MC²-2: A Code to Calculate Fast Neutron Spectra and Multigroup Cross Sections

by

H. Henryson II, B. J. Toppel, and C. G. Stenberg

ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS

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Applied Physics Division

June 1976
THIS PAGE
WAS INTENTIONALLY
LEFT BLANK
TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>CODE ABSTRACT</td>
<td>xi</td>
</tr>
<tr>
<td>ABSTRACT</td>
<td>xiv</td>
</tr>
<tr>
<td>LIST OF TABLES</td>
<td></td>
</tr>
<tr>
<td>LIST OF FIGURES</td>
<td></td>
</tr>
<tr>
<td>I.  INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>II. FUNDAMENTAL MODE SPECTRUM CALCULATION</td>
<td>4</td>
</tr>
<tr>
<td>II.A. ( P_1 ) and ( B_1 ) Extended Transport Equations.</td>
<td>4</td>
</tr>
<tr>
<td>II.B. Source Term</td>
<td>7</td>
</tr>
<tr>
<td>II.C. Continuous Slowing Down Theory</td>
<td>8</td>
</tr>
<tr>
<td>II.D. Continuous Slowing Down Moderating Parameters</td>
<td>13</td>
</tr>
<tr>
<td>II.D.1. Goertzel-Greuling Moderating Parameters</td>
<td>14</td>
</tr>
<tr>
<td>II.D.2. Improved Goertzel-Greuling Moderating Parameters</td>
<td>15</td>
</tr>
<tr>
<td>II.E. Narrow Resonance Attenuation</td>
<td>21</td>
</tr>
<tr>
<td>II.F. Ultra-Fine-Group Equations</td>
<td>23</td>
</tr>
<tr>
<td>II.F.1. Multigroup Equations</td>
<td>25</td>
</tr>
<tr>
<td>II.F.2. Continuous Slowing Down Equations</td>
<td>27</td>
</tr>
<tr>
<td>II.G. Elastic Scattering Transfer Matrix</td>
<td>32</td>
</tr>
<tr>
<td>II.G.1. Light Elements</td>
<td>32</td>
</tr>
<tr>
<td>II.G.2. Heavy Elements</td>
<td>36</td>
</tr>
<tr>
<td>II.G.3. Hydrogen Elastic Scattering</td>
<td>38</td>
</tr>
<tr>
<td>II.H. Inelastic and ( (n,2n) ) Scattering</td>
<td>39</td>
</tr>
<tr>
<td>II.H.1. Tabulated Function</td>
<td>39</td>
</tr>
<tr>
<td>II.H.2. Evaporation Spectrum</td>
<td>40</td>
</tr>
<tr>
<td>II.H.3. Discrete Levels</td>
<td>40</td>
</tr>
<tr>
<td>II.H.3.a. Approximate Treatment Neglecting Energy-Angle Correlation</td>
<td>41</td>
</tr>
<tr>
<td>II.H.3.b. Rigorous Treatment Assuming Isotropic Scattering</td>
<td>42</td>
</tr>
<tr>
<td>II.I. Ultra-Fine-Group Macroscopic Data</td>
<td>44</td>
</tr>
<tr>
<td>II.I.1. Fission Source Data</td>
<td>44</td>
</tr>
<tr>
<td>II.I.2. Ultra-Fine-Group Extended Transport Cross Section.</td>
<td>45</td>
</tr>
<tr>
<td>II.I.3. Improved Goertzel-Greuling Moderating Parameters</td>
<td>46</td>
</tr>
</tbody>
</table>
TABLE OF CONTENTS (cont'd)

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>II.J.</td>
<td>Ultra-Fine-Group Solution Strategies</td>
<td>50</td>
</tr>
<tr>
<td>II.J.1.</td>
<td>Ultra-Fine-Group Spectrum Solution</td>
<td>50</td>
</tr>
<tr>
<td>II.J.2.</td>
<td>Eigenvalue Solution</td>
<td>53</td>
</tr>
<tr>
<td>II.J.3.</td>
<td>Inhomogeneous Source Solution</td>
<td>54</td>
</tr>
<tr>
<td>II.J.4.</td>
<td>Buckling Search to Critical</td>
<td>55</td>
</tr>
<tr>
<td>II.K.</td>
<td>Group Condensation</td>
<td>56</td>
</tr>
<tr>
<td>II.K.1.</td>
<td>Broad-Group Inelastic and (n,2n) Cross Sections</td>
<td>56</td>
</tr>
<tr>
<td>II.K.2.</td>
<td>Broad-Group Absorption Cross Sections</td>
<td>57</td>
</tr>
<tr>
<td>II.K.3.</td>
<td>Elastic Scattering Cross Sections</td>
<td>58</td>
</tr>
<tr>
<td>II.K.4.</td>
<td>Total Cross Section</td>
<td>60</td>
</tr>
<tr>
<td>II.K.5.</td>
<td>Transport Cross Section</td>
<td>62</td>
</tr>
<tr>
<td>II.K.5.a</td>
<td>Inconsistent $P_1$ or $B_1$ Spectrum</td>
<td>62</td>
</tr>
<tr>
<td>II.K.5.b</td>
<td>Consistent $P_1$ or $B_1$ Spectrum</td>
<td>63</td>
</tr>
<tr>
<td>II.K.6.</td>
<td>Average Number of Neutrons per Fission</td>
<td>63</td>
</tr>
<tr>
<td>II.K.7.</td>
<td>Fission Spectrum Distribution</td>
<td>64</td>
</tr>
<tr>
<td>II.K.8.</td>
<td>XS.ISO Cross Sections</td>
<td>64</td>
</tr>
<tr>
<td>II.L.</td>
<td>Broad-Group Spectrum</td>
<td>64</td>
</tr>
</tbody>
</table>

III.  CALCULATION OF RESOLVED RESONANCE INTEGRALS

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>III.A.</td>
<td>General Formulation</td>
<td>67</td>
</tr>
<tr>
<td>III.B.</td>
<td>Calculation of Isolated Resonance Integrals</td>
<td>78</td>
</tr>
<tr>
<td>III.C.</td>
<td>Calculations of Overlap Integrals</td>
<td>79</td>
</tr>
<tr>
<td>III.C.1.</td>
<td>Selection of Overlapping Resonances</td>
<td>79</td>
</tr>
<tr>
<td>III.C.2.</td>
<td>Asymptotic Algorithms</td>
<td>80</td>
</tr>
<tr>
<td>III.C.3.</td>
<td>Gauss-Jacobi Quadrature Algorithms</td>
<td>89</td>
</tr>
</tbody>
</table>

IV.  CALCULATION OF UNRESOLVED RESONANCE INTEGRALS

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>IV.A.</td>
<td>General Formulation</td>
<td>94</td>
</tr>
<tr>
<td>IV.B.</td>
<td>Evaluation of Self-Overlap Term</td>
<td>99</td>
</tr>
<tr>
<td>IV.B.1.</td>
<td>Evaluation of $L_1$</td>
<td>100</td>
</tr>
<tr>
<td>IV.B.1.a</td>
<td>Asymptotic Algorithms for $L_1$</td>
<td>102</td>
</tr>
<tr>
<td>IV.B.1.b</td>
<td>Non-Asymptotic Algorithms for $L_1$</td>
<td>103</td>
</tr>
<tr>
<td>IV.B.2.</td>
<td>Evaluation of $L_2$</td>
<td>105</td>
</tr>
<tr>
<td>IV.B.2.a</td>
<td>Asymptotic Algorithms for $L_2$</td>
<td>106</td>
</tr>
<tr>
<td>IV.B.2.b</td>
<td>Non-Asymptotic Algorithms for $L_2$</td>
<td>106</td>
</tr>
</tbody>
</table>
# TABLE OF CONTENTS (cont'd)

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>IV.C.</td>
<td>Evaluation of Unresolved Resonance Cross Sections</td>
<td>107</td>
</tr>
<tr>
<td>IV.D.</td>
<td>Unresolved Resonance Integrals and Resolved-Unresolved Resonance Interaction</td>
<td>108</td>
</tr>
<tr>
<td>IV.E.</td>
<td>Ultra-Fine-Group Unresolved Resonance Cross Sections</td>
<td>109</td>
</tr>
<tr>
<td>V.</td>
<td>RABANL, HYPER-FINE-GROUP INTEGRAL TRANSPORT THEORY NEUTRON SLOWING DOWN</td>
<td>112</td>
</tr>
<tr>
<td>V.A.</td>
<td>Introduction</td>
<td>112</td>
</tr>
<tr>
<td>V.B.</td>
<td>Calculation of Elastic Slowing-Down Sources</td>
<td>112</td>
</tr>
<tr>
<td>V.C.</td>
<td>Calculation of Collision Rates</td>
<td>118</td>
</tr>
<tr>
<td>V.C.1</td>
<td>One Region (Homogeneous) Problems</td>
<td>118</td>
</tr>
<tr>
<td>V.C.2</td>
<td>Multi-Region (Heterogeneous) Problems</td>
<td>122</td>
</tr>
<tr>
<td>V.C.2.a</td>
<td>Slab Geometry</td>
<td>122</td>
</tr>
<tr>
<td>V.C.2.b</td>
<td>Cylindrical Geometry</td>
<td>130</td>
</tr>
<tr>
<td>V.D.</td>
<td>Calculation of Hyper-Fine-Group Cross Sections</td>
<td>132</td>
</tr>
<tr>
<td>V.D.1</td>
<td>Resonance Selection</td>
<td>133</td>
</tr>
<tr>
<td>V.D.2</td>
<td>Resolved Resonance Algorithms</td>
<td>133</td>
</tr>
<tr>
<td>V.D.2.a</td>
<td>Single Level Breit Wigner</td>
<td>133</td>
</tr>
<tr>
<td>V.D.2.b</td>
<td>Multilevel Breit Wigner</td>
<td>135</td>
</tr>
<tr>
<td>V.D.2.c</td>
<td>Multilevel Adler-Adler</td>
<td>137</td>
</tr>
<tr>
<td>V.E.</td>
<td>Broad Group Edits</td>
<td>138</td>
</tr>
<tr>
<td>VI.</td>
<td>A GUIDE TO USER APPLICATION</td>
<td>141</td>
</tr>
<tr>
<td>VI.A.</td>
<td>Standard Path STP015</td>
<td>141</td>
</tr>
<tr>
<td>VI.B.</td>
<td>Job Control Language Procedure ARCSP015</td>
<td>142</td>
</tr>
<tr>
<td>VI.C.</td>
<td>Problem Specification</td>
<td>155</td>
</tr>
<tr>
<td>VI.D.</td>
<td>Sample Problems</td>
<td>161</td>
</tr>
<tr>
<td>VI.D.1</td>
<td>Homogeneous Reference Problem</td>
<td>161</td>
</tr>
<tr>
<td>VI.D.2</td>
<td>Hyper-Fine-Group Homogeneous Integral Transport Problem</td>
<td>161</td>
</tr>
<tr>
<td>VI.D.3</td>
<td>Hyper-Fine-Group Heterogeneous Integral Transport Problem</td>
<td>162</td>
</tr>
<tr>
<td>VI.E.</td>
<td>Error Messages</td>
<td>163</td>
</tr>
<tr>
<td>VII. PROGRAMMING INFORMATION</td>
<td>182</td>
<td></td>
</tr>
<tr>
<td>-----------------------------</td>
<td>-----</td>
<td></td>
</tr>
<tr>
<td>VII.A. Program Structure.</td>
<td>182</td>
<td></td>
</tr>
<tr>
<td>VII.B. ARC System Routines.</td>
<td>182</td>
<td></td>
</tr>
<tr>
<td>VII.C. CCCC Standard Subroutines.</td>
<td>186</td>
<td></td>
</tr>
<tr>
<td>VII.C.1. SEEK</td>
<td>186</td>
<td></td>
</tr>
<tr>
<td>VII.C.2. REED/RITE</td>
<td>193</td>
<td></td>
</tr>
<tr>
<td>VII.C.3. TIMER.</td>
<td>193</td>
<td></td>
</tr>
<tr>
<td>VII.D. Machine Language Routines.</td>
<td>193</td>
<td></td>
</tr>
<tr>
<td>VII.D.1. ALLOC.</td>
<td>193</td>
<td></td>
</tr>
<tr>
<td>VII.D.2. LOCF.</td>
<td>193</td>
<td></td>
</tr>
<tr>
<td>VII.D.3. GOWEST</td>
<td>194</td>
<td></td>
</tr>
<tr>
<td>VII.D.4. FILEID</td>
<td>194</td>
<td></td>
</tr>
<tr>
<td>VII.D.5. CVD.</td>
<td>194</td>
<td></td>
</tr>
<tr>
<td>VII.D.6. TIME</td>
<td>194</td>
<td></td>
</tr>
<tr>
<td>VII.D.7. CLOCK.</td>
<td>194</td>
<td></td>
</tr>
<tr>
<td>VII.D.8. DATE</td>
<td>194</td>
<td></td>
</tr>
<tr>
<td>VII.D.9. SECOND</td>
<td>194</td>
<td></td>
</tr>
<tr>
<td>VII.D.10. ABEND.</td>
<td>194</td>
<td></td>
</tr>
<tr>
<td>VII.D.11. JOBID.</td>
<td>195</td>
<td></td>
</tr>
<tr>
<td>VII.D.12. FXP.</td>
<td>195</td>
<td></td>
</tr>
<tr>
<td>VII.D.13. DISPOS</td>
<td>195</td>
<td></td>
</tr>
<tr>
<td>VII.D.14. TRACER</td>
<td>195</td>
<td></td>
</tr>
<tr>
<td>VII.E. Program Implementation</td>
<td>195</td>
<td></td>
</tr>
<tr>
<td>VII.E.1. IBM Code Implementation</td>
<td>195</td>
<td></td>
</tr>
<tr>
<td>VII.E.2. CDC Code Implementation</td>
<td>221</td>
<td></td>
</tr>
</tbody>
</table>

APPENDICES. 230

A. Special Function Evaluation 230

A.I. Legendre Functions of the Second Kind 231

A.II. A Fast Exponential Subroutine-FXP 236

A.III. Calculation of Doppler-Broadened Line Shape Functions 237

A.IV. Numerical Methods Used in Calculating the Isolated Resonance Integral 240

A.V. Quadratures for Statistical Integration 244

A.VI. Numerical Methods Used in Calculating Slab Collision Rates 246

A.VI.a. Exponential Integrals 246

A.VI.b. Slab Collision Escape Probability 247

A.VI.c. Infinite Sum of Exponential Integrals 247

A.VII. Cylindrical Transmission Probabilities 251
# TABLE OF CONTENTS (cont'd)

<table>
<thead>
<tr>
<th>Section</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>B.</td>
<td><strong>MC²-2 BCD Input Files</strong></td>
<td></td>
</tr>
<tr>
<td>B.I.</td>
<td>A.MCC2</td>
<td>253</td>
</tr>
<tr>
<td>B.II.</td>
<td>A.NIP</td>
<td>254</td>
</tr>
<tr>
<td>B.III.</td>
<td>A.STP015</td>
<td>276</td>
</tr>
<tr>
<td>B.IV.</td>
<td>ACSE12</td>
<td>280</td>
</tr>
<tr>
<td>B.V.</td>
<td>ACS009</td>
<td>283</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C.</td>
<td><strong>MC²-2 Binary Interface Files</strong></td>
<td></td>
</tr>
<tr>
<td>C.I.</td>
<td>ISOTXS</td>
<td>285</td>
</tr>
<tr>
<td>C.II.</td>
<td>MCC2F1</td>
<td>286</td>
</tr>
<tr>
<td>C.III.</td>
<td>MCC2F2</td>
<td>315</td>
</tr>
<tr>
<td>C.IV.</td>
<td>MCC2F3</td>
<td>317</td>
</tr>
<tr>
<td>C.V.</td>
<td>MCC2F4</td>
<td>318</td>
</tr>
<tr>
<td>C.VI.</td>
<td>MCC2F5</td>
<td>324</td>
</tr>
<tr>
<td>C.VII.</td>
<td>MCC2F6</td>
<td>326</td>
</tr>
<tr>
<td>C.VIII.</td>
<td>MCC2F7</td>
<td>329</td>
</tr>
<tr>
<td>C.IX.</td>
<td>MCC2F8</td>
<td></td>
</tr>
<tr>
<td>C.X.</td>
<td>XS.ISO</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>D.</td>
<td><strong>MC²-2 Binary Files</strong></td>
<td></td>
</tr>
<tr>
<td>D.I.</td>
<td>ATNUAT</td>
<td>337</td>
</tr>
<tr>
<td>D.II.</td>
<td>BC</td>
<td>342</td>
</tr>
<tr>
<td>D.III.</td>
<td>BIGXS(I)</td>
<td>343</td>
</tr>
<tr>
<td>D.IV.</td>
<td>GEOM1</td>
<td>345</td>
</tr>
<tr>
<td>D.V.</td>
<td>IRESCS</td>
<td>348</td>
</tr>
<tr>
<td>D.VI.</td>
<td>LORENZ</td>
<td>352</td>
</tr>
<tr>
<td>D.VII.</td>
<td>MACTOT</td>
<td>355</td>
</tr>
<tr>
<td>D.VIII.</td>
<td>MICTOT</td>
<td>359</td>
</tr>
<tr>
<td>D.IX.</td>
<td>OLDSGS</td>
<td>360</td>
</tr>
<tr>
<td>D.X.</td>
<td>OPTICL</td>
<td>361</td>
</tr>
<tr>
<td>D.XI.</td>
<td>PRBCHI</td>
<td>363</td>
</tr>
<tr>
<td>D.XII.</td>
<td>PRBSPC</td>
<td>366</td>
</tr>
<tr>
<td>D.XIII.</td>
<td>RESDAT</td>
<td>379</td>
</tr>
</tbody>
</table>
# TABLE OF CONTENTS (cont'd)

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>D.XIV.</td>
<td>RESINT</td>
<td>381</td>
</tr>
<tr>
<td>D.XV.</td>
<td>SCR001</td>
<td>385</td>
</tr>
<tr>
<td>D.XVI.</td>
<td>SCR002</td>
<td>390</td>
</tr>
<tr>
<td>D.XVII.</td>
<td>SCR003</td>
<td>395</td>
</tr>
<tr>
<td>D.XVIII.</td>
<td>SCR004</td>
<td>407</td>
</tr>
<tr>
<td>D.XIX.</td>
<td>SCR005</td>
<td>409</td>
</tr>
<tr>
<td>D.XX.</td>
<td>SIGNAP</td>
<td>411</td>
</tr>
<tr>
<td>D.XXI.</td>
<td>SMSIGS</td>
<td>413</td>
</tr>
<tr>
<td>D.XXII.</td>
<td>SPECTR</td>
<td>416</td>
</tr>
<tr>
<td>D.XXIII.</td>
<td>SPECXS</td>
<td>418</td>
</tr>
<tr>
<td>D.XXIV.</td>
<td>SRATES</td>
<td>421</td>
</tr>
<tr>
<td>D.XXV.</td>
<td>UNREG.</td>
<td>424</td>
</tr>
<tr>
<td>D.XXVI.</td>
<td>UNRES.</td>
<td>427</td>
</tr>
<tr>
<td>E.</td>
<td>BPOINTER, A Dynamic Storage Allocation Program</td>
<td>431</td>
</tr>
<tr>
<td>E.I.</td>
<td>Description of Subprogram Package.</td>
<td>432</td>
</tr>
<tr>
<td>E.I.a.</td>
<td>IBM Allocation</td>
<td>433</td>
</tr>
<tr>
<td>E.I.b.</td>
<td>CDC Allocation</td>
<td>433</td>
</tr>
<tr>
<td>F.</td>
<td>MC²-2 Library Generation</td>
<td>438</td>
</tr>
<tr>
<td>ACKNOWLEDGMENTS</td>
<td>442</td>
<td></td>
</tr>
<tr>
<td>REFERENCES</td>
<td>443</td>
<td></td>
</tr>
</tbody>
</table>
**LIST OF FIGURES**

<table>
<thead>
<tr>
<th>No.</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>MC²-2 Program Flow</td>
<td>3</td>
</tr>
<tr>
<td>2</td>
<td>MC²-2 Energy Structure</td>
<td>24</td>
</tr>
<tr>
<td>3</td>
<td>Elastic Scattering Group Structure</td>
<td>34</td>
</tr>
<tr>
<td>4</td>
<td>Gauss-Jacobi Quadrature Point Selection</td>
<td>90</td>
</tr>
<tr>
<td>5</td>
<td>Unresolved Resonance Energy Grid</td>
<td>110</td>
</tr>
<tr>
<td>6</td>
<td>Linearization of Ultra-Fine-Group Data</td>
<td>121</td>
</tr>
<tr>
<td>7</td>
<td>Slab Geometry Coordinates</td>
<td>123</td>
</tr>
<tr>
<td>8</td>
<td>Slab Geometry Optical Distance</td>
<td>126</td>
</tr>
<tr>
<td>9</td>
<td>MC²-2 Module Flow Diagram</td>
<td>143</td>
</tr>
<tr>
<td>10</td>
<td>MC²-2 Path Driver Listing</td>
<td>144</td>
</tr>
<tr>
<td>11</td>
<td>MC²-2 JCL Procedure</td>
<td>148</td>
</tr>
<tr>
<td>12</td>
<td>Minimum JCL Execution Deck</td>
<td>164</td>
</tr>
<tr>
<td>13</td>
<td>Input for Sample Problem 1</td>
<td>164</td>
</tr>
<tr>
<td>14</td>
<td>Input for Sample Problem 2</td>
<td>165</td>
</tr>
<tr>
<td>15</td>
<td>Input for Sample Problem 3</td>
<td>166</td>
</tr>
<tr>
<td>16</td>
<td>IBM Overlay Control</td>
<td>183</td>
</tr>
<tr>
<td>17</td>
<td>CDC Segmentation Loader Directives</td>
<td>185</td>
</tr>
<tr>
<td>18</td>
<td>Preallocation of Object Library</td>
<td>199</td>
</tr>
<tr>
<td>19</td>
<td>Compilation of FORTRAN Subprograms</td>
<td>199</td>
</tr>
<tr>
<td>20</td>
<td>Assembly of File 2 CSECTS</td>
<td>199</td>
</tr>
<tr>
<td>21</td>
<td>Copy Object Module From File 3 of IBM Code Center</td>
<td>199</td>
</tr>
<tr>
<td></td>
<td>Tape to Disk</td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>Copy of MC²-2 IBM Binary Library Files</td>
<td>200</td>
</tr>
<tr>
<td>23</td>
<td>Compilation and Assembly of CDC Source Code to Generate Object Code</td>
<td>227</td>
</tr>
<tr>
<td>24</td>
<td>Build Segments from Object Code Using Segmentation Loader</td>
<td>228</td>
</tr>
<tr>
<td>25</td>
<td>CDC Execution of MC²-2 Problem</td>
<td>229</td>
</tr>
<tr>
<td>26</td>
<td>Gauss-Jacobi Quadrature Selection</td>
<td>241</td>
</tr>
<tr>
<td>27</td>
<td>BPOINTER Example</td>
<td>435</td>
</tr>
<tr>
<td>28</td>
<td>Generation of MC²-2 Library From Two X-Mode Binary Library Tapes</td>
<td>440</td>
</tr>
<tr>
<td>29</td>
<td>Generation of MC²-2 Library From Three BCD Data Tapes</td>
<td>441</td>
</tr>
</tbody>
</table>
# LIST OF TABLES

<table>
<thead>
<tr>
<th>No.</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>Coefficients $K_{nn}^{(a)}$</td>
<td>20</td>
</tr>
<tr>
<td>II</td>
<td>Heavy Mass Matrix Elements $A_{n}^{j} (j\rightarrow k)$</td>
<td>37</td>
</tr>
<tr>
<td>III</td>
<td>BCD Input Data Sets</td>
<td>156</td>
</tr>
<tr>
<td>IV</td>
<td>Prestored Group Structures</td>
<td>157</td>
</tr>
<tr>
<td>V</td>
<td>$MC^2$-2 Error Messages</td>
<td>167</td>
</tr>
<tr>
<td>VI</td>
<td>$MC^2$-2 File Information</td>
<td>187</td>
</tr>
<tr>
<td>VII</td>
<td>IBM Code Center Tape Description</td>
<td>198</td>
</tr>
<tr>
<td>VIII</td>
<td>Function of $MC^2$-2 Subprograms</td>
<td>201</td>
</tr>
<tr>
<td>IX</td>
<td>$MC^2$-2 ENDF/B-IV Library Files</td>
<td>217</td>
</tr>
<tr>
<td>X</td>
<td>CDC Code Center Tape Description</td>
<td>224</td>
</tr>
<tr>
<td>XI</td>
<td>Function of $MC^2$-2 Subprograms for CDC Code</td>
<td>225</td>
</tr>
<tr>
<td>XII</td>
<td>Legendre Function Evaluation</td>
<td>235</td>
</tr>
<tr>
<td>XIII</td>
<td>Ten Point Quadrature Weights and Abscissae for Statistical Integration</td>
<td>245</td>
</tr>
<tr>
<td>XIV</td>
<td>BPOINTER Subprogram Descriptions</td>
<td>436</td>
</tr>
</tbody>
</table>
MC²-2: A CODE TO CALCULATE FAST NEUTRON SPECTRA AND MULTIGROUP CROSS SECTIONS

CODE ABSTRACT

1. Program Identification: MC²-2

2. Computer for which program is designed and others on which it is operable: IBM 370/195, any IBM OS system with 600K core, CDC 7600.

3. Description of Function: MC²-2 solves the neutron slowing down equations to determine spectra for use in generating multigroup neutron cross sections.

4. Method of Solution: The extended transport $P_1$, $B_1$, consistent $P_1$, and consistent $B_1$ fundamental mode ultra-fine-group equations are solved using continuous slowing down theory and multigroup methods. Fast and accurate resonance integral methods are used in the narrow resonance resolved and unresolved resonance treatments. Multigroup neutron cross sections are generated for arbitrary group structures. A hyper-fine-group integral transport slowing down calculation is available on option to treat the low energy spectrum where the narrow resonance approximation is not valid.

5. Restrictions: Variable dimensioning is used throughout the program so that computer core requirements depend on a variety of problem parameters. Space requirements range from 400K bytes to 800K bytes on IBM equipment depending on the complexity of the problem.

6. Running Time: An 1740 group consistent $P_1$ homogeneous twelve isotope problem with 27 broad groups requires about 4.2 min. CPU and 6 min. PP time on an IBM 370/195. The same problem requires approximately 30% less CPU time on the CDC 7600.

7. Unusual Features of the Program: Extreme flexibility is provided in specifying the rigor of a calculation including a choice of four distinct slowing down treatments: multigroup, improved and standard Greuling-Goertzel continuous slowing down, and integral transport theory. All binary data transfers are localized in standard sub-routines REED/RITE. Broad group cross section files may be generated in the ARC System XS.ISO(1) and/or CCCC ISOTXS(2) formats.
8. Related and Auxiliary Programs: Input data files required by MC²-2 may be generated from ENDF/B data(3) by the code ETOE-2(4). The hyper-fine-group integral transport theory module of MC²-2, RABANL, is an improved version of the RABBLE(5)/RABID(6) codes. Many of the MC²-2 modules are used in the SDX(7) code.

9. Status:


11. Machine Requirements: A large amount of fast peripheral storage is required. Core requirements depend on problem complexity but virtually any reasonable problem may be executed on IBM equipment with 800K bytes or CDC equipment with 50,000 words of SCM and 100,000 words of directly addressable LCM.

12. Programming Language Used: FORTRAN IV. Both IBM and CDC versions of MC²-2 contain a few Assembler language routines.

13. Operating System or Monitor under which Program is Executed: The IBM version of MC²-2 may be executed under OS or VS operating systems and compiled using the Fortran H or program product compilers with the highest level of optimization. The CDC 7600 version of MC²-2 has been implemented on both the LRL Berkeley and Brookhaven National Laboratory computers with their special COKE/SCOPE operating systems. The SEGMENTATION LOADER is required and directly addressable LCM is used. The code was compiled using the FORTRAN Extended Compiler under OPT=1 optimization.

14. Any Other Programming or Operating Information or Restrictions:
15. Name and Establishment of Authors:

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16. Material Available: Separate tapes are available for the IBM and CDC versions of MC²-2. The MC²-2 package includes:

i) Source decks
ii) Test problem input decks
iii) Test problem output
iv) Eight binary library files processed from ENDF/B-IV
v) Source code and BCD library files to generate binary libraries
vi) Reference report

17. Category: B
Keywords: cross sections, group constants, spectra, multigroup, resonance, B_L method, P_L method, slowing down, infinite media, homogeneous, heterogeneous, ENDF/B, cell calculation
MC$^2$-2: A Code to Calculate Fast Neutron Spectra and Multigroup Cross Sections

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ABSTRACT

MC$^2$-2 is a program to solve the neutron slowing down problem using basic neutron data derived from the ENDF/B data files. The spectrum calculated by MC$^2$-2 is used to collapse the basic data to multigroup cross sections for use in standard reactor neutronics codes. Four different slowing down formulations are used by MC$^2$-2: multigroup, continuous slowing down using the Goertzel-Greuling or Improved Goertzel-Greuling moderating parameters, and a hyper-fine-group integral transport calculation. Resolved and unresolved resonance cross sections are calculated accounting for self-shielding, broadening and overlap effects. This document provides a description of the MC$^2$-2 program. The physics and mathematics of the neutron slowing down problem are derived and detailed information is provided to aid the MC$^2$-2 user in preparing input for the program and implementation of the program on IBM 370 or CDC 7600 computers.
I. INTRODUCTION

MC$^2$–2 is a program for solving the neutron slowing down problem to determine a detailed spectrum for use in deriving multigroup cross sections. The code has been developed to satisfy the need for a rigorous and computationally efficient capability which can serve as a standard for fast reactor calculations. Recent advances in neutron slowing down theory, resonance theory, and numerical methods have been incorporated into the MC$^2$–2 calculation. A large number of options are available which permit great flexibility in specifying the rigor of a calculation.

The MC$^2$–2 code was developed at Argonne National Laboratory in the ARC System$^{(1)}$ environment. The programming was performed with strict adherence to the standards established by the Committee on Computer Code Coordination$^{(2)}$. As a consequence the modifications required to develop standalone versions of the code for alternative computer configurations are minor. Both IBM and CDC standalone versions of the code have been implemented. The program is structured in eight principal modules (overlays):

1) Input Processor (CSI010)
2) Unresolved Resonance Calculation (CSC004)
3) Resolved Resonance Calculation (CSC005)
4) Resolved-Unresolved Resonance Interaction (CSC006)
5) Macroscopic Data Processing (CSC007)
6) Ultra-Fine-Group Spectrum Calculation and Broad-Group Cross Section Collapse (CSC008)
7) Hyper-Fine-Group Integral Transport Spectrum Calculation – RABANL (CSC009)
8) Broad-Group Spectrum Calculation (CSC010)

Figure 1 indicates the program flow through these modules. The basic data required by MC$^2$–2 are structured in eight data files. The file formats are provided in Appendix C. These data files may be created from the ENDF/B data$^{(3)}$ by the program ETOE–2$^{(4)}$. Multigroup cross sections generated by MC$^2$–2 are processed in the ARC System XS.ISO$^{(1)}$ and/or the CCCC ISOTXS$^{(2)}$ formats. These structures are included in Appendix C for the sake of completeness.

The major features of MC$^2$–2 include:

1. the ability to specify the rigor of a calculation through input options,
2. $P_1$, $B_1$, consistent $P_1$ and consistent $B_1$ extended transport theory algorithms,
3. multigroup, improved or standard Greuling-Goertzel continuous slowing down theory solutions,
4. hyper-fine-group integral transport theory solutions,
5. flexible broad group structures in a choice of formats,
6. consistent treatment of all ENDF/B Version III and Version IV data formats,
7. fast and accurate resonance integral treatment of Breit-Wigner and Adler-Adler resolved resonances,
8. fast and accurate treatment of unresolved resonances including interference scattering and same-sequence overlap effects,
9. isotope dependent fission spectra,
10. inhomogeneous source calculation,
11. buckling search or group dependent buckling calculations,
12. flexible output options.

This report is organized into seven chapters which are intended to provide the physics, mathematics and code user documentation for the program MC²-2. Chapter II contains the theoretical development of all the methods and approximations used in the ultra-fine-group fundamental mode spectrum calculation of MC²-2. Chapter III contains the information relevant to the calculation of resonance integrals from resolved resonance parameters and Chapter IV is concerned with the calculation of cross sections and resonance integrals from average parameters in the unresolved resonance energy regions. Chapter V describes the RABANL module of the code MC²-2. The RABANL calculation is a hyper-fine-group integral transport slowing down calculation which treats resolved resonance absorption rigorously. The module is modeled after the resonance absorption codes RABBLE\(^5\) and RABID.\(^6\) Chapter VI provides a guide for user application and Chapter VII contains information relevant to the programming of MC²-2.
Fig. 1. MC²-2 Program Flow
II. FUNDAMENTAL MODE SPECTRUM CALCULATION

A. $P_1$ and $B_1$ Extended Transport Equations

The time independent transport equation is written

$$\nabla \cdot \Omega \psi + \Sigma_t \psi(\mathbf{r}, u, \Omega) = \iiint dV' d\Omega' \psi(\mathbf{r}, u', \Omega') \cdot$$

$$\Sigma_s (u' \rightarrow u, \Omega \cdot \Omega') + S(\mathbf{r}, u)/4\pi$$

(II.1)*

where $\psi$ is the flux defined such that $\psi dVdud\Omega$ is the flux in the volume $dV$ about $\mathbf{r}$, in the element of solid angle $d\Omega$ about $\Omega$, in the lethargy range $du$ about $\nu$. The lethargy $u$ is defined as $ln(E_0/E)$. Similarly $S$ is the isotropic source density in the same element of phase space and includes contributions due to fission and/or sources independent of the flux $\psi$. The macroscopic total cross section is denoted by $\Sigma_t$ and the macroscopic scattering transfer cross section by $\Sigma_s$. If one assumes a homogeneous mixture so that the above quantities are not space dependent and makes use of the fundamental mode ansatz

$$\psi(\mathbf{r}, u, \Omega) \equiv \psi(u, \Omega)e^{iB'' \mathbf{r}}; \quad S(\mathbf{r}, u) \equiv S(u)e^{iB'' \mathbf{r}}$$

(II.2)

then Eq. II.1 may be written,

$$\langle \Sigma_t + iB'' \cdot \Omega \rangle \psi(u, \Omega) = \iiint dV' d\Omega' \psi(u', \Omega') \Sigma_s (u' \rightarrow u, \mu_o)$$

$$+ S(u)/4\pi$$

(II.3)

where $\mu_o \equiv \Omega \cdot \Omega'$. In order to simplify the notation, consider only plane geometry. Expanding the flux and scattering transfer cross section in spherical harmonics,

$$2\pi \psi(u, \Omega) = \psi(u, \mu) = \sum_{\ell=0}^{\infty} \frac{2\ell + 1}{2} \phi_\ell(u) P_\ell(\mu)$$

$$\Sigma_s (u' \rightarrow u, \mu_o) = \sum_{\ell=0}^{\infty} \frac{2\ell + 1}{2} \Sigma_s^\ell (u' \rightarrow u) P_\ell(\mu_o)$$

(II.4)

where $P_\ell(\mu)$ is the $\ell$th order Legendre polynomial, substituting into Eq. II.3 and making use of the addition theorem for Legendre polynomials yields

*Equation numbering convention of the form N,n is used where N is the chapter number and n is the equation number in Chapter N.
Multiplying by \( P_\ell (u) \), integrating over the range of \( u \), and using the recursion relation gives

\[
\frac{\ell + 1}{2\ell + 1} iB\phi_{\ell+1}(u) + \frac{\ell}{2\ell + 1} iB\phi_{\ell-1}(u) + \Sigma_{t} \phi_{\ell}(u) = S(u) \delta_{\ell}^0
\]

\[
+ \int du' \Sigma_{s}^\ell (u' + u) \phi_{\ell}(u') \quad \ell = 0, 1, \ldots, \infty
\]

\[
\phi_{-1}(u) = 0.
\]

Two well known approximations to this infinite set of coupled equations are the \( P_N \) and \( B_N \) methods (8). The \( P_N \) approximation assumes

\[
\phi_{N+1} = 0,
\]

and the \( B_N \) approximation assumes

\[
\int du' \Sigma_{s}^\ell (u' + u) \phi_{\ell}(u') = 0 \quad \ell > N
\]

which is equivalent to taking

\[
\phi_{N+1} = \phi_{N} \frac{Q_{N+1} (- \Sigma_t / iB)}{Q_{N} (- \Sigma_t / iB)}
\]

where \( Q_{\ell}(x) \) is a Legendre function of the second kind. Using Eq. II.7a or II.7b, Eqs. II.6 may be written

\[
\frac{\ell + 1}{2\ell + 1} iB\phi_{\ell+1} + \frac{\ell}{2\ell + 1} iB\phi_{\ell-1} + \Sigma_{t} \phi_{\ell} = S(u) \delta_{\ell}^0
\]

\[
+ \int du' \Sigma_{s}^\ell (u' + u) \phi_{\ell}(u') \quad \ell = 0, 1, \ldots, N - 1
\]

\[
\frac{N}{2N + 1} iB\phi_{N+1} + \gamma \Sigma_{t} \phi_{N} = \int du' \Sigma_{s}^{N} (u' + u) \phi_{N}(u')
\]

\[
\phi_{-1} = 0
\]

\[
\gamma = \left\{ \begin{array}{ll}
1 & P_N \\
1 + \frac{N + 1}{2N + 1} \frac{iB}{\Sigma_t} \frac{Q_{N+1} (- \Sigma_t / iB)}{Q_{N} (- \Sigma_t / iB)} & B_N
\end{array} \right.
\]
The set of Eqs. II.8 may be further simplified by use of the extended transport approximation (9) which assumes that anisotropic scattering takes place without a change in lethargy so that

\[ \int du' \Sigma_s^E(u' + u) \phi_L(u') = \Sigma_s^E(u) \phi_L(u) \quad L = 2, \ldots, N \]  

(II.9)

where

\[ \Sigma_s^E(u) \equiv \int du' \Sigma_s^E(u + u'). \]

Using Eq. II.9 in Eqs. II.8 one obtains the consistent \( P_1 \) and \( B_1 \) order \( N \) extended transport equations.

\[ iB \phi_1(u) + \Sigma_t \phi_0(u) - \Sigma(u) + \int du' \Sigma_s^E(u' + u) \psi_0(u') \]

\[ \frac{iB}{3} \phi_2(u) + A_1(B, u, N) \phi_1(u) = \int du' \Sigma_s^E(u' + u) \phi_1(u') \]  

(II.10)

where

\[ \phi_L(u) = - \frac{\lambda}{2\lambda + 1} iB \phi_{L-1}(u)/A_\lambda(B, u, N) \quad L = 2, \ldots, N \]

and

\[ A_\lambda(B, u, N) = b_{\lambda-1} + \frac{a_\lambda}{b_\lambda} + \frac{a_{\lambda+1}}{b_{\lambda+1}} + \cdots + \frac{a_{N-1}}{b_{N-1}} \]

\[ a_\lambda = \frac{\lambda + 1}{2\lambda + 1} \frac{\lambda + 1}{2(\lambda + 1) + 1} B^2 \quad 1 \leq \lambda \leq N - 1 \]  

(II.11)

The consistent \( P_1 \) and \( B_1 \) Eqs. II.10 with the continued fraction definitions of Eqs. II.11 reduce to the standard forms programmed in the MC2(10) and GAM(11) codes if one takes the order of the extended transport approximation, \( N \), as unity.
The inconsistent $P_1$ and $B_1$ equations are obtained by assuming that Eq. II.9 is applicable for $\ell = 1$. In this case the $P_1$ integral of Eqs. II.10 disappears and the coefficient $b_0$ of the continued fraction is modified,

$$b_\ell = \begin{cases} 
E_t(u) - E_s^{\ell+1}(u), & \ell = 0, 1, \ldots, N - 1 \\
E_t(u) - E_s^{\ell+1}(u) + \frac{N + 1}{2N + 1} iB \frac{Q_{N+1}(-E_t/iB)}{Q_N(-E_t/iB)} \delta N - 1 , & B_1
\end{cases} \quad (II.12)$$

The sets of Eqs. II.10, II.11 and II.12 define the four spectrum options, consistent and inconsistent $P_1$ and $B_1$ extended transport approximations, which are available in the ultra-fine-group spectrum calculations of the $MC^2$-2 code. The following sub-sections will discuss the methods by which these equations are solved.

B. Source Term

The source term of Eqs. II.10, $S(u)$, describes neutron sources due to fission and inhomogeneous sources independent of the flux. The source is assumed to be isotropic in the laboratory system. In $MC^2$-2 scattering sources due to inelastic and $(n,2n)$ scattering are also assumed isotropic and it is convenient to include these scattering sources as components of $S(u)$. With this convention the equations of Section II.A above are applicable if $E_s^{\ell}(u' + u)$ is taken to be the elastic scattering transfer cross section and $S(u)$ is defined

$$S(u) = \frac{1}{k} S_f(u) + S_{ne}(u) + S_{fix}(u) \quad (II.13)$$

with

$$S_f(u) \equiv \text{fission source}$$
$$S_{ne}(u) \equiv \text{non-elastic scattering source}$$
$$S_{fix}(u) \equiv \text{inhomogeneous source}$$

The fission source has the form

$$S_f(u) = \sum \chi_i(u) N_i \int du' \nu_i(u') \sigma_{fi}(u') \phi(u') \quad (II.14)$$

where the sum is over all isotopes in the mixture, $N_i$ is the atom density of isotope $i$, $\chi_i(u)$ is the fraction of fission neutrons emitted in the lethargy range $du$ about $u$ for isotope $i$, $\nu_i(u)$ is the number of neutrons emitted per fission for isotope $i$, $\sigma_{fi}(u)$ is the microscopic fission cross section for isotope $i$. The fission spectrum distribution $\chi_i(u)$ may actually depend upon the fission lethargy, but such a possibility is not permitted by the $MC^2$-2 code. An option is available in the code to assign library fission
spectra to problem isotopes thus permitting a single fission spectrum distribution for all fissionable isotopes. The scalar $k$ of Eq.II.13 has the value unity if $S_{\text{fix}}(u) \neq 0$. If $S_{\text{fix}}(u) = 0$, then Eqs.II.10 have a solution only if $k$ is the eigenvalue of the system of equations.

C. Continuous Slowing Down Theory

Two sets of algorithms for the solution of Eqs.II.10 are available in the MC$^2$-2 code, multigroup and continuous slowing down theory. In this section the form of the continuous slowing down equations treated by MC$^2$-2 is derived. The algorithms are based on the work of Stacey (12) and are included in this report to provide a self-contained presentation for the convenience of the reader. A general review of continuous slowing down theory has been prepared by Stacey (13).

The $\ell$-th order angular component of the elastic slowing down density is defined

$$q_{\ell}(u) = \sum \int_{u-\ln/a_i}^{u} \frac{du'}{u-\ln/a_i} \left( \int_{u}^{u'+\ln/a_i} \frac{du''}{u''} \Sigma_{s_i}^{\ell}(u' + u'' \phi_{\ell}(u')) \right)$$

where

$$a_i = \left( \frac{A_i - 1}{A_i + 1} \right)^2$$

$A_i = \text{mass of isotope } i / \text{neutron mass}$

$\Sigma_{s_i}^{\ell}(u' + u) \equiv \text{macroscopic elastic scattering transfer cross section for isotope } i$

The scattering transfer cross sections of Eqs.II.4 and II.10 are given by

$$\Sigma_{s_i}^{\ell}(u' + u) = \sum \Sigma_{s_i}^{\ell}(u' + u)$$

as a consequence of the conventions assumed in Section II.B. It is convenient to define an elastic transfer kernel $P_{\ell}^{\ell}(u' + u)$ and a slowing down kernel $K_{\ell}^{\ell}(u' + u)$ in the following manner,

$$\Sigma_{s}^{\ell}(u' + u) = \sum \Sigma_{s_i}^{\ell}(u') P_{\ell}^{\ell}(u' + u)$$

$$K_{\ell}^{\ell}(u' + u) = \int_{u}^{u'+\ln/a_i} \frac{du''}{u''} P_{\ell}^{\ell}(u' + u').$$

Differentiation of Eq.II.15 gives

$$\frac{dq_{\ell}(u)}{du} = \Sigma_{s_i}^{\ell}(u) \phi_{\ell}(u) - \sum \int_{u-\ln/a_i}^{u} \frac{du}{u-\ln/a_i} \left( \int_{u}^{u'+\ln/a_i} \frac{du''}{u''} \Sigma_{s_i}^{\ell}(u') P_{\ell}^{\ell}(u' + u) \phi_{\ell}(u') \right).$$

(II.18)
A continuous slowing down approximation results from assuming
\[ F^\ell_i(u') = g^\ell_i(u') \phi^\ell_i(u') = F^\ell_i(u) + (u' - u) \frac{d}{du} F^\ell_i(u) \]  
\( u' \geq u \geq u - \ln(1/u) \)

where \( g^\ell_i(u') \) is taken to be either the isotopic scattering cross section, \( \Sigma^i (u') \), or the macroscopic total cross section \( \Sigma^i_T (u') \). The validity of either approximation depends upon the mixture and the lethargy range in question. Since the total collision density is likely to be a more slowly varying quantity than each of the isotopic scattering collision densities, the latter choice of \( g^\ell_i(u') \) has a greater range of validity. As the scattering band for Hydrogen (\( A_H \lesssim 1 \)) is infinite, the two term expansion of Eq.II.19 is not valid in this case for either choice of \( g^\ell_i(u) \). Hydrogen is therefore treated separately and the slowing down density is represented as
\[ q^\ell_i(u) = q^\ell_i(u) + \eta^\ell_i(u) \]

where \( \eta^\ell_i(u) \) is the Hydrogen slowing down density and \( q^\ell_i(u) \) is given by Eq.II.15 with the sum excluding Hydrogen. Substitution of Eq.II.19 into Eqs.II.15 and II.18 gives
\[ q^\ell_i(u) = \sum_{i \neq H} [\xi^\ell_i(u) F^\ell_i(u) + a^\ell_i(u) \frac{d}{du} F^\ell_i(u)] \]  
\[ \frac{dq^\ell_i(u)}{du} = \sum_{i \neq H} [c^\ell_i F^\ell_i(u) - e^\ell_i(u) \frac{d}{du} F^\ell_i(u)] \]

with the moderating parameters given by
\[ \xi^\ell_i(u) = \int_{u - \ln 1/\alpha_i}^{u} \frac{\Sigma^i (u')} {g^\ell_i(u')} \ K^\ell_i(u' + u) \]
\[ a^\ell_i(u) = \int_{u - \ln 1/\alpha_i}^{u} (u' - u) \frac{\Sigma^i (u')} {g^\ell_i(u')} \ K^\ell_i(u' + u) \]
\[ c^\ell_i(u) = \frac{\Sigma^i (u)} {g^\ell_i(u)} - \int_{u - \ln 1/\alpha_i}^{u} \frac{\Sigma^i (u')} {g^\ell_i(u')} \ P^\ell_i(u' + u) \]
If consideration is limited to the case, \( g_i(u') = \Sigma_s(u') \), then composite moderating parameters may be defined

\[
\xi_{\mathcal{L}}(u) = \sum_{i \notin \mathcal{H}} \xi^\mathcal{L}_i(u), \quad a_{\mathcal{L}}(u) = \sum_{i \notin \mathcal{H}} a^\mathcal{L}_i(u),
\]

\[
c_{\mathcal{L}}(u) = \sum_{i \notin \mathcal{H}} c^\mathcal{L}_i(u), \quad e_{\mathcal{L}}(u) = \sum_{i \notin \mathcal{H}} e^\mathcal{L}_i(u)
\]

and Eqs. II.20 and II.21 may be combined to give

\[
\frac{d \xi_{\mathcal{L}}(u)}{du} = \varepsilon_{\mathcal{L}}(u) \dot{\varepsilon}_{\mathcal{L}}(u) \Phi_{\mathcal{L}}(u) - \varepsilon_{\mathcal{L}}(u) \Phi_{\mathcal{L}}(u)
\]

where

\[
\varepsilon_{\mathcal{L}}(u) = \frac{1}{\gamma_{\mathcal{L}}(u)} = \frac{e_{\mathcal{L}}(u)}{a_{\mathcal{L}}(u)}
\]

\[
\dot{\varepsilon}_{\mathcal{L}}(u) = \xi_{\mathcal{L}}(u) + \gamma_{\mathcal{L}}(u) c_{\mathcal{L}}(u)
\]

and

\[
\Phi_{\mathcal{L}}(u) = \Sigma_t(u) \phi_{\mathcal{L}}(u).
\]

If one considers the case \( g_i(u') = \Sigma_s(u') \), and defines the composite moderating parameters

\[
\xi_{\mathcal{L}}(u) = -e_{\mathcal{L}}(u) = \sum_{i \notin \mathcal{H}} \frac{\Sigma_s(u)}{\Sigma_s(u')} \xi^\mathcal{L}_i
\]

\[
a_{\mathcal{L}}(u) = \sum_{i \notin \mathcal{H}} \frac{\Sigma_s(u)}{\Sigma_s(u')} a^\mathcal{L}_i
\]

\[
c_{\mathcal{L}}(u) = 0
\]

then combination of Eqs. II.20 and II.21 gives Eq. II.24 with the parameter \( \hat{\xi}_{\mathcal{L}} \) defined

\[
\hat{\xi}_{\mathcal{L}}(u) = \xi_{\mathcal{L}}(u) \left[ 1 - \frac{d \gamma_{\mathcal{L}}(u)}{du} \right]
\]

A result formally similar to Eq. II.24 was obtained by Goertzel and Greuling. They obtained their results by replacing the slowing down kernel \( K_i(u' + u) \) by a synthetic kernel and preserving moments. The standard Goertzel-Greuling approximation corresponds to Eqs. II.24, II.25, II.27 and II.28 with \( \frac{d \gamma_{\mathcal{L}}}{du} = 0 \).
The set of Eqs. II.23, II.24, II.25 and II.26 defines the "Improved Goertzel-Greuling Approximation" derived by Stacey. The microscopic moderating parameters for both approximations are given by Eqs. II.22 with

\[ g_1(u) = \begin{cases} 
\sum_{s_i} (u) & \text{Goertzel-Greuling} \\
\sum_{t}(u) & \text{Improved Goertzel-Greuling}
\end{cases} \]

In Section II.D of this report explicit definitions of the moderating parameters will be given.

The slowing down Eq. II.24 may be combined with the \( P_1/B_1 \) balance Eqs. II.10 to obtain solutions for the flux and slowing down density. For the inconsistent \( P_1/B_1 \) approximations, one sets

\[ \frac{dq_1(u)}{du} = 0 \]

which is equivalent to Eq. II.9 for \( \varepsilon = 1 \). Equation II.10 may then be written

\[ \sum_{ne} (u) \phi_o(u) = S(u) - \frac{dq_o}{du} \]  \hspace{1cm} (II.29)

where the non-elastic cross section has been defined

\[ \sum_{ne} (u) = \sum_t(u) + \frac{B^2}{3A_1 (B, u, N)} - \sum_s(u). \]  \hspace{1cm} (II.30)

Equations II.24 and II.29 are combined to obtain:

**Inconsistent \( P_1/B_1 \) Approximation**

\[ \frac{dq_o(u)}{du} = \frac{[-(\sum_{ne}(u) + \sum_{s_H}(u)) q_o(u) + \hat{\xi}_o(u) \sum_t(u) (S(u) + \eta_o(u))]}{M(u)} \]  \hspace{1cm} (II.31)

\[ \phi_o(u) = \frac{q_o(u) + \gamma_o(u) [S(u) + \eta_o(u)]}{M(u)} \]  \hspace{1cm} (II.32)

\[ M(u) = \hat{\xi}_o(u) \sum_t(u) + \gamma_o(u) [\sum_{ne}(u) + \sum_{s_H}(u)] \]  \hspace{1cm} (II.33)
Equation II.31 may be integrated directly

\[
q_o(u) = \exp \left[ - \int_0^u du' \frac{[\Sigma ne(u') + \Sigma sH(u')]}{M(u')} \right] \cdot \left\{ q_o(0) + \int_0^u du' \frac{\hat{\xi}_o(u') \Sigma_t(u') (S(u') + \eta_o(u'))}{M(u')} \exp \left[ - \int_0^{u'} du'' \frac{[\Sigma ne(u'') + \Sigma sH(u'')]}{M(u'')} \right] \right\}
\]

Equations II.31-II.34 have been written for the general situation which includes Hydrogen in the mixture. If there were no Hydrogen, the above equations are applicable with \(\Sigma_s(u) = 0, \eta_o(u) = 0\).

If one retains both the \(\ell = 0, 1\) terms of Eqs. II.10 and II.24, the consistent \(P_1/B_1\) coupled equations are obtained,

Consistent \(P_1/B_1\) Approximation

\[
\frac{1}{\Delta(u)} \left\{ \left[ \Sigma_t - \Sigma_s + \Sigma sH \right] (A_1 - \Sigma_1^s + \frac{2}{3} \Sigma sH + \epsilon_1 \hat{\xi}_1 \Sigma_t) + \frac{1}{3} B^2 \right\}.
\]

\[
\left[ \epsilon_o q_o + S + \eta_o \right] + iB \epsilon_o \hat{\xi}_o \Sigma_t \left[ \epsilon_1 q_1 + \frac{3}{2} \eta_1 \right]
\]

\[
+ \frac{dq_o}{du} = S(u) + \eta_o(u)
\]

\[
\frac{1}{\Delta(u)} \left\{ \left[ (A_1 - \Sigma_1^s + \frac{2}{3} \Sigma sH) (\Sigma_t - \Sigma_s + \Sigma sH + \epsilon_o \hat{\xi}_o \Sigma_t) + \frac{B^2}{3} \right] \right\}.
\]

\[
\left[ \epsilon_1 q_1 + \frac{3}{2} \eta_1 \right] + \frac{3}{2} \epsilon_1 \hat{\xi}_1 \Sigma_t \left[ \epsilon_o q_o + S + \eta_o \right]
\]

\[
+ \frac{dq_1}{du} = \frac{3}{2} \eta_1(u)
\]

\(\Delta(u) = (A_1 - \Sigma_1^s + \frac{2}{3} \Sigma sH + \epsilon_1 \hat{\xi}_1 \Sigma_t) (\Sigma_t - \Sigma_s + \Sigma sH + \epsilon_o \hat{\xi}_o \Sigma_t) + \frac{1}{3} B^2\)

and

\[
\phi_o(u) = \frac{1}{\Delta(u)} \left\{ (A_1 - \Sigma_1^s + \frac{2}{3} \Sigma sH + \epsilon_1 \hat{\xi}_1 \Sigma_t) (\epsilon_o q_o + S + \eta_o)
\]

\[
- iB \left[ \epsilon_1 q_1 + \frac{3}{2} \eta_1 \right]
\]

\(\phi_1(u) = \frac{1}{\Delta(u)} \left\{ (\Sigma - \Sigma_s + \Sigma sH + \epsilon_o \hat{\xi}_o \Sigma_t) (\epsilon_1 q_1 + \frac{3}{2} \eta_1)
\]

\[
- \frac{iB}{3} \left( \epsilon_o q_o + S + \eta_o \right) \right\}.
\]
In writing Eqs. II.35 and II.36 hydrogen elastic scattering has been assumed isotropic in the center of mass system so that

\[ \Sigma_{H}^{1}(u) = \frac{2}{3} \Sigma_{H}(u) \]

\[ \eta_{0}(u) = \int_{u}^{u'} du' \Sigma_{H}^{1}(u') \phi_{0}(u') e^{-(u-u')} \] (II.37)

\[ \eta_{1}(u) = \frac{2}{3} \int_{u}^{u'} du' \Sigma_{H}^{1}(u') \phi_{1}(u') e^{-\frac{3}{2}(u-u')} \]

The difference equations used by MC2-2 in the solution of Eqs. II.32-II.36 will be discussed in Section F.

D. Continuous Slowing Down Moderating Parameters

It is well known that the microscopic Legendre moments of the elastic scattering transfer cross section defined in Eq. II.14 may be represented in the form,

\[ \sigma_s^{L}(u') = \frac{\sigma_s(u') P_L[\mu_c(u' + u)] e^{-(u'-u)}}{1-\alpha} \sum_{n=0}^{N} \frac{(2n+1) f_n(u')}{P_n[\mu_c(u' + u)]} \] (II.38)

where

\[ f_n(u') = \text{nth Legendre expansion coefficient at lethargy u'} \]

in the center of mass system. \( f_0(u') = 1 \)

The MC2-2 code permits all \( N \leq 20 \).

\[ \mu_c = \text{cosine of scattering angle in the center of mass system.} \]

\[ \mu_c = \frac{(A+1)^2 e^{-(u-u')}}{2A} - \frac{(A^2 + 1)}{1-\alpha} \left[ 2e^{-(u-u')} - (1 + \alpha) \right] \] (II.39)

\[ \mu_o = \text{cosine of scattering angle in the laboratory system} \]

\[ \mu_o = \frac{(A+1) e^{-(u-u')}}{2} - \frac{(A-1) e^{-(u-u')}}{2} \] (II.40)

and all other terms have been defined previously. To simplify the notation, the isotope index \( i \) has been dropped. Equation II.38 along with Eqs. II.16, II.17 may be used to obtain explicit forms for the isotopic moderating parameters of Equations II.22.
1. Goertzel-Greuling Moderating Parameters

Setting $S_i(u') = \sum_{i} S_i (u')$ and dropping the isotope index $i$,
Eqs. II.22 may be written,

$$\xi^L = -e^L = \frac{1}{1-\alpha} \sum_{n=0}^{N} (2n + 1) \int_{u - \ln 1/\alpha}^{u} du' \int_{u}^{u + \ln 1/\alpha} du'' f_n(u') e^{-(u''-u')}.$$

$$P_L \left[ \mu_o (u' \to u'') \right] P_n \left[ \mu_c (u' \to u'') \right]$$

$$a^L = \frac{1}{1-\alpha} \sum_{n=0}^{N} (2n + 1) \int_{u - \ln 1/\alpha}^{u} du' (u' - u) \int_{u}^{u + \ln 1/\alpha} du'' f_n(u') e^{-(u''-u')}.$$

$$P_L (\mu_o) P_n (\mu_c)$$

$$c^L = 0.$$

Transforming variables to $U = u'' - u'$ and switching orders of integration gives

$$\xi^L = \sum_{n=0}^{N} \frac{(2n + 1)}{2} \int_{u - \ln 1/\alpha}^{u} dU P_n(\mu_c (U)) P_L[\mu_o (U)] \left( - \frac{d\mu_c}{dU} \right) \int_{u - U}^{u} du' f_n(u')$$

$$a^L = \sum_{n=0}^{N} \frac{(2n + 1)}{2} \int_{u - \ln 1/\alpha}^{u} dU P_n(\mu_c) P_L[\mu_o] \left( - \frac{d\mu_c}{dU} \right) \int_{u - U}^{u} du' (u' - u) f_n(u').$$

If the scattering coefficients $f_n(u)$ are assumed constant in the scattering band $[u - \ln(1/\alpha), u]$, the Goertzel-Greuling moderating parameters may be written

$$\xi^L_1(u) = -e^L_1(u) = -\sum_{n=0}^{N} f_n(u) T_1^L(\alpha_1)$$

$$a^L_1(u) = -\sum_{n=0}^{N} f_n(u) T_2^L(\alpha_1) \quad \text{(II.41)}$$

$$c^L_1(u) = 0.$$

where

$$T_m^L(\alpha_1) = \frac{(-)^m}{m!} \frac{(2n + 1)}{2} \int_{u - \ln 1/\alpha}^{u} dU U^m P_L[\mu_o (U)] P_n(\mu_c (U)).$$

$$\left( - \frac{dU}{dU} \right)^m.$$
The quantities $T_{\ell n}^m$ relate Legendre moments of the scattering cross sections in the center of mass and laboratory systems and have been studied in detail.\(^{(16-18)}\) Precalculated values of $T_{\ell n}^m$ are provided in the MC\(^2\)-2 library (MCC2F8 of Appendix C) for each isotope. Numerical experience has shown that six terms in the sums of Eqs.II.41 suffice to calculate the parameters accurately. This is a consequence of the fact that $T_{\ell n}^m(\alpha)$ approaches zero at least as fast as the faster of $A^{-m}$ and $A^{-|\ell-n|}$.\(^{(6)}\)

2. Improved Goertzel-Greuling Moderating Parameters

Setting $g_i(u') = \Sigma_t(u')$ Eqs.II.22 may be written

$$
\xi^\ell_i(u) = \frac{1}{1-\alpha_i} \sum_{n=0}^{N} (2n + 1) \int_{u-Ln^1/\alpha_i}^{u} \frac{\Sigma^s_i(u')}{\Sigma^t(u')} \frac{\Sigma^s_i(u')}{f_{n_i}(u')} du' e^{-(u''-u')} P_{\ell}(\mu_o) P_n(\mu_c)
$$

$$
a^\ell_i(u) = \frac{1}{1-\alpha_i} \sum_{n=0}^{N} (2n + 1) \int_{u-Ln^1/\alpha_i}^{u} \frac{\Sigma^s_i(u')}{\Sigma^t(u')} (u' - u) f_{n_i}(u').
$$

$$
b^\ell_i(u) = \frac{1}{1-\alpha_i} \sum_{n=0}^{N} (2n + 1) \int_{u-Ln^1/\alpha_i}^{u} \frac{\Sigma^s_i(u')}{\Sigma^t(u')} (u' - u) f_{n_i}(u').
$$

$$
e^{-(u-u')} P_{\ell}(\mu_o) P_n(\mu_c)
$$

$$
c^\ell_i(u) = \frac{\Sigma^\ell_i(u)}{\Sigma^t(u)} - \frac{1}{1-\alpha_i} \sum_{n=0}^{N} (2n + 1) \int_{u-Ln^1/\alpha_i}^{u} \frac{\Sigma^s_i(u')}{\Sigma^t(u')} f_{n_i}(u').
$$

For heavy isotopes which have a small scattering band width, it is reasonable to assume

$$
\frac{\Sigma^s_i(u')}{\Sigma^t(u')} f_{n_i}(u') \sim \left(\frac{\Sigma^s_i f_{n_i}}{\Sigma^t}ight) u - Ln^1/\alpha_i \leq u' \leq u
$$
where \( \langle \cdot \rangle_u \) denotes an average over the lethargy band. With this approximation the same operations which led to Eqs. II.41 give

\[
\xi_i^L(u) = - \xi_i^L(u) = - N \sum_{n=0}^{\infty} \left( \frac{\xi_s^i}{\xi_t} f_n^i \right) u T_{\xi n}^1 (\alpha_i)
\]

\[
a_i^L(u) = \sum_{n=0}^{\infty} \left( \frac{\xi_s^i}{\xi_t} f_n^i \right) u T_{\xi n}^2 (\alpha_i)
\]

\[
c_i^L(u) = \sum_{n=0}^{N} \left[ \frac{\xi_s^i(u)}{\xi_t(u)} t_n^i(u) - \left( \frac{\xi_s^i}{\xi_t} f_n^i \right) u \right] T_{\xi n}^0 (\alpha_i) \approx 0
\]

where the definition

\[
\xi_s^L(u) = \sum_{n=0}^{N} \xi_s^L(u) f_n^i(u) T_{\xi n}^i (\alpha_i)
\]

has been used. The setting of \( c_i^L(u) \) to zero is an approximation required in MC\(^2\)-2 to avoid numerical difficulties. In the MC\(^2\)-2 code Eqs. II.44 are used for isotopes of mass \( A_i \geq 200 \) (\( \ell n^2 / \alpha_i < 0.02 \)) so that the averaging assumption is expected to be valid. Numerical experience has shown that four terms in the sums of Eqs. II.44, \( N = 3 \), suffice to calculate the parameters accurately for the heavy isotopes.

For lighter materials \( (A_i < 200) \) the Improved Coertzel-Greuling moderating parameters are derived in the following manner. Define the quantity

\[
\varphi^i_n(u) \equiv \sum_{n=n'-1}^{N} \frac{2n+1}{2} f_n^i(u) K_{nn'}^i (\alpha_i)
\]

where

\[
K_{nn'}^i (\alpha_i) \equiv \frac{1}{2^n(n'-1)!} \left( \frac{2}{1 + \alpha_i} \right)^n K_{\max} \sum_{k=0}^{n'/2} \left( \frac{-1}{(n-k)!} \right)^{n' + 1 - k} \frac{(2n - 2k)!}{(n+1-2k-n')!} \left( \frac{i + \alpha_i}{1 - \alpha_i} \right)^{n+1-2k}
\]

\[
K_{\max} = \min \left\{ \left[ \frac{n}{2} \right], \left[ \frac{n+1}{2} - n' \right] \right\}
\]

Noting that the Legendre Polynomials \( P_n(\mu) \) may be expanded

\[
P_n(\mu) = \sum_{k=0}^{[n/2]} \frac{(-1)^{2n-2k} (2n - 2k)!}{2^n k! (n-k)! (n-2k)!} \mu^{n-2k}
\]

and using Eqs. II.39 and II.40 it can be shown that the \( \ell = 0, 1 \) Eqs. II.43 may be written in the form
\[ \xi_1^0(u) = \sum_{n' = 1}^{N+1} \frac{1}{n'} \left\{ \int_{u - n'u^1/\alpha_i}^{u} \frac{\Sigma_{s_i^n}(u')}{\Sigma_t(u')} \, \rho_{n'}^i(u') \, e^{-n'(u-u')} \right. \\
- \alpha_i^{n'} \int_{u - n'u^1/\alpha_i}^{u} \frac{\Sigma_{s_i^n}(u')}{\Sigma_t(u')} \, \rho_{n'}^i(u') \left. \right\} \]

\[ a_1^0(u) = -\sum_{n' = 1}^{N+1} \frac{1}{n'} \left\{ \int_{u - n'u^1/\alpha_i}^{u} \frac{\Sigma_{s_i^n}(u')}{\Sigma_t(u')} \, \rho_{n'}^i(u') \, (u - u') \, e^{-n'(u-u')} \right. \\
- \alpha_i^{n'} \int_{u - n'u^1/\alpha_i}^{u} \frac{\Sigma_{s_i^n}(u')}{\Sigma_t(u')} \, (u - u') \, \rho_{n'}^i(u') \left. \right\} \]

\[ c_1^0(u) = \sum_{n' = 1}^{N+1} \left\{ \frac{\Sigma_{s_i^n}(u)}{\Sigma_t(u)} \, \left( 1 - \alpha_i^{n'} \right) \rho_{n'}^i(u) - \int_{u - n'u^1/\alpha_i}^{u} \frac{\Sigma_{s_i^n}(u')}{\Sigma_t(u')} \, \rho_{n'}^i(u') \, e^{-n'(u-u')} \right. \\
= \frac{\Sigma_{s_i^n}(u)}{\Sigma_t(u)} - \sum_{n' = 1}^{N+1} \int_{u - n'u^1/\alpha_i}^{u} \frac{\Sigma_{s_i^n}(u')}{\Sigma_t(u')} \, \rho_{n'}^i(u') \, e^{-n'(u-u')} \left. \right\} \]

\[ e_1^0(u) = \sum_{n' = 1}^{N+1} \int_{u - n'u^1/\alpha_i}^{u} \frac{\Sigma_{s_i^n}(u')}{\Sigma_t(u')} \, \rho_{n'}^i(u') \, (u - u') \, e^{-n'(u-u')} \quad (II.48) \]

\[ \xi_1^1(u) = \sum_{n' = 1}^{N+1} \left\{ \frac{(A_i^1 + 1)}{2n'^{1} + 1} \left[ \int_{u - n'u^1/\alpha_i}^{u} \frac{\Sigma_{s_i^n}(u')}{\Sigma_t(u')} \, \rho_{n'}^i(u') \, e^{-(n'^{1}+1/2)(u-u')} \right. \right. \\
- \alpha_i^{n'^{1}+1/2} \int_{u - n'u^1/\alpha_i}^{u} \frac{\Sigma_{s_i^n}(u')}{\Sigma_t(u')} \, \rho_{n'}^i(u') \left. \right\} \right. \\
- \frac{(A_i^1 - 1)}{2n'^{-1} - 1} \left[ \int_{u - n'u^1/\alpha_i}^{u} \frac{\Sigma_{s_i^n}(u')}{\Sigma_t(u')} \, \rho_{n'}^i(u') \, e^{-(n'^{-1}-1/2)(u-u')} \right. \\
- \alpha_i^{n'^{-1}-1/2} \int_{u - n'u^1/\alpha_i}^{u} \frac{\Sigma_{s_i^n}(u')}{\Sigma_t(u')} \, \rho_{n'}^i(u') \left. \right\} \right. \]
\[ a_{i_1}^{n_1}(u) = - \frac{N+1}{2n_1 + 1} \left\{ \frac{(A_i + 1)}{2^{n_1 + 1}} \left[ \int_{u - \ln^1 / \alpha_i}^{u} \frac{\Sigma_{s_1}^{i}(u')}{\Sigma_{s_1}^{i}(u') \left( u - u' \right)} \left( u - u' \right) \right] \right\} \]

\[ \mathcal{D}_{n_1}^{i}(u') \left( u - u' \right) e^{-(n_1+1/2)} \left( u - u' \right) \]

\[ - \alpha_{i_1}^{n_1 + 1/2} \int_{u - \ln^1 / \alpha_i}^{u} du' \frac{\Sigma_{s_1}^{i}(u')}{\Sigma_{t}^{i}(u')} \left( u - u' \right) \mathcal{D}_{n_1}^{i}(u') \]

\[ \left( u - u' \right) e^{-(n_1-1/2)} \left( u - u' \right) \]

\[ - \alpha_{i_1}^{n_1 - 1/2} \int_{u - \ln^1 / \alpha_i}^{u} du' \frac{\Sigma_{s_1}^{i}(u')}{\Sigma_{t}^{i}(u')} \left( u - u' \right) \mathcal{D}_{n_1}^{i}(u') \]

\[ c_{i_1}^{n_1}(u) = \frac{N+1}{2^n - 1} \left\{ \frac{\Sigma_{s_1}^{i}(u)}{\Sigma_{t}^{i}(u)} \right\} \]

\[ \mathcal{D}_{n_1}^{i}(u') \left( u - u' \right) e^{-(n_1+1/2)} \left( u - u' \right) \]

\[ - \frac{(A_i - 1)}{2^{n_1 - 1}} \left[ \int_{u - \ln^1 / \alpha_i}^{u} \frac{\Sigma_{s_1}^{i}(u')}{\Sigma_{t}^{i}(u')} \left( u - u' \right) \right] \]

\[ \mathcal{D}_{n_1}^{i}(u') \left( u - u' \right) e^{-(n_1-1/2)} \left( u - u' \right) \]

\[ - \frac{(A_i - 1)}{2^{n_1 - 1}} \left[ \int_{u - \ln^1 / \alpha_i}^{u} \frac{\Sigma_{s_1}^{i}(u')}{\Sigma_{t}^{i}(u')} \left( u - u' \right) \right] \]

\[ \mathcal{D}_{n_1}^{i}(u') \left( u - u' \right) e^{-(n_1-1/2)} \left( u - u' \right) \]
Numerical experience has shown that only four terms need be retained in the sums of Eqs. II.48, \( N = 3 \). The mass dependent coefficients \( K_{\mu\nu}(\alpha) \) defined by Eq. II.47 are given in Table I. These coefficients are provided in the MC\(^2\)-2 library (MCC2F8 of Appendix C).
<table>
<thead>
<tr>
<th>( n/n' )</th>
<th>( 1 )</th>
<th>( 2 )</th>
<th>( 3 )</th>
<th>( 4 )</th>
<th>( 5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>( \frac{2}{1-\alpha} )</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>1</td>
<td>( -\frac{2}{(1-\alpha)} \left( \frac{1+\alpha}{1-\alpha} \right) )</td>
<td>( \frac{4}{(1-\alpha)^2} )</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>( \frac{1}{1-\alpha} \left[ 3 \left( \frac{1+\alpha}{1-\alpha} \right)^2 - 1 \right] )</td>
<td>( -\frac{12}{(1-\alpha)^3} )</td>
<td>( \frac{12}{(1-\alpha)^3} )</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
<td>( \frac{1}{(1-\alpha)^2} \left[ -5 \left( \frac{1+\alpha}{1-\alpha} \right)^2 + 3 \right] )</td>
<td>( \frac{6}{(1-\alpha)^2} \left[ 5 \left( \frac{1+\alpha}{1-\alpha} \right)^2 - 1 \right] )</td>
<td>( -\frac{60}{(1-\alpha)^4} )</td>
<td>( \frac{40}{(1-\alpha)^4} )</td>
<td>-</td>
</tr>
<tr>
<td>4</td>
<td>( \frac{1}{4(1-\alpha)} \left[ 35 \left( \frac{1+\alpha}{1-\alpha} \right)^4 - 30 \left( \frac{1+\alpha}{1-\alpha} \right)^2 + 3 \right] )</td>
<td>( \frac{10}{(1-\alpha)^3} \left[ -7 \left( \frac{1+\alpha}{1-\alpha} \right)^2 + 3 \right] )</td>
<td>( \frac{30}{(1-\alpha)^3} \left[ 7 \left( \frac{1-\alpha}{1-\alpha} \right)^2 - 1 \right] )</td>
<td>( -\frac{280}{(1-\alpha)^5} )</td>
<td>( \frac{140}{(1-\alpha)^5} )</td>
</tr>
</tbody>
</table>
E. Narrow Resonance Attenuation

The formalism developed in the previous sections is directly applicable to narrow resonances provided that effective resonance cross sections could be calculated. Such a calculation is quite time consuming as evidenced by the fact that the resonance calculation of the code MC$^2$(10) is about one-half of the total computing time for typical problem executions. It is, therefore, advantageous to ignore these resonances in defining the moderating parameters of Section D and then superimpose their effect by attenuating the slowing down density. This is the strategy employed by the code MC$^2-2$ for the treatment of narrow resolved resonances. In particular, the wide resonances of light materials are treated by the code which prepares the library for MC$^2-2$ from basic nuclear data, e.g. ETOE-2\(^{(4)}\). MC$^2-2$ treats these resonance cross sections as effective smooth cross sections and includes their contribution in the calculation of moderating parameters. Similarly, effective smooth cross sections for heavy isotopes are calculated by MC$^2-2$ from unresolved resonance parameters according to the algorithms specified in Chapter IV and included in the calculation of the moderating parameters. An asymptotic slowing down density, $q_{\text{asy}}(u)$, is calculated using these parameters in Eqs. II.34 or II.35 and the effects of the narrow resolved resonances are superimposed on $q_{\text{asy}}(u)$ by use of attenuation factors. The form of the narrow resonance attenuation factors is derived below.

For the sake of simplicity consider the $P_1/B_1$ equations for a single material and assume zero buckling,

$$F(u) = \int_{0}^{u} \text{d}u' P^O(u - u') h(u') F(u') + S(u)$$  (II.49)

where

$$F(u) = \Sigma_t(u) \phi_o(u)$$

$$h(u) = \Sigma_s(u)/\Sigma_t(u)$$

and all other terms have been defined previously. If one neglects the narrow resolved resonance cross sections, Eq. II.49 has the form

$$F_{\text{asy}}(u) = \int_{0}^{u} \text{d}u' P^O(u - u') h_{\text{asy}}(u') F_{\text{asy}}(u') + S(u)$$  (II.50)

where the asymptotic cross sections are defined

$$\Sigma_{\text{asy}}(u) = \Sigma_t(u) - \Sigma_r(u), \text{ etc.}$$

and $r$ represents the narrow resolved resonance cross sections. Subtracting Eq. II.50 from Eq. II.49,

$$F(u) = F_{\text{asy}}(u) + \int_{0}^{u} \text{d}u' P^O(u - u') [h(u') F(u') - h_{\text{asy}}(u') F_{\text{asy}}(u')]$$
Following the methods used by Corngold, \(^{(19)}\) define the Laplace transform as

\[
\tilde{f}(s) = L[f(u)] = \int_{0}^{\infty} du \ e^{-su} f(u)
\]

so that

\[
\tilde{F}(s) = \tilde{F}_{as}(s) + \tilde{F}_{0}(s) [L(hf) - L(h_{as} F_{as})].
\]

Define

\[
\begin{align*}
    h(u) &= 1 - g(u) \\
    h_{as}(u) &= 1 - g_{as}(u)
\end{align*}
\]

where

\[
\begin{align*}
    g(u) &= \frac{\Sigma_{ne}^{as} + \Sigma_{ne}^{r}}{\Sigma_{t}^{as} + \Sigma_{t}^{r}} \\
    g_{as}(u) &= \frac{\eta_{as}}{\sigma_{as}}
\end{align*}
\]

and

\[
\begin{align*}
    \tilde{F}(s) &= \tilde{F}_{as}(s) - \frac{\tilde{F}_{0}(s) [L(gF) - L(g_{as} F_{as})]}{1 - \tilde{F}_{0}(s)}.
\end{align*}
\] (II.51)

Defining

\[
\tilde{\psi}(s) = \frac{\tilde{F}_{0}(s)}{1 - \tilde{F}_{0}(s)}
\]

Equation II.51 may be inverted to obtain

\[
F(u) = F_{as}(u) - \int_{0}^{u} du' \ \psi(u - u') \ [g(u') F(u') - g_{as}(u') F_{as}(u')]
\] (II.52)

where the kernel \(\psi\) satisfies

\[
\psi(u) = \int_{0}^{u} du' \ F_{0}(u - u') \ \psi(u') + F_{0}(u).
\] (II.53)

It is obvious from Eq. II.53 that \(\psi(u)\) is the solution of Eq. II.49, for a delta function source in the absence of absorption. It is well known that asymptotically

\[
\psi(u) = \frac{1}{\xi} \frac{\Sigma_{ne}^{as}}{\phi_{as}^{as}}.
\] (II.54)
Using Eq.II.54 in Eq.II.52 an expression for the attenuation in the asymptotic (non-resonance) collision density is obtained,

\[ F(u) \approx F_{as}(u) \prod_{r} (1 - p_r) \]  \hspace{1cm} (II.55)

where the product is taken over all resonances in the interval \(0 \leq u_r \leq u\) and

\[ p_r = \left\{ \begin{array}{l}
\Gamma_r \frac{J^*}{a_r} \left[ 1 - \frac{\Sigma_{as}}{E_r} \frac{\Gamma_r}{\Sigma_{as}} \right] \frac{\Sigma_{as} \phi_{as}}{q_{as}} \\
\end{array} \right. \]  \hspace{1cm} (II.56)

\[ J^*_r = \frac{1}{\Gamma_r} \int_{-\infty}^{x_r} \frac{\Sigma_t}{\Sigma_{as} + \Gamma_r} \, du \]  \hspace{1cm} (II.57)

The method for calculating the \(J^*_r\) function will be discussed in Chapter III.

Stacey \cite{12} derived an attenuation factor formalism by considering the resonance as a point absorber. This leads to Eq.II.56 without the second term in the brackets, thus neglecting the competition between scattering and absorption of the resonance.

**F. Ultra-Fine-Group Equations**

The lethargy (energy) domain of interest is assumed to be partitioned into equal lethargy intervals of width \(\Delta u\). The corresponding energy widths are denoted \(\Delta E^g\). By convention, increasing \(g\) represents increasing lethargy (decreasing energy),

\[ u_{g+1} = u_g + \Delta u \]

\[ E_{g+1} = E_g e^{-\Delta u} \]

The lethargy group width is assumed to be small and, following the \(MC^2\) \cite{10} conventions, calculations performed in this structure are called ultra-fine-group calculations. The group structure is fixed by the \(MC^2\)-2 library (Appendix C). It is usually set at \(\Delta u = 1/120\), corresponding to the \(MC^2\) structure, giving 2040 groups from 10 MeV to 0.414 eV.

Figure 2 gives a schematic representation of the \(MC^2\)-2 group structure. From the maximum problem energy, \(E_{\text{max}}\), to a user specified energy, \(E_{\text{CSD}}\), the code uses a multigroup form of Eqs.II.10-II.12 in the spectrum calculation. From \(E_{\text{CSD}}\) to \(E_{\text{min}}\), the equations of Section II.C, Continuous Slowing Down Theory, are applicable. The user specified energy \(E_{\text{CSD}}\) must satisfy the relationship
Fig. 2. MC²-2 Energy Structure
\[
\frac{E_R}{E_{CSD}} \leq E_{\text{max}}
\]  

where \(E_R\) = energy of highest energy resolved resonance in the problem mixture.

This restriction is a consequence of the use of the attenuation factor treatment of resolved resonances (c.f. Section II.E) in the continuous slowing down energy domain.

The remainder of this section presents the ultra-fine-group equations for the multigroup and continuous slowing down formulations.

1. Multigroup Equations

Integrating Eqs.II.10 and II.11 over a group one obtains

\[
i B \phi_g + \Sigma_t^g \phi_g = S^g + \sum_{g' \leq g} \Sigma_s^g (g' \rightarrow g) \phi_{g'}^g
\]

\[
i \frac{B}{3} \phi_o + A^g \phi_{g-1}^g = \sum_{g' \leq g} \Sigma_s^1 (g' \rightarrow g) \phi_{g-1}^g
\]  

(II.59)

\[
\phi_g^\ell = - \frac{\ell}{2\ell + 1} i B \phi_g^{\ell-1} / A^g_{\ell-1} \quad \ell = 2, \ldots, N
\]

(II.60)

where

\[
\phi_g^\ell = \int_{u_{g-1}}^{u_g} \phi_L(u) \text{ du}
\]

and

\[
\Sigma_t^g = \frac{1}{\phi_g^o} \int_{u_{g-1}}^{u_g} \Sigma_t(u) \phi_o(u) \text{ du}
\]

\[
\Sigma_s^g (g' \rightarrow g) = \frac{1}{\phi_g^0} \int_{u_{g-1}}^{u_g} \int_{u_{g'-1}}^{u_{g'}} \Sigma_s^g (u' \rightarrow u) \phi_{g'}^L(u')
\]

(II.61)

\[
A^g_{\ell-1} = \int_{u_{g-1}}^{u_g} A_{\ell} (B, u, N) \text{ du}
\]

Since the flux moments \(\phi_L(u)\) are unknown a spectrum must be assumed in order to derive the ultra-fine-group cross sections defined by Eqs.II.61. This averaging is performed by the processing code which prepares the library files for MC\(^2\)-2. These ultra-fine-group data are the basic input to MC\(^2\)-2 and later sections of this report will describe how these data are processed to permit a solution of Eqs. II.59.
As noted earlier in this report, an option of the code permits group dependent buckling. In this case one is solving Eqs.II.59 with $B$ replaced by $B_g$. To simplify notation, only the group independent buckling equations will be developed.

In writing Eqs.II.59 it has been assumed that a neutron cannot gain energy as a result of scattering thus precluding the use of $MC^2-2$ in the thermal energy domain.

Equations II.59 may be written:

Consistent $P_1/B_1$ Approximation

$$
\begin{align*}
\phi^g &= \frac{\Sigma^g_{r_0} + \frac{B^2}{3\Sigma^g_{r_1}}}{\Sigma^g_{r_1}} \\
J^g &= \frac{\frac{B}{3} \phi^g + \sum_{g' < g} \Sigma^1_{s}(g' \to g) J^{g'}}{\Sigma^g_{r_1}}
\end{align*}
$$

$$
\phi^g = -\frac{\ell}{2\ell + 1} iB \phi^g_{\ell-1}/\phi^g
$$

$$
\phi^g = \phi^g_0
$$

$$
J^g = i\phi^g_1
$$

and

$$
\begin{align*}
\Sigma^g_{r_0} &= \Sigma^g_t - \Sigma^0_{s}(g \to g) - \Sigma_{ine}(g \to g) - 2\Sigma_{n,2n}(g \to g) \\
\Sigma^g_{r_1} &= A^g_1 - \Sigma^1_{s}(g \to g) \\
s^g &= \frac{1}{k} s^g + s^g_{fix} + \sum_{g' < g} \left[ \Sigma_{ine}(g' \to g) + 2\Sigma_{n,2n}(g' \to g) \right] \phi^{g'}
\end{align*}
$$
In Eqs. II.63 explicit account has been taken of the elastic \( (E_{\text{el}}) \), inelastic \( (E_{\text{inel}}) \), and \( (n,2n) \), \( (E_{n,2n}) \) scattering sources and the source term \( S^g \) has been redefined to exclude non-elastic in-group scattering which has been incorporated in the removal cross section \( \Sigma_{ro}^g \). Equations II.62 and II.63 define the multigroup consistent \( P_1/B_1 \) approximation. The inconsistent \( P_1/B_1 \) equations are written:

\[
\phi^g = S^g + \sum_{g' < g} L^S_{g'}(g' + g) \phi^{g'}
\]

\[
\phi^g = \frac{S^g + \frac{L^2}{r_0}}{3A^g_1} \phi^g
\]

\[
j^g = \frac{B^g}{3A^g_1} \phi^g
\]

2. Continuous Slowing Down Equations

If one assumes

\[
\int_{u_{g-1}}^{u_g} f(u) \, du = [\theta f_+ + (1 - \theta) f_-] \Delta u
\]

where

\[
f_+ \equiv f(u) = f(u) \quad \text{for} \quad u > u_g - \theta \Delta u
\]

\[
f_- \equiv f(u_{g-1}) = f(u) \quad \text{for} \quad u_{g-1} < u < u_g - \theta \Delta u
\]

\[
\theta \equiv \text{integration factor} \quad 0 \leq \theta \leq 1
\]

\[
\Delta u \equiv u_g - u_{g-1}
\]

then the inconsistent \( P_1/B_1 \) slowing down Eq.II.34 may be written
where

\[ \Sigma_{ne}^{g} = \Sigma_{t}^{g} + \frac{B^2}{3A_1} - \Sigma_{s}^{g} \]

\[ M_{+}^{g} = \xi_{o}(u_{g}) \Sigma_{t}^{g} + \gamma_{o}(u_{g}) \left[ \Sigma_{ne}^{g} + \Sigma_{s}^{g} \right] \]

\[ M_{-}^{g} = \xi_{o}(u_{g-1}) \Sigma_{t}^{g} + \gamma_{o}(u_{g-1}) \left[ \Sigma_{ne}^{g} + \Sigma_{s}^{g} \right] \]

The group flux \( \phi_{g} \) may be derived from Eq. II.32

\[ \phi_{g} = \left[ \frac{\theta \xi_{o}(u_{g}) + (1 - \theta) \xi_{o}(u_{g-1})}{M_{+}^{g}} + \frac{(S_{g} + \eta_{o}^{g}) (1 - \theta) \gamma_{o}(u_{g})}{M_{-}^{g}} \right] \Delta u \]

or from the balance Eq. II.29

\[ \phi_{g} = \frac{S_{g} + \eta_{o}^{g} + \xi_{o}(u_{g-1}) - \xi_{o}(u_{g})}{\Sigma_{ne}^{g} + \Sigma_{s}^{g}} \]
The consistent $P_{1}/B_{1}$ recursion relations are derived by differencing of Eqs. II.35 and II.36 using the approximations

$$
\frac{dq}{du} \approx \frac{q(u) - q(u_{g-1})}{\Delta u}
$$

$$
f(u)q(u) \approx \theta f_{+}q(u_{g}) + (1 - \theta) f_{-}q(u_{g-1}).
$$

Consistent $P_{1}/B_{1}$ Approximation

$$
q_{o}(u_{g}) = \frac{1}{n_{g}} \left\{ \left[ (\theta z_{+}^{g} + \frac{1}{\Delta u}) [1 - \theta] \nu_{-}^{g} - \frac{1}{\Delta u} \nu_{-}^{g} + \theta \chi_{+}^{g} (1 - \theta) \nu_{-}^{g} \right] q_{o}(u_{g-1}) 
+ \left[ (\theta z_{+}^{g} + \frac{1}{\Delta u}) [1 - \theta] \chi_{-}^{g} - \theta \chi_{+}^{g} (1 - \theta) \nu_{-}^{g} - \frac{1}{\Delta u} \right] q_{1}(u_{g-1}) 
- \left[ (\theta z_{+}^{g} + \frac{1}{\Delta u}) [1 - \gamma_{o}(u_{g}) \theta \nu_{+}^{g} - (1 - \theta) \gamma_{o}(u_{g-1}) \nu_{-}^{g}] \right] \right\} (II.70)
$$

$$
+ \theta \chi_{+}^{g} [\gamma_{o}(u_{g}) \theta \nu_{+}^{g} + \gamma_{o}(u_{g-1}) (1 - \theta) \nu_{-}^{g}] \left( \frac{s_{g}^{g} + \eta_{o}^{g}}{\Delta u} \right)
$$

$$
+ \left[ \gamma_{1}(u_{g}) \theta \chi_{+}^{g} + \gamma_{1}(u_{g-1}) (1 - \theta) \chi_{-}^{g} \left( \theta z_{+}^{g} + \frac{1}{\Delta u} \right) \right]
+ \theta \chi_{+}^{g} [1 - \gamma_{1}(u_{g}) \theta \chi_{+}^{g} - \gamma_{1}(u_{g-1}) (1 - \theta) \nu_{-}^{g}] \left( \frac{s_{g}^{g} + \eta_{o}^{g}}{2 \Delta u} \right)
$$

$$
q_{1}(u_{g}) = \frac{-1}{(\theta z_{+}^{g} + \frac{1}{\Delta u})} \left\{ [(1 - \theta) \nu_{-}^{g} - \frac{1}{\Delta u}] q_{1}(u_{g-1}) 
+ \theta \nu_{+}^{g} q_{o}(u_{g}) + (1 - \theta) \nu_{-}^{g} q_{o}(u_{g-1}) \right\} (II.71)
$$

$$
+ \left[ \gamma_{o}(u_{g}) \theta \nu_{+}^{g} + \gamma_{o}(u_{g-1}) (1 - \theta) \nu_{-}^{g} \right] \left( \frac{s_{g}^{g} + \eta_{o}^{g}}{\Delta u} \right)
$$

$$
+ \left[ \gamma_{1}(u_{g}) \theta \chi_{+}^{g} + \gamma_{1}(u_{g-1}) (1 - \theta) \chi_{-}^{g} \left( \frac{s_{g}^{g} + \eta_{o}^{g}}{2 \Delta u} \right) \right]
$$
where
\[ N^g = (\theta Y^g)(\theta X^g) - (\theta Z^g + \frac{1}{\Delta u})(\theta \omega^g + \frac{1}{\Delta u}) \]
\[ W^g = \frac{1}{\gamma_o} \left[ (\varepsilon^g_t - \varepsilon^g + \varepsilon^g_H) (\Lambda^g_1 - \varepsilon^g + \frac{2}{3} \varepsilon^g_H + \frac{\xi^g_1}{\gamma o} \varepsilon^g_t) + \frac{B^2}{3} \right] / \Delta g \]
\[ X^g = \frac{1}{\gamma_o \gamma_1} \frac{\zeta_o \varepsilon^g}{B / \Delta g} \]
\[ Y^g \equiv -\frac{B}{3} \frac{1}{\gamma_o \gamma_1} \xi^g_1 \varepsilon^g / \Delta g \]
\[ Z^g = \frac{1}{\gamma} \left[ (\Lambda^g_1 - \varepsilon^g + \frac{2}{3} \varepsilon^g_H + \frac{\xi^g_1}{\gamma_1} \varepsilon^g_t) (\varepsilon^g - \varepsilon^g + \varepsilon^g_H + \frac{\xi^g_o \varepsilon^g_t}{\gamma_o} + \frac{B^2}{3} \right] / \Delta g \]
\[ \Delta^g = (\Lambda^g_1 - \varepsilon^g + \frac{2}{3} \varepsilon^g_H + \frac{\xi^g_1}{\gamma_1} \varepsilon^g_t) (\varepsilon^g - \varepsilon^g + \varepsilon^g_H + \frac{\xi^g_o \varepsilon^g_t}{\gamma_o} + \frac{B^2}{3} \right] \]

Expressions for the flux and current follow directly from Eqs. 36,
\[ \phi^g = \left[ \theta R^g + q_o(u_g) + (1 - \theta) R_g q_o(u_{g-1}) - \theta T^g + q_1(u_g) \right. \]
\[ - (1 - \theta) R^- q_1(u_{g-1}) \Delta u + (s^g + n^g_o) \left[ \gamma O(u_g) \theta R^g + \gamma O(u_{g-1}) (1 - \theta) R_g \right. \]
\[ - \frac{3}{2} n^g_1 \left[ \gamma_1(u_g) \theta T^g_1 + \gamma_1(u_{g-1}) (1 - \theta) T^- \right] \]
\[ J^g = \left[ \theta V^g + q_o(u_g) + (1 - \theta) V_g q_o(u_{g-1}) + \theta V^g + q_1(u_g) \right. \]
\[ + (1 - \theta) V^- q_1(u_{g-1}) \Delta u + (s^g + n^g_o) \left[ \gamma O(u_g) \theta V^g + \gamma O(u_{g-1}) (1 - \theta) V_g \right. \]
\[ + \frac{3}{2} n^g_1 \left[ \gamma_1(u_g) \theta V^g_1 + \gamma_1(u_{g-1}) (1 - \theta) V^- \right] \]
where
\[ R^g = \frac{1}{\gamma_0} \int A_1^g \mathcal{L}_{\text{Mod}} \, \mathcal{L}_{\text{Mod}} + \frac{2}{3} \Sigma_{s_H}^g + \frac{1}{\gamma_1} \Sigma_{s_H}^g / \Delta^g \]
\[ T^g = \frac{B}{\gamma_1} \frac{1}{\Delta^g} \]
\[ U^g = \frac{1}{\gamma_1} \left[ \Sigma_t^g - \Sigma_s^g + \frac{\xi_o}{\gamma_0} \Sigma_t^{g-1} \right] / \Delta^g \]
\[ V^g = \frac{B}{3\gamma_0} \frac{1}{\Delta^g} \]

The calculation of the moderating parameters required in Eqs. II.66-II.75 will be described in Section I. The Hydrogen slowing down density \( \eta^g_{\epsilon} \) may be calculated recursively. From Eqs. II.37 it follows that

\[
\eta^g_{\epsilon}(u) \sim \eta^g_{\epsilon}(u_{g-1}) e^{-\frac{(2\ell+1)}{(\ell+1)} \Delta u} + \frac{(\ell + 1)}{(2\ell + 1)} \frac{\Sigma_{s_H}^g \phi_{\ell}^g}{\Delta u} \left[ 1 - e^{-\frac{(2\ell+1)}{(\ell+1)} \Delta u} \right] \quad \ell = 0, 1
\]

\[
\eta^g_{\epsilon} = \int_{u_{g-1}}^{u_{g-1}} \eta^g_{\epsilon}(u) \, du \sim \eta^g_{\epsilon}(u_{g-1}) \Delta u .
\]

The initial conditions for the continuous slowing down calculation are given by

\[
\eta_{\epsilon}(0) = 0
\]
\[
q_{\epsilon}(0) = 0
\]
\[
q_{\epsilon}(u_{\text{CS})} = \sum_{i \neq H} \sum_{g=1}^{G-1} \sum_{g'=G}^{G+1} \Sigma_{s_i}^\epsilon (g + g') \phi_{\ell}^g \quad G > 1
\]

where
\[
u_{\text{CS}} = \nu_{G} = \ln \left( \frac{E_{\text{max}}}{E_{\text{CS}}} \right)
\]
\[ G = \frac{u_G}{\Delta u}, \quad NG = \frac{1}{\Delta u} \ln \left( \frac{E_{\text{max}}}{E_{\text{min}}} \right) .
\]
G. Elastic Scattering Transfer Matrix

The multigroup spectrum calculation of $MC^2-2$ requires ultra-fine-group elastic scattering transfer matrices. Using Eqs. II.38 and II.61, the transfer matrices are defined

$$
\sigma_s^\ell(g' \rightarrow g) = \frac{1}{\phi_s^\ell} \int_{E_{g-1}}^{u^*} du \int_{E_{g'-1}}^{u^*} du' \frac{\sigma_s(u')}{1 - \alpha} \phi_s^\ell[\mu_o(u' + u)] e^{-(u-u')} \phi_s^\ell(u')
$$

\[\cdot \sum_{n=0}^{N} (2n + 1) f_n(u') P_n[\mu_c(u' + u)] \cdot \] (II.79)

Noting that $\sigma_s(u')$ does not include the heavy element resolved resonance structure so that in the ultra-fine-group $g'$, $\sigma_s(u') \approx \sigma_s^{g'}$ and assuming a constant weighting function, Eq. II.79 may be written

$$
\sigma_s^\ell(g' \rightarrow g) = \frac{\sigma_s^{g'}}{(1 - \alpha) \Delta u} \sum_{n=0}^{N} (2n + 1) \int_{E_{g-1}}^{u^*} du \int_{E_{g'-1}}^{u^*} du' f_n(u') .
$$

$$
P_s^\ell(\mu) \, P_n(\mu_c) \, e^{-(u-u')} . \quad \text{(II.80)}
$$

The code evaluates $\sigma_s(g' \rightarrow g)$ in three different options depending upon the mass $A$ of the scattering material.

1. Light Elements

For light materials other than Hydrogen which scatter more than three ultra-fine-groups

$$1 < A < \frac{e^{1.5\Delta u} + 1}{e^{1.5\Delta u} - 1}$$

an algorithm similar to that of the $MC^2$ code is used to evaluate the transfer matrix. Writing Eq. II.80

$$
\sigma_s^\ell(g' \rightarrow g) = \frac{\sigma_s^{g'}}{\Delta u} \int_{E_{g'-1}}^{u^*} du' P_s^\ell(u' + g) \quad \text{(II.81)}
$$

$$
P_s^\ell(u' + g) = \sum_{n=0}^{N} \frac{2n + 1}{1 - \alpha} \int_{E_{g-1}}^{u^*} du f_n(u') P_s^\ell(\mu) \, P_n(\mu_c) \, e^{-(u-u')} \quad \text{(II.82)}
$$
it is clear that $P_{\ell}(u' + g)$ may be evaluated analytically. Considering the case $\ell = 0$, define the variable

$$r = \frac{1 - e^{-(u-u')}}{1 - \alpha} \leq 1$$

so that

$$P_0(u' + g) = \sum_{n=0}^{N} (2n + 1) \int_{r_{g-1}}^{r_g} f_n(u') P_n(1 - 2r) \, dr$$

$$= \sum_{n=0}^{N} (2n + 1) \int_{r_{g-1}}^{r_g} f_n(u') \sum_{m=0}^{n} (-)^m \frac{(n + m)!}{(n - m)!} \frac{r^m}{m!} \, dr$$

$$= \sum_{m=0}^{N} A_m \left( r_{g}^{m+1} - r_{g-1}^{m+1} \right)$$

where

$$A_m = \sum_{n=m}^{N} f_n(u') \left( - \right)^m \frac{(2n + 1)(n + m)!}{m!(m + 1)!(n - m)!}.$$

Using the analytical expression, Eq.II.83, the transfer matrix of Eq.II.81 is evaluated in the following manner. Each ultra-fine-group, $\Delta u$, is subdivided into $M$ hyper-fine-groups, as shown in Fig. 3, such that

$$M \Delta u = \Delta u$$

$$u_{g_0} = u_g$$

$$u_{g_{M+1}} = u_{g+1}$$

$$u_{g_n} = u_g + n \Delta u$$

The number of hyper-fine-groups per ultra-fine-group, $M$, is chosen so that (i) $M$ does not exceed a user input number; (ii) $M = 1$ if scattering is isotropic or linearly anisotropic in the center of mass system ($N \leq 1$); (iii) $M = 1$ if isotope scatters at least twenty ultra-fine-groups, (iv) $M$ is calculated to ensure that isotope scatters at least twenty hyper-fine-groups, $M = -20 \Delta u \ln(\alpha)$ the scattering from lethargy $u'$ to hyper-fine-group $g_0$, $P_0(u' + g_0)$ is calculated using Eq. II.83 with the factorial coefficients for $A_m$ precalculated. The transfer matrix is then obtained using a trapezoidal rule integration,
Fig. 3. Elastic Scattering Group Structure
For the last group which can be reached from \( g' \), the matrix element is calculated by balance,

\[
\sigma_s^{\text{o}}(g' \to g) = \frac{s}{2M} \left[ P_o(g'_{-1} \to g) + P_o(u_g \to g) \right] + 2 \sum_{m=1}^{M-1} P_o(u_{g'_{-1} + m\Delta u} \to g) \tag{II.84}
\]

For the last group which can be reached from \( g' \), the matrix element is calculated by balance,

\[
\sigma_s^{\text{o}}(g' \to g^*) = \sigma_s^{g'} - \sum_{g'=g}^{g^*} \sigma_s^{\text{o}}(g' \to g) \tag{II.85}
\]

where

\[ u_{g^*} < u_{g'}, \quad \frac{1}{\alpha} < u_{g^*} \]

For the consistent \( P_1/B_1 \) options of MC\(^n\)-2, the matrix elements of Equations II.81-II.82 for \( \ell = 1 \) are required. Although it is possible to derive \( P_1(u' \to g) \) analytically as with Eq. II.83, this expression is time consuming and difficult to evaluate numerically. It is furthermore possible to obtain a fast and accurate evaluation of the integral by taking

\[
P_1(u' \to g_n) \approx \mu_o(u' \to g_n) P_o(u' \to g_n). \tag{II.86}
\]

The small group size, \( \delta u \leq \Delta u \% 0.008 \) makes this a good approximation. The code uses the energy midpoint of the hyper-fine sink group in this calculation. From Eq. II.40, \( \mu_o \) is given by

\[
\mu_o(u' \to g_n) = \frac{1}{2} \frac{\bar{X}_n}{X_n} (1 + A - \frac{A - 1}{\bar{X}_n}) \tag{II.87}
\]

\[
\bar{X}_n = \frac{1}{2} e^{-(n-1)\delta u} [1 + e^{-\delta u}] .
\]

Equations II.86 and II.87 are used to calculate the \( P_1 \) matrix in a manner analogous to that of the \( P_0 \) matrix,

\[
P_1(u' \to g) = \sum_{g_n} \mu_o(u' \to g_n) P_o(u' \to g_n)
\]

\[
\sigma_s^{1}(g' \to g) = \frac{s_1}{2M} \left[ P_1(g'_{-1} \to g) + P_1(u_g \to g) \right] + 2 \sum_{m=1}^{M-1} P_1(u_{g'_{-1} + m\Delta u} \to g) \tag{II.88}
\]
where $\sigma^g_{s_1}$ is calculated from Eq. II.45,

$$
\sigma^g_{s_1} = \sum_{n=0}^{N} \sigma^g_{s_n} f^n T^0_{ln}(\alpha) \tag{II.89}
$$

and scattering into the last group is calculated by balance as in Eq. II.85

$$
\sigma^l_{s}(g' + g, s) = \sigma^g_{s_1} - \sum_{g=g'}^{g^k} \sigma_s (g' + g) \tag{II.90}
$$

The accuracy of these methods has been documented by Henryson, et al. (20)

2. Heavy Elements

For materials which scatter less than four ultra-fine-groups ($A > 160$ for $\Delta u = 1/120$) the method reported by Henryson (21) is used. Equation II.79 is written

$$
\sigma_s^g (g' + g) = \frac{\sum_{n=0}^{N} \left< \sigma_n^g (u') \phi_n^g (u') \right>_A}{\Delta u \left< \phi_n^g (u') \right>_{g'}} \tag{II.91}
$$

where $\left< \right>$ designates a suitable average over the group, and

$$
A_n^g (g' + g) = \frac{(2n + 1)}{1 - \alpha} \int_g^{g'} du' \int_g^0 du \ P_n (\mu_o) \ P_n (\mu_c) \ e^{-u-u'} \tag{II.92}
$$

As with the light elements, one takes the group width to be small enough to permit a constant weight function so that

$$
\left< \sigma_n^g (u') \phi_n^g (u') \right>_{g'} \sim 1/2 \sigma^g_{s_1} [f_n^g (u'_{g'}) + f_n^g (u_1)].
$$

As shown in Ref. 21, it is possible to change variables and switch the order to integration so as to write Eq. II.92 in terms of a function

$$
\overline{T}_{\ln}^m (\alpha, \beta) = \frac{(-)^m}{m!} \frac{(2n + 1)}{2} \int_0^\beta du \ u^m P_n (\mu_o) \ P_n (\mu_c) \ (- \frac{du}{dU}). \tag{II.93}
$$

It is not difficult to show that on integrating Eq. II.92 over all sink groups,

$$
A_n^g (g') = \Delta u T^0_{\ln} (\alpha) = \Delta u \overline{T}_{\ln}^0 (\alpha, \ln \frac{1}{\alpha})
$$

where the $T$ function was defined by Equation II.42. The matrix elements $A_n^g (g' + g)$ are given in Table II. These precalculated elements are given on File 8 of the MC$^2-2$ library (Appendix C) for each of the heavy isotopes and are used by MC$^2-2$ in the calculation of Equation II.91.
<table>
<thead>
<tr>
<th>k</th>
<th>( \text{Group Width/Mass} ) ((q = \ell n \ 1/\alpha))</th>
<th>( A_n^\ell(j\rightarrow k) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1/3 \ q \leq \Delta u &lt; 1/2 \ q )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(j)</td>
<td>(\Delta u T_{\ell n}^0(\alpha, \Delta u) + T_{\ell n}^1(\alpha, \Delta u))</td>
<td></td>
</tr>
<tr>
<td>(j + 1)</td>
<td>(2\Delta u[T_{\ell n}^0(\alpha, 2\Delta u) - T_{\ell n}^0(\alpha, \Delta u)] + T_{\ell n}^1(\alpha, 2\Delta u) - 2T_{\ell n}^1(\alpha, \Delta u))</td>
<td></td>
</tr>
<tr>
<td>(j + 2)</td>
<td>(3\Delta u T_{\ell n}^0(\alpha) + T_{\ell n}^1(\alpha) - 2T_{\ell n}^1(\alpha, 2\Delta u) + T_{\ell n}^1(\alpha, \Delta u) - \Delta u[4T_{\ell n}^0(\alpha, 2\Delta u) - T_{\ell n}^0(\alpha, \Delta u)])</td>
<td></td>
</tr>
<tr>
<td>(j + 3)</td>
<td>(-2\Delta u T_{\ell n}^0(\alpha) - T_{\ell n}^1(\alpha) + 2\Delta u T_{\ell n}^0(\alpha, 2\Delta u) + T_{\ell n}^1(\alpha, 2\Delta u))</td>
<td></td>
</tr>
<tr>
<td>(1/2 \ q \leq \Delta u &lt; q )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(j)</td>
<td>(\Delta u T_{\ell n}^0(\alpha, \Delta u) + T_{\ell n}^1(\alpha, \Delta u))</td>
<td></td>
</tr>
<tr>
<td>(j + 1)</td>
<td>(2\Delta u T_{\ell n}^0(\alpha) + T_{\ell n}^1(\alpha) - 2\Delta u T_{\ell n}^0(\alpha, \Delta u) - 2T_{\ell n}^1(\alpha, \Delta u))</td>
<td></td>
</tr>
<tr>
<td>(j + 2)</td>
<td>(-T_{\ell n}^1(\alpha) - \Delta u T_{\ell n}^0(\alpha) + \Delta u T_{\ell n}^0(\alpha, \Delta u) + T_{\ell n}^1(\alpha, \Delta u))</td>
<td></td>
</tr>
<tr>
<td>(\Delta u \geq q )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(j)</td>
<td>(\Delta u T_{\ell n}^0(\alpha) + T_{\ell n}^1(\alpha))</td>
<td></td>
</tr>
<tr>
<td>(j + 1)</td>
<td>(-T_{\ell n}^1(\alpha))</td>
<td></td>
</tr>
</tbody>
</table>
3. **Hydrogen Elastic Scattering**

It is impossible to treat Hydrogen elastic scattering in the manner outlined for the light elements above because of the computer storage problems associated with a full ultra-fine-group scattering band. Simple recursive relationships exist which are used by MC²-2 in lieu of storing the Hydrogen matrix. These relationships are given below.

Let $S_{H}^{g}$ be the $F_{\ell}$ elastic scattering source into group $g$ from all groups above $g$ due to scattering from Hydrogen. Assuming the scattering to be isotropic in the center of mass system, and taking $\Delta=1$, Eqs. II.40 and II.79 are used to give

$$S_{H}^{g} = \int_{u_{g-1}}^{u_{g}} du \int_{0}^{u_{g-1}} du' \Sigma_{H}(u') \phi_{\ell}(u') e^{-(1 - \frac{\ell}{2})(u-u')} \left(1 - \frac{\ell}{2}\Delta u\right), \quad \ell = 0, 1. \quad (I1.94)$$

Performing the integration over group $g$ it is simple to show

$$S_{H}^{g} = \eta_{\ell}(u_{g-1}) [1 - e^{-(1 + \frac{\ell}{2})\Delta u}], \quad \ell = 0, 1 \quad (I1.95)$$

where the Hydrogen slowing down density $\eta_{\ell}(u)$ is given by Eqs.II.37 and II.76.
H. Inelastic and (n,2n) Scattering

As noted in Section B above, non-elastic scattering (inelastic, (n,2n)) is treated as a source term in the ultra-fine-group spectrum calculation. The development of the continuous slowing down equations made use of this separation explicitly. In the multigroup formulation this separation is implicit since the code does not prepare a non-elastic ultra-fine-group scattering matrix because of the excessive storage requirements for such a matrix. Rather, the non-elastic scattering source is calculated directly on each pass through the ultra-fine-groups. This is the most time consuming part of the ultra-fine-group spectrum calculation in MC²-2.

For both inelastic and (n,2n) scattering, the MC²-2 code permits three descriptions of the secondary energy distributions: (i) tabulated function; (ii) evaporation spectrum; (iii) discrete levels. The remainder of this section will be concerned with the methods used to calculate the ultra-fine-group non-elastic scattering source for each of these descriptions.

1. Tabulated Function

The following data are provided on the MC²-2 library file MCC2F6 (c.f. Appendix C),

\[ P_x (g \rightarrow E_{\text{tab}}) \]

Probability that a neutron is scattered by process \( x \) (inelastic or \( (n,2n) \)) from group \( g \) to energy point \( E_{\text{tab}} \)

\[ E_{\text{tab}} \]

An array of "sink" energy points

\[ \text{KT} \]

An interpolation law on the sink energies \( E_{\text{tab}} \)

\[ \sigma^g_{\text{tab}} \]

Cross section in group \( g \) for process \( x \) multiplied by the fraction of scattering events described by the \( P_x \) law

From these definitions it is obvious that the non-elastic scattering source into group \( g \) described by the tabulated law is given by

\[
S_{n\text{e tab}}^g = \sum_{g'} \phi^{g'} \left\{ \sigma^g_{\text{inel tab}} \int_{E_{g-1}}^{E_g} dE P_{\text{inel}} (g' + E) \right. \\
+ 2 \sigma^{g',2n}_{\text{tab}} \int_{E_{g-1}}^{E_g} dE P_{\text{n,2n}} (g' + E) \right\} \quad (\text{II.96})
\]

The integrals of Eq. II.96 are evaluated analytically using the interpolation law defined by the KT data.
2. Evaporation Spectrum

For both inelastic and (n,2n) scattering, the MC\textsuperscript{2}-2 library provides evaporation temperatures and fractional probabilities such that

\[
S_{\text{evap}}^g = S_{\text{evap,inel}}^g + 2 S_{\text{evap,n,2n}}^g
\]

\[
S_{\text{evap}}^g = \sum_{g'} \sigma_{x}^{g'} \phi_{x}^{g'} \sum_{n} \frac{w_{n,x}^{g'}}{I_{n,x}^{g'}} \int_{E_1}^{E_2} dE P_{ev,x,n}(g' \to E) \tag{II.97}
\]

\[
P_{ev,x,n}(g' \to E) = \begin{cases} 
0 & E > E_{g' - 1} - U_{x,n} \\
E \exp \left( - \frac{E}{\phi_{x,n}^{g'}} \right) & E < E_{g' - 1} - U_{x,n}
\end{cases}
\]

where the subscript n is used to indicate a sum over all evaporation spectra for process x and \( I_{n,x}^{g'} \) is a normalization factor,

\[
I_{n,x}^{g'} = \int_{0}^{E_{g' - 1} - U_{x,n}} dE P_{ev}(g' \to E).
\]

For (n,2n) events the constant \( U \) is assumed to be zero.

The evaluation of Eq.II.97 requires an exponential for each ultra-fine sink group, and it is this calculation which controls the computing time of an MC\textsuperscript{2}-2 spectrum calculation. A fast exponential function (22) (Appendix A) is used by MC\textsuperscript{2}-2 to evaluate the required exponentials. Furthermore, the calculation over sink groups g is terminated once the criterion

\[
\frac{\int_{E_{g' - 1} - U_{x,n}}^{E} dE P_{ev,x,n}(g' \to E)}{\int_{E_{g' - 1} - U_{x,n}}^{E_{g' - 1}} dE P_{ev,x,n}(g' \to E)} \leq 10^{-6}
\]

is met. The integrals of Eq.II.97 are calculated analytically.

3. Discrete Levels

The MC\textsuperscript{2}-2 library file MCC2F6 provides Q values and ultra-fine-group level cross sections for all inelastic and (n,2n) discrete scattering levels. In addition the library provides the average cosine of the scattering angle in the center of mass system for discrete inelastic scattering by level and group. These data are processed in the manner indicated below.
a. Approximate Treatment Neglecting Energy-Angle Correlation

It is well known that energy and momentum conservation give

\[
E = \frac{1 + \frac{A^2}{(1 + A)^2}}{E'} - \frac{A}{A + 1} Q_\lambda + \frac{2A}{(1 + A)^2} \mu E' \left[ 1 - \frac{A + 1}{A \frac{Q_\lambda}{E'}} \right]^{1/2} \tag{II.98}
\]

where

\begin{align*}
E &= \text{lab energy after collision} \\
E' &= \text{lab energy before collision} \\
\mu &= \text{cosine of c.m. angle of scatter} \\
Q_\lambda &= -Q \text{ value of reaction for level } \lambda \\
A &= \text{mass of scattering isotope.}
\end{align*}

The threshold energy of the reaction is

\[
E_\lambda = \frac{A + 1}{A} Q_\lambda, \tag{II.99}
\]

A rigorous evaluation of the group to group transfer probability accounting for the energy-angle correlation of Eq. II.98 is quite complicated.\(^{(23)}\) Two assumptions serve to simplify the situation without much loss in accuracy:

(i) angle of scattering is fixed;

(ii) \( \left( 1 - \frac{E_\lambda}{E'} \right)^{1/2} \approx 1 - 1/2 \frac{E_\lambda}{E'} \).

With these assumptions one can write

\[
E = E' \left[ \frac{1 + \frac{A^2}{(1 + A)^2}}{1 + \frac{A}{A + 1} \frac{Q_\lambda}{E'}} \right] - \frac{(A + <\mu>)}{A + 1} Q_\lambda \tag{II.100}
\]

\[
E' = \frac{(1 + A)^2}{1 + \frac{A^2}{2} \frac{Q_\lambda}{<\mu>}} E + \frac{(A + <\mu>)(A + 1)}{1 + \frac{A^2}{2} \frac{Q_\lambda}{<\mu>}} \tag{II.101}
\]

It is clear from Eq. II.100 that the probability of scattering from group j to group k for discrete level \( \lambda \) is identically zero unless group k lies between the energy boundaries

\[
E_{j-1} = \left[ \frac{1 + \frac{A^2}{(1 + A)^2}}{1 + \frac{A}{A + 1} \frac{Q_\lambda}{E'}} \right] - \frac{(A + <\mu>)}{1 + A} Q_\lambda,
\]
and it has been assumed that at least a part of group j lay above the threshold, 
\[ E_{j-1} > E_\lambda. \]

For those groups, k, which fall partially or totally within this range, the probability of scattering from group j to group k is given by the fractional part of group j which scatters into group k. This can be derived directly from Eq. II.101,

\[ P_\lambda(j \rightarrow k) = \frac{E_{j-1}^\ast - E_j^\ast}{E_{j-1} - E_j} \]  

where

\[ E_{j-1}^\ast = \min \left[ \left( 1 + A^2 \right) E_{k-1} + (A + 1) (A + \langle \mu \rangle) Q_\lambda \right] \]

\[ E_j^\ast = \max \left[ E_j, E_\lambda, \frac{(1 + A^2) E_k + (A + 1) (A + \langle \mu \rangle) Q_\lambda}{1 + A^2 + 2A \langle \mu \rangle} \right]. \]  

The Eqs. II.102-II.104 are used by MC~2\~2 to calculate the discrete scattering source,

\[ S^g_{ne,d} = \sum_{g'} \phi^g' \left\{ \sum_{\lambda, \text{inel}} \sigma_{\lambda, \text{inel}}^g P_{\lambda}(g' + g) 
+ 2 \sum_{\lambda, n, 2n} \sigma_{n, 2n}^g P_{\lambda}(g' + g) \right\}. \]

The average cosine of the scattering angle is taken to be zero (isotropic in center of mass) for scattering from all \((n, 2n)\) levels. The \(\lambda, \lambda'\) sums represent sums over all discrete levels.

The complete microscopic non-elastic scattering source is given by

\[ S^g_{ne} = S^g_{ne, \text{tab}} + S^g_{ne, \text{cvp}} + S^g_{ne, d}. \]

The macroscopic sources are defined by summing over all materials using the appropriate atom densities.

b. **Rigorous Treatment Assuming Isotropic Scattering**

The approximations made above are quite good for source energies far above threshold where the level cross sections of \(g\) are large. The simplicity of the formulation along with its accuracy suggest that Eqs. II.102-II.104 provide the recommended procedure for evaluating the discrete inelastic source. On option the user may, however, specify a more rigorous, and correspondingly more time consuming, treatment of discrete level scattering. The option follows the work of Segev,\(^{(23)}\) which accounts
explicitly for the fact that a neutron scattered at energy $E'$ scatters into a band of energies defined from Eq. II.98 as

$$ \left[ 1 + A \left( \frac{E' - E_\lambda}{E + 1} \right)^{1/2} \right]^{2} E'. $$

(II.105)

This band of energies must be used instead of Eq. II.100 to define the possible sink groups. Similarly, a neutron scattered into energy $E'$ may be scattered from a range of source energies defined by

$$ \left[ 1 + A \left( \frac{1 + A - 1}{A + 1} E_\lambda \right)^{1/2} \right]^{2} E. $$

(II.106)

and

$$ \max \left\{ E^{(c)}_\lambda, \left[ 1 - A \left( \frac{1 + A - 1}{A + 1} E_\lambda \right)^{1/2} \right]^{2} E \right\} $$

where

$$ E^{(c)}_\lambda = \frac{A^2}{A^2 - 1} E_\lambda $$

is a pseudo-threshold energy defined to avoid the need to consider the double valued nature of $E'$ for a given $E$. This source group band width replaces Eq. II.101 of the approximate treatment. Accounting for the above energy bands leads to four domains of integration in evaluating the probability of scattering from group $j$ to group $k$ as

$$ P_\lambda(j \rightarrow k) = \frac{1}{E_{j-1} - E_j} \int_{\text{group } j} dE' \int_{\text{group } k} dE \sum_n \frac{(2n + 1)}{n (1 - \alpha) E'} \frac{f_n(E')}{\left[ 1 - \frac{E_\lambda}{E'} \right]^{1/2}} P_n(\mu). $$

(II.107)

In the more rigorous option of MC²-2, Eq. II.107 is evaluated analytically taking proper account of the four domains of integration as discussed in Ref. 23. Because of the time consuming nature of the calculation, Eq. II.107 is solved assuming isotropic scattering in the center-of-mass. For standard fast reactor configurations, it has been found that the discrete inelastic calculation using the approximate method defined by Eqs. II.103-II.104 is quite accurate and significantly faster than the algorithms discussed above which account explicitly for the energy-angle correlation of discrete level scattering as defined by Eq. II.98.
I. **Ultra-Fine-Group Macroscopic Data**

The macroscopic data required for solution of the spectrum equations discussed in Section F may in almost all cases be derived from the simple expression

\[
\Sigma^g_x = \sum_i \frac{N_i \sigma^g_{x_i}}{1}
\]

(II.108)

where \(N_i\) is the atom density of isotope \(i\) in the homogeneous mix and \(\sigma^g_{x_i}\) is the ultra-fine-group cross section for isotope \(i\) and process \(x\). This expression is clearly applicable to the scattering matrix data discussed in Sections G and H above. The ultra-fine-group microscopic reaction cross sections are available on the MC\(^2\)-run library file MCC2F5 (c.f. Appendix C). These data are generally processed directly from the ENDF/B data files by the code ETOE-2 assuming a constant weighting.

The unresolved resonance cross sections are treated in the same manner as the above data. The calculation of the ultra-fine-group unresolved cross sections is discussed in Chapter IV. The remainder of this section is concerned with the calculation of macroscopic data which require more processing than that given by Eq. II.108.

1. **Fission Source Data**

The fission source of Eq. II.14 may be written in group form as

\[
S^g_f = \sum_i \chi_i^g N_i \sum_g \nu^g_i \sigma^g_{x_i} \phi^g_i .
\]

(II.109)

The number of neutrons per fission, \(\nu^g_i\), is derived from the expression

\[
\nu^g_i = \frac{1}{E - E^g} \int_{E^g}^{E_{\text{max}}} \nu^g_i(E) \, dE
\]

\[
\nu^g_i(E) = A_o^i + A_1^i E + A_2^i E^2 + A_3^i E^3 .
\]

(II.110)

The fission spectrum distribution is given by

\[
\chi^g_i = \frac{\int_{E_{\text{min}}}^{E_{\text{max}}} dE \chi_i(E)}{\int_{E_{\text{min}}}^{E_{\text{max}}} \chi_i(E)} = \frac{\hat{\chi}^g_i}{\sum_i \hat{\chi}^g_i}
\]

(II.111)

with

\[
\chi^g_i(E) = \alpha^i_1 \frac{E}{\tau_1^i} e^{-E/\tau_1^i} + (1 - \alpha^i_1) \frac{4E}{\pi^3 \beta^i_1} e^{-E/\beta^i_1} .
\]
This combination of a Maxwellian plus an evaporation spectrum suffices to describe all but one of the fission spectra for the most recent release of the ENDF/B data files. Integration of Eq. II.111 gives

$$\chi_i = \alpha_i \left[ \left( 1 + \frac{E}{T_i} \right) e^{-E/T_i} - \left( 1 + \frac{E_{g-1}}{T_i} \right) e^{-E_{g-1}/T_i} \right]$$

$$+ (1 - \alpha_i) \left[ \text{erf} \left( \frac{E_{g-1}/\beta_1}{\beta_1} \right) - \text{erf} \left( \frac{E_g/\beta_1}{\beta_1} \right) \right] - \left( \frac{4E_{g-1}}{\beta_1} \right) e^{-E_{g-1}/\beta_1} + \left( \frac{4E_g}{\beta_1} \right) e^{-E_g/\beta_1} \right].$$

Equation II.112 is used by MC2-2 to evaluate the fission spectrum distribution. It should be noted that the "temperatures" $T_i$ and $\beta_i$ are not energy dependent in the MC2-2 formulation although such a description is not rigorous. In practice the temperatures in the MC2-2 library are those characteristic of the average fission energy of a typical fast reactor assembly. It is possible on user option to input the fission spectrum temperature $\beta_i$ by isotope which the code will use in lieu of the library data taking $\alpha_i$ to be zero.

2. **Ultra-Fine-Group Extended Transport Cross Section**

The transport-like cross sections $A^g_{\ell}$ defined as

$$A^g_{\ell} = \int_{u_{g-1}}^{u_g} A_{\ell}(B, u, N) \, du$$

are required in solution of the ultra-fine-group spectrum equations. $A_{\ell}(B, u, N)$ is defined by the continued fraction expansion of Eqs.II.11 and II.12. The MC2-2 code does not actually perform the required integration. Rather the parameters $b_{\ell}$ are simply defined in terms of the group cross sections, so that, for example,

$$A^g_{\ell} = \frac{B \tan^{-1} \left( \frac{\gamma^g_{\ell}}{B} \right)}{3 \left( 1 - \frac{\gamma^g_{\ell}}{B} \tan^{-1} \left( \frac{\gamma^g_{\ell}}{B} \right) \right)}$$

in the consistent $B_1$ approximation. The cross sections $A^g_{\ell}$ are clearly dependent upon the buckling $B^2$ which may change during the course of a calculation if the user specifies a buckling search option. The code does not recalculate $A^g_{\ell}$ in that case. Rather, a special user input buckling, $\kappa^2$ is used in the calculation of $A^g_{\ell}$. This same value of $\kappa^2$ is also used
in the leakage correction to the background cross section in the resonance
calculation of MC$^2$-2, as described in Chapters III and IV. The value of $\kappa^2$
is set by the user and may or may not equal the $B^2$ used in the ultra-fine
group spectrum calculation.

The continued fraction coefficients depend upon the ratio of Legendre
functions of the second kind which cannot be calculated for all arguments
using the standard forward recurrence relation without a significant loss
of accuracy. The algorithms used in MC$^2$-2 to calculate this ratio are
summarized in Appendix A.

3. Improved Goertzel-Greuling Moderating Parameters

In Section D.2 integral expressions were derived defining the
isotopic moderating parameters $\xi_i$, $a_i$, $c_i$, and $e_i$. The numerical evaluation
of these expressions is described below.

The heavy isotope moderating parameters are given by Eq. II.44. The
effective ratios are calculated by integrating over the scattering
bandwidth,

$$
\left\langle \frac{\Sigma_s}{\Sigma_t} \ln \left( \frac{f_{n_1}}{u} \right) \right\rangle_u \approx \frac{1}{\ln \frac{1}{a_i}} \left\{ \frac{N_i \sum_s (u - (n - \frac{1}{2}) \Delta u)}{\Delta u} \sum_{n=1}^{N_i} \frac{\sum_s (u - (n - \frac{1}{2}) \Delta u)}{f_{n_1} (u - (n - 1) \Delta u)} \right. 
$$

$$
+ \left. \left( \ln \frac{1}{a_i} - N_i \Delta u \right) \frac{\sum_s (u - (N_i + \frac{1}{2}) \Delta u)}{\sum_s (u - (N_i + \frac{1}{2}) \Delta u)} \right\} 
$$

(II.113)

where $N_i$ is the nearest whole integer to the ratio $\frac{\ln a_i}{\Delta u} = \left[ \frac{\ln a_i}{\Delta u} \right]$.

The ratio is evaluated at ultra-fine-group boundaries and group cross
sections are used so that

$$
\frac{\Sigma_s (u - \frac{1}{2} \Delta u)}{\Sigma_t (u - \frac{1}{2} \Delta u)} = \frac{\Sigma_s^G}{\Sigma_t^G}. 
$$

The evaluation of the light element moderating parameters as
defined by Eqs. II.48 is somewhat more complex. The first step in the
development is the definition of integrating factors which permit an
accurate numerical evaluation of the integrals:

$$
\int_{u-\ln \frac{1}{a_i}}^{u} du' \frac{\Sigma_s (u')}{\Sigma_t (u')} D_{m}^i (u') \approx \sum_{n=1}^{N_i} \frac{\Sigma_s (u - (n - \frac{1}{2}) \Delta u)}{\sum_s (u - (n - \frac{1}{2}) \Delta u)} D_{m}^i (u - (n - \frac{1}{2}) \Delta u) 
$$
It is clear from the development of the improved Goertzel-Greuling slowing down theory that if

\[
\frac{\sum_{i} s_i(u')}{\sum_{i} t(u')} \int_{u-Ln^1/a_i}^{u} du' \frac{P^i_m(u')}{\sum_{i} t(u')} (u - u') e^{-x(u-u')} \propto n_i \frac{\sum_{i} s_i(u - (n - \frac{1}{2}) \Delta u)}{\sum_{i} t(u - (n - \frac{1}{2}) \Delta u)} P^i_m(u - (n - \frac{1}{2}) \Delta u) (n - \frac{1}{2}) e^{-x(n-\frac{1}{2})\Delta u}.
\]

If this characteristic of the moderating parameters is retained, then it is possible to define integration factors in the following manner:

\[
W^x_1 \equiv \frac{Ln^1/a_i}{N_i},
\]

\[
W^x_2 \equiv \left(\frac{Ln^1/a_i}{N_i}\right)^2,
\]

\[
W^x_3 \equiv \frac{1}{x(1 - \alpha^x_i)} \frac{\sum_{i=1}^{N_i} e^{-x(n-\frac{1}{2})\Delta u}}{\sum_{i=1}^{N_i} e^{-x(n-\frac{1}{2})\Delta u}}.
\]

\[
W^x_4 \equiv \frac{1}{x^2} \frac{(1 - \alpha^x_i (1 + x \cdot Ln^1/a_i))}{\sum_{i=1}^{N_i} (n - \frac{1}{2}) e^{-x(n-\frac{1}{2})\Delta u}}.
\]

The improved Goertzel-Greuling moderating parameters are then calculated by replacing the integrals of Eqs. II.48 by the numerical approximations.
\[ \xi_1^0(u) = \sum_{n'=1}^{N+1} \frac{1}{n'!} \left[ w_{3i}^n b_{i1}^{n',n'}(u) - \alpha_{1i}^{n'} w_{11} d_{i1}^{n'}(u) \right] \]

\[ a_1^0(u) = -\sum_{n'=1}^{N+1} \frac{1}{n'!} \left[ w_{4i}^n f_{i1}^{n',n'}(u) - \alpha_{2i}^{n'} w_{21} g_{i1}^{n'}(u) \right] \]

\[ c_1^0(u) = \frac{\Sigma_{s_i}^0(u)}{\Sigma_{t_i}^0(u)} - \sum_{n'=1}^{N+1} w_{3i}^n b_{i1}^{n',n'}(u) \]

\[ c_1^0(u) = \sum_{n'=1}^{N+1} w_{4i}^n f_{i1}^{n',n'}(u) \quad (II.116) \]

\[ \xi_1^1(u) = \sum_{n'=1}^{N+1} \left\{ \frac{(A_1+1)}{2n'+1} \left[ w_{3i}^{n'+\frac{1}{2}} b_{i1}^{n'+\frac{1}{2},n'}(u) - \alpha_{1i}^{n'+\frac{1}{2}} w_{11} d_{i1}^{n'}(u) \right] \right. \]

\[ - \frac{(A_1-1)}{2n'-1} \left[ w_{3i}^{n'-\frac{1}{2}} b_{i1}^{n'-\frac{1}{2},n'}(u) - \alpha_{1i}^{n'-\frac{1}{2}} w_{11} d_{i1}^{n'}(u) \right] \} \]

\[ a_1^1(u) = -\sum_{n'=1}^{N+1} \left\{ \frac{(A_1+1)}{2n'+1} \left[ w_{4i}^{n'+\frac{1}{2}} f_{i1}^{n'+\frac{1}{2},n'}(u) - \alpha_{2i}^{n'+\frac{1}{2}} w_{21} g_{i1}^{n'}(u) \right] \right. \]

\[ - \frac{(A_1-1)}{2n'-1} \left[ w_{4i}^{n'-\frac{1}{2}} f_{i1}^{n'-\frac{1}{2},n'}(u) - \alpha_{2i}^{n'-\frac{1}{2}} w_{21} g_{i1}^{n'}(u) \right] \} \]

\[ c_1^1(u) = \frac{\Sigma_{s_i}^0(u)}{\Sigma_{t_i}^0(u)} \sum_{n'=0}^{N} T_{1n_1}(\alpha_1) f_{i1}^{n',n'}(u) - \frac{1}{2} \sum_{n'=1}^{N+1} (A_1+1) w_{3i}^{n'+\frac{1}{2}} b_{i1}^{n'+\frac{1}{2},n'}(u) \]

\[ + \frac{1}{2} (A_1 - 1) \sum_{n'=1}^{N+1} w_{3i}^{n'-\frac{1}{2}} b_{i1}^{n'-\frac{1}{2},n'}(u) \]

\[ e_1^1(u) = \frac{1}{2} \sum_{n'=1}^{N+1} \left\{ (A_1+1) w_{4i}^{n'+\frac{1}{2}} f_{i1}^{n'+\frac{1}{2},n'} - (A_1-1) w_{4i}^{n'-\frac{1}{2}} f_{i1}^{n'-\frac{1}{2},n'}(u) \right\} \]

where

\[ b_{i1}^{x,m} = \sum_{n=1}^{N_i} \frac{\Sigma_{s_i}^0(u-(n-\frac{1}{2}) \Delta u)}{\Sigma_{t_i}^0(u-(n-\frac{1}{2}) \Delta u)} D_m^{i}(u-(n-\frac{1}{2}) \Delta u) e^{-x(n-\frac{1}{2}) \Delta u} \]

\[ d_{i1}^{m}(u) = \sum_{n=1}^{N_i} \frac{\Sigma_{s_i}^0(u-(n-\frac{1}{2}) \Delta u)}{\Sigma_{t_i}^0(u-(n-\frac{1}{2}) \Delta u)} D_m^{i}(u-(n-\frac{1}{2}) \Delta u) \quad (II.117) \]
The Eqs. II.117 are used to calculate the coefficients at the lethargy $U_{CS}$ between the multigroup and continuous slowing down regions of the calculation. For the lethargy boundaries $u_g > U_{CS}$ recursion relations are used:

\[
b_{i}^{x,m}(u + \Delta u) = b_{i}^{x,m}(u) e^{-x\Delta u} + e^{-N_{i}^2 \Delta u} \left\{ \frac{\Sigma_{s_i} (u + \Delta u)}{\Sigma_{t} (u + \Delta u)} - \Sigma_{s_i} (u + \Delta u) \right\} e^{-xN_{i}^2 \Delta u},
\]

\[
d_{i}^{m}(u + \Delta u) = d_{i}^{m}(u) + \left\{ \frac{\Sigma_{s_i} (u + \Delta u)}{\Sigma_{t} (u + \Delta u)} - \Sigma_{s_i} (u + \Delta u) \right\} e^{-N_{i}^2 \Delta u}.
\]

\[
f_{i}^{x,m}(u + \Delta u) = e^{-x\Delta u} f_{i}^{x,m}(u) + b_{i}^{x,m}(u + \Delta u)
\]

\[
- e^{-x\Delta u/2} \left\{ \frac{1}{2} \left\{ \frac{\Sigma_{s_i} (u + \Delta u)}{\Sigma_{t} (u + \Delta u)} - \Sigma_{s_i} (u + \Delta u) \right\} e^{-xN_{i}^2 \Delta u} + (N_{i} - \frac{1}{2}) \frac{\Sigma_{s_i} (u - (N_{i} - \frac{1}{2}) \Delta u)}{\Sigma_{t} (u - (N_{i} - \frac{1}{2}) \Delta u)} e^{-xN_{i}^2 \Delta u} \right\}
\]

\[
f_{i}^{x,m}(u) = \sum_{n=1}^{N_i} \frac{\Sigma_{s_i} (u - (n - \frac{1}{2}) \Delta u)}{\Sigma_{t} (u - (n - \frac{1}{2}) \Delta u)} - \frac{\Sigma_{s_i} (u - (n - \frac{1}{2}) \Delta u)}{\Sigma_{t} (u - (n - \frac{1}{2}) \Delta u)} e^{-x(n - \frac{1}{2}) \Delta u}.
\]
As noted in Section D.2, the sums over Legendre coefficients of Eqs. 11.116 are limited to four terms \((N = 3)\) within the MC\(^2\)-2 code.

J. **Ultra-Fine-Group Solution Strategies**

Once the resonance, transfer matrix, moderating parameter and cross section data have been processed on an ultra-fine-group mesh the solution of the spectrum equations presented in Section F must be performed. In this section the strategies involved in treating the resonance attenuation, buckling search, flux iterations and fixed source or eigenvalue problems are discussed.

1. **Ultra-Fine-Group Spectrum Solution**

Given an initial fission source, \(S^g_f\), and a buckling, \(B^2\), it is possible to solve both the multigroup equations, II.62 or II.64 and the continuous slowing down equations II.66 or II.70 and II.71 by sweeping down the energy mesh from group 1 to the last ultra-fine-group in the problem. Both the sources due to inelastic and/or \((n,2n)\) scattering and the Hydrogen slowing down density are updated after calculating the flux (and current) for a given ultra-fine-group. In the continuous slowing down region, the equations II.66 or II.70 are used to obtain \(q_o^{asy}(u)\) from the values \(q(u_{g-1})\). The \(q_o^{asy}(u)\) so obtained does not feel any effects of narrow resonances in the group \(g\). The attenuation of the asymptotic slowing down density is performed in the manner outlined in Section E. One defines

\[
q_o(u_g) = Q_g q_o^{asy}(u_g)
\]

where the attenuation factor \(Q_g\) is defined

\[
Q_g = \prod_{r \in g} (1 - p_r)
\]

\[
p_r = \begin{cases} a_r & \text{if } g \text{ is neutron} \\ E_r & \text{if } g \text{ is electron} \\ a_r + \frac{\Sigma_g}{\Sigma_t} J^* t_r \end{cases} \left( \frac{\Sigma_g}{\Sigma_t} t_r + \frac{B^2}{3A_g} \right) \left( C_0 + C_1 \right)
\]

and

\[
g_i^m(u + \Delta u) = g_i^m(u) + d_i^m(u + \Delta u)
\]

\[
\frac{\Sigma_s}{\Sigma_t} \left( u + \frac{\Delta u}{2} \right) - \frac{1}{2} \frac{\Sigma_s}{\Sigma_t} \left( u + \frac{\Delta u}{2} \right) = \frac{\Sigma_s}{\Sigma_t} \left( u - \left( N_i - \frac{1}{2} \right) \Delta u \right) - \frac{\Sigma_s}{\Sigma_t} \left( u - \left( N_i - \frac{1}{2} \right) \Delta u \right)
\]

\[
\frac{\Sigma_s}{\Sigma_t} \left( u - \left( N_i - \frac{1}{2} \right) \Delta u \right)
\]

\[
d_i^m(u + \Delta u)
\]
In the absence of resonances the slowing down density $q_\ell(u)$ is assumed to vary linearly between group boundaries,

$$q_\ell^{as}(u) = q_\ell^{as}(u_{g-1}) + \left[q_\ell^{as}(u_g) - q_\ell^{as}(u_{g-1})\right] \frac{(u - u_{g-1})}{\Delta u}.$$

The presence of a resonance $r$ introduces a discontinuity such that

$$q_\ell^{as}(u_{r+}) = (1 - p_r)q_\ell^{as}(u_{r-}).$$

With these conventions and the Eqs. II.32 and II.36 expressions may be derived for the ultra-fine-group flux and current as well as resonance reaction rates.

If $A_x^r$ is the reaction rate for process $x$ (capture, fission, total) of resonance $r$, then

$$A_x^r = \int x_r \phi \, du$$

which using the narrow resonance approximation can be written

$$A_x^r \sim \frac{\Gamma_x}{E_r} \frac{x_r}{x} \left(\frac{G^r}{3A^l} + \frac{B^2}{3A^l}\right) \phi(u_r).$$

The flux of Eq. II.119 is obtained from Eq. II.32 or II.36 using the attenuated slowing down density $q_\ell^{as}(u_r)$,

$$\phi(u_r) = \begin{cases} \begin{aligned} \Gamma_x \frac{G^r}{3A^l} q_\ell^{as}(u_r) + \frac{S^r + \eta^o_{\ell}}{M^+} \frac{\theta \gamma_{\ell}^{as}(u_g)}{\Delta u} + \frac{(S^r + \eta^o_{\ell})}{M^+} \frac{\theta \gamma_{\ell}^{as}(u_{g-1})}{\Delta u}, \end{aligned} & \text{Inconsistent $P_1/B_1$} \\
\left[\begin{array}{c} \theta R^g + (1 - \theta) R^g_- \\ \frac{(S^r + \eta^o_{\ell})}{\Delta u} \end{array}\right] q_\ell^{as}(u_r) - \left[\begin{array}{c} \theta T^g + (1 - \theta) T^g_- \\ \frac{(S^r + \eta^o_{\ell})}{\Delta u} \end{array}\right] q_1^{as}(u_r) & \text{Consistent $P_1/B_1$} \end{cases}.$$

$$= \begin{cases} \begin{aligned} \Gamma_x \frac{G^r}{3A^l} q_\ell^{as}(u_r) + \frac{S^r + \eta^o_{\ell}}{M^+} \frac{\theta \gamma_{\ell}^{as}(u_g)}{\Delta u} + \frac{(S^r + \eta^o_{\ell})}{M^+} \frac{\theta \gamma_{\ell}^{as}(u_{g-1})}{\Delta u}, \end{aligned} & \text{Inconsistent $P_1/B_1$} \\
\left[\begin{array}{c} \theta R^g + (1 - \theta) R^g_- \\ \frac{(S^r + \eta^o_{\ell})}{\Delta u} \end{array}\right] q_\ell^{as}(u_r) - \left[\begin{array}{c} \theta T^g + (1 - \theta) T^g_- \\ \frac{(S^r + \eta^o_{\ell})}{\Delta u} \end{array}\right] q_1^{as}(u_r) & \text{Consistent $P_1/B_1$} \end{cases}.$$
The group flux $\phi^g$ and current $J^g$ are obtained in a similar manner,

\[
\phi^g = \left\{
\begin{align*}
\left[ \frac{\theta}{M_+^g} + \frac{(1 - \theta)}{M_-^g} \right] (1 - f) \int q_o(u) \, du \\
+ (S_g + \eta_o^g) \left[ \frac{\theta \gamma_0(u_g)}{M_+^g} + \frac{(1 - \theta) \gamma_o(u_{g-1})}{M_-^g} \right], & \quad \text{Inconsistent } P_1/B_1 \\
\left[ \theta R_+^g + (1 - \theta) R_-^g \right] (1 - f) \int q_o(u) \, du \\
- \left[ \theta T_+^g + (1 - \theta) T_-^g \right] \int q_1(u) \, du \\
+ (S_g + \eta_o^g) \left[ \theta \gamma_0(u_g) + (1 - \theta) R_-^g \gamma_o(u_{g-1}) \right] \\
- 1.5 \eta_1^g \left[ \theta T_+^g + \gamma_1(u_g) + (1 - \theta) T_-^g \gamma_1(u_{g-1}) \right]. & \quad \text{Consistent } P_1/B_1
\end{align*}
\right.
\] (II.121)

\[
J^g = \left[ \theta v_+^g + (1 - \theta) v_-^g \right] \int q_o(u) \, du \\
+ \left[ \theta u_+^g + (1 - \theta) u_-^g \right] \int q_1(u) \, du
\] (II.122)

\[+ (S_g + \eta_o^g) \left[ \theta \gamma_0(u_g) \gamma_v^g + \gamma_o(u_{g-1}) + (1 - \theta) \gamma_v^g \right] \\
+ 1.5 \eta_1^g \left[ \gamma_1(u_g) \theta u_+^g + \gamma_1(u_{g-1}) + (1 - \theta) \theta u_-^g \right].
\]

The flux depression factor $(1 - f)$ is defined by use of the narrow resonance approximation,

\[
f = \frac{1}{\int q_o(u) \, du} \sum_{\text{res}} \frac{\Gamma_t}{E} J^* q_o(u_r).
\] (II.123)

The thermal flux $\phi^{th}$ is given by
The thermal cross sections are either provided by the user or given by the cross sections of the last ultra-fine-group of the problem \((g = NG)\).

2. Eigenvalue Solution

By decomposing the source term \(S^g\) of the ultra-fine-group spectrum equations, it is possible to write the equations in matrix form as

\[
H\Phi = \lambda M\Phi + S_{\text{fix}}.
\]  

If \(S_{\text{fix}}\), the inhomogeneous source vector, is zero Eq. II.125 represents an eigenvalue problem with

\[
\lambda = \frac{1}{k_{\text{eff}}}.
\]

From Eq. II.14 it is clear that the non-zero elements of the vector \(M\Phi\) have the form

\[
S^g_f = \sum_i \chi_i^g \sum_{g'} (\nu \Sigma_{f}^{g'})_i \phi^{g'}
\]  

If the fission spectrum distribution is isotope independent, then one can take

\[
S^g_f = \chi^g
\]

and

\[
k_{\text{eff}} = \sum_{g'} \nu \Sigma_{f}^{g'} \phi^{g'}
\]

so that no flux iterations are required in the spectrum solution. If the fission spectrum distribution is isotope dependent then one assumes a flux, calculates \(S^g_f\) from Eq. II.127, solves the spectrum equations as detailed in the previous section, and calculates a new fission source and eigenvalue \(k_{\text{eff}}\). This process is repeated until the eigenvalue has converged. Convergence is assumed if on the first iteration

\[
\max \left| \frac{S^g_f(1) - S^g_f(0)}{S^g_f(0)} \right| < .001
\]

or on following iterations

\[
\left| \frac{k^{(n+1)} - k^{(n)}}{k^n} \right| < .0001 \quad n \geq 1.
\]
3. **Inhomogeneous Source Solution**

If there are no fissionable isotopes in the problem mixture then Eq. II.125 becomes

\[ H\Phi = S_{\text{fix}} \]

which may be solved directly by sweeping through the ultra-fine-group equations once in precisely the same manner as that used to solve the eigenvalue equation with isotope independent fission spectra. If both fission and inhomogeneous sources are present a different solution strategy is required. Assuming an isotope independent fission spectrum distribution for the sake of simplicity, Eq. II.25 may be written

\[ (I - H^{-1} M)\Phi = H^{-1} S_{\text{fix}} \] (II.132)

where

\[ M = \chi f^T = \begin{pmatrix} \chi^1 \\ \chi^2 \\ \vdots \end{pmatrix} (\nu E_f^1, \nu E_f^2, \ldots) \ldots \] (II.133)

Substituting Eq. II.133 into Eq. II.132 and multiplying through by \( f^T \)

\[ f^T\Phi = \frac{f^T H^{-1} S_{\text{fix}}}{I - f^T H^{-1} \chi} \] (II.134)

but

\[ \Phi = H^{-1} S_{\text{fix}} + H^{-1} \chi (f^T\Phi) \] (II.135)

or from Eq. II.134

\[ \Phi = H^{-1} S_{\text{fix}} + H^{-1} \chi \frac{f^T H^{-1} S_{\text{fix}}}{I - f^T H^{-1} \chi} \] (II.136)

If the eigenvalue equation is defined

\[ H\Phi = \chi \] (II.137)
\[ f^T\Phi = \lambda \]

then

\[ \Phi = H^{-1} S_{\text{fix}} + \frac{\Phi_0}{1 - \lambda_0} f^T H^{-1} S_{\text{fix}} \]

or

\[ \Phi = \Phi_1 + \frac{\lambda_0 \Phi_0}{1 - \lambda_0} \] (II.138)

where

\[ H\Phi_1 = S_{\text{fix}} \]
\[ \lambda_1 = f^T\Phi_1 \] (II.139)
Based on these equations a three-step strategy is involved in the solution of the inhomogeneous equations:

(a) Solve the eigenvalue problem of Eqs. II.137 for $\Phi_0$ and $\lambda_0$ as outlined in the previous section iterating on the flux if isotope fission spectra are in problem mixture;

(b) Solve the inhomogeneous problem of Eqs. II.139 for $\phi_1$ and $\lambda_1$;

(c) Construct the fission source from Eq. II.137 as $\chi f^T \Phi$ and solve Eq.II.135 for the flux $\phi$.

Step (c) is not strictly necessary since the flux is given by Eq.II.138 but it is required to calculate the resonance reaction rates $A_x^R$ of Eq. II.119 which are used in the broad-group cross-section calculation.

4. Buckling Search to Critical

The spectrum and eigenvalue are clearly dependent upon the buckling $B^2$. For eigenvalue problems ($S^\text{fix} = 0$) with group independent buckling, the code MC$^2$-2 provides an option to search on $B^2$ to $k_{\text{eff}} = 1$. In order to invoke this option of the code, the user provides two starting guesses, $B_1^2$, $B_2^2$ and a convergence criterion $\epsilon_{B^2}$. The code solves the slowing down problem and calculates an eigenvalue for each of these values of $B^2$. Later estimates of $B^2$ are based upon linear or parabolic fits to the best available $k_{\text{eff}}$ vs. $B^2$ data. The search procedure ends if

$$|k_{\text{eff}}^{(n)} - 1| \leq \epsilon_{B^2}.$$

For problems with isotope dependent fission spectra data, the flux iteration discussed above is not converged until the buckling search has been completed. The algorithms invoked in choosing the points for the linear or parabolic fit are based upon those used in the ARC System neutronics search modules$^{(4)}$, and depend upon both the sign and magnitude of $1 - k_{\text{eff}}$. Several checks are made to insure that a search is not permitted to continue if a pathological situation arises, e.g. search to critical for a highly subcritical (blanket) composition.
K. Group Condensation

The individual material microscopic broad-group cross sections are obtained by averaging the ultra-fine-group data over the flux and current spectra obtained by solving the multigroup and continuous slowing down equations. The broad groups are user specified but must be defined such that broad-group energy boundaries fall on ultra-fine-group boundaries.

The broad group data are written in the ISOTXS(2) and/or XS.ISO(1) formats as defined in Appendix C. On user option it is possible to neglect the contributions of resolved and unresolved resonances in the edited cross sections thus making it possible to use MC²-2 for the generation of fine-group SDX libraries. (7) The broad-group averaging algorithms are defined below.

1. Broad-Group Inelastic and (n,2n) Cross Sections

The broad-group inelastic and (n,2n) transfer matrices are calculated using the algorithms defined in Section H above. In particular

\[
\sigma^m_{xG'\rightarrow G} = \sum_{g \in G} \sum_{g' \in G'} \left[ S^{g' 
rightarrow g}_{\text{tab}} + S^{g' 
rightarrow g}_{\text{evap}} + S^{g' 
rightarrow g}_{\text{d}} \right] \phi_{g'}
\]

where

- \( x \) = inelastic or (n,2n)
- \( \sum_{g \in G} \) = sum over ultra-fine-groups g contained in broad-group G
- \( S^{g' 
rightarrow g}_{\text{tab}} \) = tabulated law contribution as given inside g' sum of Eq. II.96
- \( S^{g' 
rightarrow g}_{\text{evap}} \) = evaporation law contribution as given inside g' sum of Eq. II.97
- \( S^{g' 
rightarrow g}_{\text{d}} \) = discrete law contribution as given inside g' sum of equation following Eq. II.104 using either rigorous or approximate \( P_A \)

and the broad-group flux is given by

\[
\phi^{G'} = \sum_{g' \in G'} \phi_{g'}
\]

The total inelastic and (n,2n) cross sections are obtained by summing over all sink groups

\[
\sigma^m_{xG'} = \sum_{G} \sigma^m_{x}(G' + G)
\]
Since the microscopic ultra-fine-group data required by Eq.II.140 are not saved during the course of the MC²-2 spectrum calculation, the data required for the broad-group condensation are calculated specifically for the cross section edits. It is this calculation which controls both the timing and space requirements of the MC²-2 condensation calculation. As the number of broad-groups increases beyond approximately 100, I/O times become quite large because of the data management requirements for calculation of Eq.II.140.

2. Broad-Group Absorption Cross Sections

The MC²-2 library file MCC2F5 (Appendix C) contains ultra-fine-group cross section data which are averaged over the flux spectrum as

\[ \sigma_x^m = \sum_{g \in G} \sigma_x^m \phi_g^G / \phi^G \]  

(II.143)

where \( x \) includes the six reactions \((n, H^1), (n, H^2), (n, H^3), (n, f), (n, \gamma)\) and \((n, \alpha)\). The \((n, \alpha)\) cross section calculated from Eq.II.143 is actually a sum of \((n, He^+)\) and \((n, He^3)\) cross sections. This summing was performed since the ISOTXS format does not allow editing of both the partials. Since the \( \sigma^m_x \) data from the file MCC2F5 do not include either resolved or unresolved resonance contributions, the fission and radiative capture cross sections of Eq.II.143 are not complete. The contributions from unresolved resonances are obtained using Eq.II.143 with the ultra-fine-group \((n, \gamma)\) and \((n, f)\) cross sections given by Eq.IV.68. The contribution of resolved resonances to the broad-group radiative capture and fission cross sections is derived from the resonance reaction rates, \( A_x^r \), defined by Eq.II.119. Using this equation it is clear that the resolved resonance contribution to the broad group cross section is given by

\[ \text{Resolved Resonance Reaction Rate in Broad-Group } G = \frac{1}{N \phi_g^G} \sum_{r \in G} A_x^r \]  

(II.144)

where the sum is over all resolved resonances of material \( m \) which fall into group \( G \),

\[ E_g^r < E_x^r < E_g^{r-1} \]

Thus the broad-group \((n, \gamma)\) and \((n, f)\) cross sections for a material with both resolved and unresolved data would be given by

\[ \sigma_x^m = \left\{ \sum_{g \in G} \left( \sigma_x^m + \sigma_x^m \phi_g^G + \frac{1}{N} \sum_{r \in G} A_x^r \right) \phi_g^G / \phi^G \right\} / \phi^G \]  

(II.145)
where
\[ \sigma^m_{\chi g} \equiv \text{floor cross sections from MCC2F5} \]
\[ \sigma^m_{\chi g} \equiv \text{unresolved cross sections from Eq.IV.68} \]
\[ A^r_{\chi} \equiv \text{resolved resonance reaction rate from Eq.II.119.} \]

3. Elastic Scattering Cross Sections

In Section G of this chapter the calculation of ultra-fine-group elastic transfer matrices was discussed. The ultra-fine-group cross sections derived from that calculation \( \sigma^f_{g'}(g' + g) \) include contributions from the ultra-fine-group library (MCC2F5) and the unresolved resonances from Chapter IV. The group condensation of these data are accomplished as

\[ \sigma^{om}_{eG}(G' \rightarrow G) = \sum_{g' \in G'} \sum_{g \in G} \sigma^{om}_{eG}(g' + g) \phi^{g'} \tag{II.146} \]

\[ \sigma^{lm}_{eG}(G' \rightarrow G) = \sum_{g' \in G'} \sum_{g \in G} \sigma^{lm}_{eG}(g' + g) \phi^{G'} \tag{II.147} \]

The \( P_l \) calculation is performed only for the consistent \( P_N \) or consistent \( B_N \) spectrum options in which case the ultra-fine-group current \( J^G \) is calculated directly using Eqs.II.62 and II.122 and the broad-group current is given by

\[ J^G = \sum_{g \in G} J^G. \tag{II.148} \]

The contributions of resolved resonances to the elastic transfer matrix cannot be calculated by use of Eqs.II.146-II.147 since ultra-fine-group resolved resonance scattering cross sections are not available. An approximate method adapted from the work of Stacey (39) which accounts for the position of the resonance in the group and the shape of the resonance is used in lieu of requiring ultra-fine-group resonance cross sections. The method adopted assumes that resolved resonance materials can scatter only one broad-group. Since the current MC2-2 library described in Table VIII has resolved data only for materials of mass greater than one hundred, this assumption fixes the smallest broad-group lethargy width at .04 (\( \sqrt{5} \) ultra-fine-groups). Following the methods used in calculating the resolved absorption cross sections we take
\[
\sigma_{\text{res}}^{m}(G \to G') = \frac{1}{N_{m}^{G}} \sum_{r \in G} \frac{A_{s}^{r} P(r \to G')}{r \in m} \quad (\text{II.149})
\]

where

\[A_{s}^{r} \text{ resolved resonance } r \text{ elastic reaction rate}
\]

\[P(r \to G') \text{ probability of scattering a neutron by resonance } r
\]

into Group G'.

The resonance reaction rate is calculated directly from the resonance integrals discussed in Chapter III,

\[
A_{s}^{r} = \frac{1}{E_{r}} (\Gamma_{r} J_{r}^{*} - \Gamma_{r} J_{r}^{*} - \Gamma_{r} J_{r}^{*}) \left( \Sigma_{t}^{G} + \frac{B^{2}}{3A_{1}^{G}} \right) \phi (u_{r}) \quad (\text{II.150})
\]

which is the scattering equivalent of Eq. II.119. The resonance integrals of Eq. II.150 take account of overlap, self-shielding, and Doppler broadening effects as described in Chapter III. The removal probability is taken as

\[
P(r \to G + 1) \approx \epsilon \frac{\int_{0}^{u_{G}} du \frac{K(u, u_{G})}{\Sigma_{t}^{G}(u)} \frac{\sigma_{s}^{r}(u)}{\Sigma_{t}^{G}(u)}}{\int_{0}^{u_{G-1}} du \frac{\sigma_{s}^{r}(u)}{\Sigma_{t}^{G}(u)}} \quad (\text{II.151})
\]

where

\[K(u, u_{G}) = \frac{-(u_{G}-u) - \alpha}{1 - \alpha}
\]

and \(\epsilon\) is the larger of \(u_{G-1}\) and \(u_{G} - \ln \frac{1}{\alpha} \).

It is further assumed that the resonance is isolated and that natural line shapes\(^{(26)}\) are applicable so that

\[
\frac{\sigma_{s}^{r}}{\Sigma_{t}^{G}(u)} \approx \frac{\psi + a\chi}{\beta + \psi + a\chi} \quad (\text{II.152})
\]

\[\psi(u) \approx \frac{1}{1 + \Delta^{2}[e^{u_{r}-u} - 1]^{2}}
\]

\[\chi(u) \approx \frac{\Delta[e^{u_{r}-u} - 1]}{1 + \Delta^{2}[e^{u_{r}-u} - 1]^{2}}
\]

\[\Delta \equiv \frac{2E_{r}}{\Gamma}
\]
The terms are defined in detail in Chapter III. The above assumptions make it possible to integrate Eq. II.151 analytically. The integrals are reported in Eqs. 12, 13, 19, 20, 23 of Reference 39. It is important to note that the above approximations are used only to distribute the resolved elastic reaction rate between in-group and removal and have no impact on the ultra-fine-group spectrum or the far more general resonance integral calculations of Chapters III and IV. The in-group probability is given by

$$P(r + G) = 1 - P(r + G + 1)$$

so that the elastic transfer matrix may be calculated from Eqs. II.149-II.151. The $P_{\perp}$ transfer matrix is calculated in the consistent spectrum options as

$$\sigma_{res}^{1m}(G \rightarrow G') = \frac{2}{3A N m G} \sum_{r} J(u_r) \frac{J(u_r)}{\phi(u_r)} A_s^r P(r + G')$$

where $J(u_r)$ is the current at lethargy $u_r$ in direct analogy with Eq. II.120.

The total elastic scattering matrix is given by the sums of II.146 and II.149 or for the $P_{\perp}$ matrix, II.147 and II.153. The elastic cross section is obtained by summing over sink groups according to Eq. II.142.

The Hydrogen elastic scattering cross sections are collapsed by assuming that scattering is isotropic in the center of mass system. With this assumption it is not difficult to show

$$\sigma_{el}^0 H(G \rightarrow G') = \frac{(E_{G'} - E_G)}{\phi G} (e^{\Delta u} - 1) \sum_{E G} \sigma_s^G \phi_s^G$$

$$\sigma_{el}^1 H(G \rightarrow G') = \frac{4}{9} \frac{(E_{G'}^{3/2} - E_G^{3/2})}{J G} (e^{3/2\Delta u} - 1) \sum_{E G} \sigma_s^G \phi_s^G$$

Eq. II.155 is used only for the consistent spectrum options. The corrections required to Eqs. II.154-II.155 to treat in-group scattering are straightforward.

4. Total Cross Section

The flux weighted total cross section is obtained by summing all of the partials discussed above,

$$\sigma_{t}^0 G = \sigma_{inel}^m G + \sigma_{n,2n}^m G + \sigma_{el}^m G + \sigma_{f}^m + \sigma_{nY}^m G + \sigma_{nh1}^m G + \sigma_{nh2}^m G + \sigma_{nh3}^m G + \sigma_{n^2}^m G$$

$$\sigma_{t}^1 G = \frac{2}{3A N m G} \sum_{r} J(u_r) \frac{J(u_r)}{\phi(u_r)} A_s^r P(r + G')$$
and the broad-group partial cross sections include floor, unresolved and resolved resonance contributions as discussed above. A current weighted total cross section is calculated as

\[
\sigma^m_{t_G} = \frac{1}{J} \sum_{g \in G} \gamma^m_{t_g} \phi^m_{t_g} + \frac{1}{N_m \phi} \sum_{r \in \mathcal{G}} \sum_{r \in \mathcal{M}} \frac{\Gamma_r}{E_r} J^r (\Sigma^r_{t_r} + \frac{B^2}{3A^r_{t_r}} \phi (u_r)) \quad (II.157)
\]

where

\[
\begin{align*}
J^g & \equiv \text{ultra-fine-group current calculated from Eqs. II.62 and II.122 for consistent options and Eq. II.64 for inconsistent options.} \\
J^G & \equiv \text{broad group current from Eq. II.148.} \\
\sigma^m_{t_g} & \equiv \text{ultra-fine-group total floor cross section from library file MCC2F5 plus ultra-fine-group total unresolved cross sections from Eq. IV.68.} \\
\gamma_g & \equiv \text{spectrum coefficient}
\end{align*}
\]

\[
\begin{cases}
\frac{B \tan^{-1} B}{\eta^g_{t_g}} & \text{consistent } B_1 \\
3(1 - \frac{B}{B \tan^{-1} B}) & \eta^g_{t_g} \\
1 & \eta^g_{t_g}
\end{cases}
\]

and the resolved resonance contribution is simply the reaction rate integral used with the flux weighted cross section of Eq. II.156.

For spectrum calculations using the extended transport approximation, higher order flux moments \( \phi^N_{t_G} \) are calculated recursively from Eq. II.62. Total cross section moments equivalent to Eq. II.157 are then calculated,

\[
\sigma^m_{t_G} = \frac{1}{\phi^N_{t_G}} \sum_{g \in G} \gamma_{t_g} \phi^m_{t_g} + \sigma^m_{t_G} \quad (II.158)
\]

where

\[
\begin{align*}
\eta^g_{t_g} & \equiv \begin{cases} 
\frac{N + \frac{1}{2} \frac{B}{\Sigma^g_{t_g}}}{N + 1} & \text{for } B_N \\
\frac{Q_{N+1} (-\Sigma^g_{t_g} / IB)}{Q_N (-\Sigma^g_{t_g} / IB)} \delta^N_{t_G} & \text{for } P_N
\end{cases} \\
\gamma_g & \equiv \begin{cases} 
1 & \text{for } P_N
\end{cases}
\end{align*}
\]

and all other terms have been defined.
5. **Transport Cross Section**

In analogy with the total cross section, the MC$^2$-2 code calculates moments of the transport cross section if the order of the extended transport approximation is greater than unity. The transport cross section algorithms are spectrum option dependent. In all cases, however, the algorithms are defined to conserve the relation

$$L_{\ell}^{tr} = \frac{-\ell}{2\ell + 1} iB \phi_{\ell-1}^{G}$$

or for the special case of $\ell = 1$

$$J = -\frac{B}{3\Sigma^{tr}_m} \phi$$

The algorithms further conserve the relation

$$\Sigma^{tr} = \sum_i N_i \sigma^{tr}_i$$

a. **Inconsistent $P_1$ or $B_1$ Spectrum**

$$\sigma_{tr}^m = \sigma_{G}^m - \sigma_{e}^m$$

where

$$\sigma_{tr}^m = P_1 \text{ moment of total cross section given by Eq.II.157 or II.158.}$$

$$\sigma_{e}^m = P_1 \text{ moment of elastic scattering cross section.}$$

The elastic scattering cross section moments are calculated from Eq.II.45 and II.150 and it is assumed that resolved resonances do not contribute to the cross sections for moments greater than unity,

$$\sigma_{e}^m = \left\{ \sum_{g \in G} \sum_{n} c_{e} g T_{n}^{o} (\alpha_{m}) \phi_{\ell}^{r} \right. + \frac{2 \delta_{\ell}}{3A N_{m}} \sum_{r \in G} \sum_{rr' \in m} A_{r}^{r'} \frac{J(u_{r'})}{\phi(u_{r'})} \left\} \phi_{G}^{G}, \quad \ell = 1,2, \ldots, N \right.$$
b. Consistent $P_1$ or $B_1$ Spectrum

The Eqs.II.160 and II.161 are used in the consistent spectrum options as well as the inconsistent options for moments greater than unity ($\ell > 1$). The $P_1$ moment is however calculated directly from the elastic transfer matrices in direct analogy with Eqs.II.147 and II.153. In particular

$$
\sigma_{tr_G}^m = \frac{1}{J_G} \sum_{g' \leq g} \sigma_{el}^m (g \to g') J_{g'G} \\
- \frac{1}{J_G} \sum_{r} \frac{2}{3A_{mN_m}} \sum_{g} J(u_r) \frac{\phi(u_r)}{A_s^r} P(r + G). \tag{II.162}
$$

6. Average Number of Neutrons per Fission

The average number of neutrons per fission is given by

$$
\nu^m_G = \frac{\sum_{g \in G} \nu_{Gm}^G \phi_g + \frac{1}{N_m} \sum_{r \in G} \nu_{A_r}^G \phi_r G}{\sigma_{fG}^m \phi_f G} \tag{II.163}
$$

where

- $\nu^G_m$ = number of neutrons per fission for material $m$ in ultra-fine-group $g$ from Eq.II.110.
- $\sigma^m_{fG}$ = floor plus unresolved ultra-fine-group fission cross section.
- $\sigma^m_{fG}$ = broad-group fission cross section.
- $A_r^f$ = resolved resonance fission reaction rate from Eq.II.119.

7. Fission Spectrum Distribution

The isotopic fission spectrum distributions are derived by summing the ultra-fine-group vectors of Eq.II.112,

$$
\chi^G_m = \sum_{g \in G} \chi^g_m. \tag{II.164}
$$
The MC²-2 code edits a set-wide fission spectrum vector as well as the isotopic vectors of Eq.II.164. The set-wide vector is defined

\[
\chi_{\text{set}}^G = \frac{\sum_{g \in G} \sum_{m} \chi_m^g S_f^m}{\sum_{m} S_f^m}
\]  

(II.165)

where \(\chi_m^g\) are the ultra-fine-group vectors of Eq.II.112 and \(S_f^m\) are the fission sources for material \(m\),

\[
S_f^m = \sum_g N_g^m \phi_g^m + \sum_{r \in m} \gamma_r^m A_r^m
\]  

(II.166)

8. XS.ISO Cross Sections

The ARC System\(^{(1)}\) cross section file XS.ISO (c.f. Appendix B) is less general than the CCCC file ISOTXS and contains derived cross sections in addition to the standard cross sections given above. The following conversions for XS.ISO cross sections are consistent with the MC² derived cross sections of Reference 10:

\[
\begin{bmatrix}
\sigma_{tr_G}^m \\
\sigma_{e(G \rightarrow G)}^m
\end{bmatrix}_\text{ARC} = \sigma_{tr_G}^m
\]  

(II.167)

\[
\begin{bmatrix}
\sigma_{e(G \rightarrow G)}^m
\end{bmatrix}_\text{ARC} = \sigma_{tr_G}^m - \sigma_{t_G}^m + \sigma_{e(G \rightarrow G)}^m
\]  

(III.168)

Equations II.168 and II.169 are consistent with Equations 116-118 of Ref. 10.

L. Broad Group Spectrum

The microscopic broad-group cross section data calculated according to the algorithms of Section K are appropriate for use in general multigroup neutronics calculations. One such calculation, extended transport \(p_{1}\) real and adjoint fundamental mode spectrum, is available in MC²-2 at user option. The module (overlay) CSC010 solves the following broad-group flux equations
\[ \sum_{G'}^G \phi_{G'} - B \Phi_1^G = Q^G + \sum_{G' < G} \Sigma_s^{\text{o}}(G' \rightarrow G) \phi_{G'} \]

\[ \frac{B}{3} \phi_o^G + \frac{2}{3} \Phi_1^G + \frac{2}{3} B \phi_2^G = \sum_{G' < G} \Sigma_s^1(G' \rightarrow G) \phi_{G'} \]

\[ -i \frac{2 \ell}{2 \ell + 1} B \phi_G^{\ell - 1} + \Sigma_{\text{tr}}^G \phi_{\ell}^G - i \frac{2 \ell}{2 \ell + 1} B \phi_{\ell + 1}^G = 0 \quad \ell = 2, \ldots, N \]  

(II.170)

\[ \phi_{N+1} = 0 \]

where

\[ \Sigma_s^{\text{o}}(G' \rightarrow G) = \sum_m N_m \left[ \sigma_{\text{el}}^{\text{o}}(G' \rightarrow G) + \sigma_{\text{inel}}^{\text{o}}(G' \rightarrow G) + 2 \sigma_{\text{n},2n}^{\text{o}}(G' \rightarrow G) \right] \]

\[ \Sigma_s^1(G' \rightarrow G) = \sum_m N_m \sigma_{\text{el}}^{1m}(G' \rightarrow G) \]

\[ \Sigma_{\text{tr}}^G = \sum_m N_m \sigma_{\text{tr}}^{1m}(G' \rightarrow G) \]

\[ \Sigma_{\text{ro}}^G = \sum_m N_m \left[ \sigma_{\text{el}}^{\text{o}}(G \rightarrow G) - \sigma_{\text{inel}}^{\text{o}}(G \rightarrow G) - 2 \sigma_{\text{n},2n}^{\text{o}}(G \rightarrow G) \right] \]

\[ \Sigma_{\text{rl}}^G = \sum_m N_m \left[ \sigma_{\text{el}}^{1m}(G \rightarrow G) \right] \]

\[ Q^G = \frac{1}{K} \chi_s^G \sum_m N_m \sum_{G'}^G \nu_{G'}^{\text{m}} \sigma_{G'}^{\text{m}} \phi_{G'} + \sum_{G \in \mathbb{G}} S_{\text{fix}}^G \]

The inconsistent spectrum option is defined by setting \( \Sigma_s^1(G' \rightarrow G) \) to zero and taking

\[ \Sigma_{\text{ro}}^G = \Sigma_{\text{tr}}^G \]

If there are no inhomogeneous sources, \( S_{\text{fix}} = 0 \), then Equations II.170 specify an eigenvalue problem. In this case the code will search on \( B^2 \) to \( K = 1 \) according to the procedures noted in Section J.4 and reference 4. The first buckling used will be the critical \( B^2 \) from the
ultra-fine-group calculation and the second guess increases (decreases) $B^2$ by 1% if the eigenvalue of the ultra-fine-group calculation is greater (less) than 1.0. The buckling search is stopped when

$$|K - 1| \leq 10^{-6}.$$  

The adjoint eigenvalue problem is also solved by MC$^2$-2,

$$\sum_{G_o}^{G} \phi_{G_o}^* - B \phi_1^* = Q^G + \sum_{G' > G} E_s^{G}(G \to G') \phi_{G'}^*$$

$$\frac{B}{3} \phi_{G_0}^* + \sum_{G_1}^{G} \phi_{G_1}^* + \frac{2}{3} B \phi_2^* = \sum_{G' > G} E_s^1(G \to G') \phi_{G'}^*$$  (II.171)

$$-(1)^{2\ell} \frac{\ell}{2\ell + 1} B \phi_{\ell-1}^* + \sum_{G}^{\ell} \phi_{G}^* - (1)^{2\ell} \frac{\ell + 1}{2\ell + 1} B \phi_{\ell+1}^* = 0 \quad \ell = 2, \ldots, N$$

$$\phi_{N+1}^* = 0$$

with

$$Q^G = \frac{1}{K} \langle \Sigma_f \rangle G \sum_{G'} \chi_{G'} \phi_{G'}^*.$$

The solution of the tridiagonal equations II.170 and II.171 is performed using the forward elimination-backward substitution technique (41), a specialization of the standard Gauss reduction. Since the flux equations II.170 are obtained by summing the ultra-fine-group equations II.59 and using the flux weighted broad-group cross section definitions of Section K, the fluxes, currents and eigenvalue calculated by the module CSC010 should agree with those obtained from the ultra-fine-group spectrum solution. In practice the differences in resonance treatments, slowing down formulations and computational precision limit this agreement. Eigenvalue agreement tends always to be better than 0.1% and spectrum agreement is excellent down to the resolved resonance energy domain where the ultra-fine-group spectrum tends to attenuate faster than the broad group spectrum. Because flux weighting is used to collapse the cross section data, it is clear that the broad-group adjoint spectrum of Eq. II.171 is not equivalent to the adjoint of the ultra-fine-group equations.
III. CALCULATION OF RESOLVED RESONANCE INTEGRALS

A. General Formulation

The algorithms involved in the resolved resonance integral calculation developed by R. Hwang (25) assume the narrow resonance approximation and account for interference scattering and the effects of overlap with neighboring resolved resonances. Both single level Breit-Wigner and multilevel Breit-Wigner or Adler-Adler representations are accommodated including interaction of single and multilevel resonances.

The effective macroscopic capture cross section over the lethargy range \( u_1, u_2 \) of width \( \Delta u \) due to resonances \( i \) for an isotope having atom density \( N_i \) can be written as

\[
\bar{\Sigma}_c = N_i \bar{\sigma}_c = \frac{\sum_{i}^{u_2} \frac{N_i \sigma_i (u) F(u) \, du}{\Sigma_t (u)}}{\sum_{i}^{u_2} \frac{F(u) \, du}{\Sigma_t (u)}}
\]

(III.1)

where \( F(u) \) is the collision density, \( \sigma_i \) is the microscopic capture cross section due to resonance \( i \), and \( \Sigma_t \) is the total macroscopic cross section for the mixture. If we consider the case of Breit-Wigner single level resonances, extend the range of integration to cover all lethargies, replace \( du \) by \( -dE/E \), assume \( E \) remains constant at the resonance energy \( E_{o_i} \), and assume a constant collision density over each resonance, we may rewrite Eq. III.1 as

\[
\bar{\Sigma}_c = \frac{\sum_{i}^{\infty} \frac{N_i \sigma_i \frac{\Gamma_i}{\Gamma_i} \psi(\theta_i, \chi_i) \frac{\Gamma_i}{2} \, dx_i \frac{1}{E_{o_i}}}{\Sigma_t (u)}}{\Delta \Sigma_p / \sum_{p}}
\]

\[
= \sum_{i} \frac{\Sigma_p \frac{\Gamma_i}{\Gamma_i}}{\Delta u E_{o_i} f} \cdot \frac{1}{2} \int_{-\infty}^{\infty} \frac{N_i \sigma_i \psi_i \, dx_i}{\Sigma_t (u)}
\]
where \( C_t(u) = L + N_i \sigma_o \psi(\theta_1, x_1) + N_i \sigma_o a_i \chi(\theta_1, x_1) + \sum_{i' \neq i} N_i \sigma_o \psi(\theta_1, x_1) \)

\[ + N_i \sigma_o a_i \chi(\theta_1, x_1) \]

\( F_i \) is the constant collision density for resonance \( i \) and \( f \) is the so-called flux correction factor which can be written as

\[ f = \sum_i F_i \frac{1}{\Delta u} \sum_j F_j \frac{J^* \Delta I_j}{E_{0_j}} \]

The sum in \( f \) extends over all resonances in the mixture, and \( J^* \Delta I_j \) is the total resonance integral defined later in Eq. III.24. The \( \Delta I \) superscript refers to single level and Eq. III.2 defines the resonance integral \( J^* \Delta I_i \).

Eq. III.2 is the starting point in defining the ultra-fine-group reaction rates and fluxes as given in Chapter II Equations II.119, II.121-II.123. The weighting functions \( F_i \) are calculated from the slowing down density attenuated by higher energy resonances.

In deriving Eq. III.2, we have used the approximation that \( E = E_{0_i} \) so that

\[ \sigma_{c_i} = \sigma_o \frac{\Gamma_i}{\Gamma_1} \psi(\theta_1, x_1) = \sigma_o \frac{\Gamma_i}{\Gamma_1} \psi_1 \] (III.3)

with a similar expression for \( \sigma_f \), where \( \Gamma_f \) replaces \( \Gamma \), and

\[ \sigma_{f_i} = \sigma_p + \sigma_o \psi_i + \sigma_o a_i \chi(\theta_1, x_1) = \sigma_p + \sigma_o \psi_i + \sigma_o a_i \chi \] (III.4)

where

\[ \sigma_o = \text{the peak cross section of the resonance} \]

\[ = 2.6039953 \times 10^6 \left| \frac{A_i + 1}{A_i} \right|^2 g_j \frac{\Gamma_{n_1}}{\Gamma_1} \]

\( A_i = \text{the mass number of the nucleus having resonance } i \)
\[ \mathcal{g}_{J_i} = \frac{2J + 1}{2(2I + 1)} \] where \( J \) is the total spin of the compound nucleus and \( I \) is the spin of the target nucleus

\[ \Gamma_{\gamma_i} \] the radiative capture line width

\[ \Gamma_i \] the total line width

\[ \Gamma_{n_{oi}} \] the neutron width evaluated at the resonance energy

\[ \psi(\theta_i, x_i) \equiv \psi_i \] the Doppler broadened symmetric line shape function given in Eq. A.1 of Appendix A and calculated as described there

\[ \beta_i = \gamma_{\gamma_i}/\Delta_i \] the ratio of natural width to Doppler width

\[ \Delta_i = \left[ \frac{4kT_i E_{\gamma_i}}{A_i} \right]^{1/2} \] with Boltzmann's constant

\[ k = 8.6168 \times 10^{-5} \text{ eV/degree Kelvin} \]

\[ T_i \] temperature of isotope having resonance \( i \) in degrees Kelvin

\[ x_i = \frac{2(E - E_{\gamma_i})}{\Gamma_i} \]

\[ a_i = \left[ \frac{\mathcal{g}_{J_i} \Gamma_{n_{oi}} \sigma_{p_{ai}}}{\Gamma_i \sigma_{o_i}} \right]^{1/2} \] the atom potential scattering cross section

\[ \chi(\theta_i, x_i) \equiv \chi_i \] the Doppler broadened antisymmetric line shape function given in Eq. A.2 of Appendix A and calculated as described there.

The summation in the denominator of Eq. III.2 is over all other resonances \( i' \neq i \) in the mixture and

\[ A_i' = \frac{N_{i',o_i'}}{N_{i,o_i}} \]

\[ B_i' = a_i' A_i' \]

\[ \beta_i = \frac{\Sigma P}{N_{i,o_i}} = \frac{\sigma_{p_{ai}}}{\sigma_{o_i}} \]
The code computes resonance integrals for a homogeneous mixture, and for heterogeneous slab geometries or cylindrical geometries. Whether the system is homogeneous or heterogeneous, and whether slab or cylinder determines the value used for \( \Sigma \) and hence for \( \beta \) by use of an equivalence principle.

For homogeneous mixtures, \( \Sigma \) is given by

\[
\Sigma = \sum_m N_m \sigma_{t_m} + \frac{\kappa^2}{3 \sum_m N_m \sigma_{t_m}}
\]  

where the summation is over all isotopes in the homogeneous mixture, \( N_m \) is the atom density of isotope \( m \), \( \sigma_{t_m} \) is the smooth total cross section library data for the ultra fine group into which the resonance in question falls, and \( \kappa^2 \) is the user supplied extended-transport approximation buckling as used in the continuous slowing down calculation.

For slab geometries, for each slab \( k \) and for the material \( i \) whose resonance integral is being calculated

\[
\Sigma^k_{pi} = \sum_{m \in k} N_m \sigma_{t_m} + \frac{\kappa^2}{3 \sum_m N_m \sigma_{t_m}} + \Sigma^{*k}_{ei}
\]  

where the first summation is over all isotopes \( m \) contained in slab region \( k \) and the second summation as in Eq. III.6 is over all isotopes in the equivalent homogeneous mixture obtained by homogenizing all slab regions. The so-called "escape" cross section (for the material \( i \) whose resonance integral is being calculated) intended to account for the heterogeneity is calculated using

\[
\Sigma^{*k}_{ei} = \Sigma^k_{ei} \frac{a_1 (1 - C^k_i)}{1 + (a_2 - 1) C^k_i}
\]  

where

\[
\Sigma^k_{ei} = \frac{S^k_e}{4V^k}
\]  

with \( S^k \) and \( V^k \) the surface area and volume of region \( k \), \( a_1 \) and \( a_2 \) are user supplied with default values of 1.09, and the Dancoff factor \( C^k_i \) is given by

\[
C^k_i = E_3(\tau^k_{Ri}) + E_3(\tau^k_{Li}).
\]  

In Eq. III.10, \( E_3 \) is the exponential integral of order three defined in Eq. A.37 of Appendix A. The optical thicknesses to the left and right of slab region \( k \) for material \( i \) denoted by, respectively, \( \tau^k_{Li} \) and \( \tau^k_{Ri} \), are computed as follows,
\[ \tau_{L1}^{k} = \sum_{j \neq i} \sum_{r \text{ left of } k} N_{j}^{r} \Delta x_{r} \sigma_{r}^{j} \]  \hspace{2cm} (III.11) \\

\[ \tau_{R1}^{k} = \sum_{j \neq i} \sum_{r \text{ right of } k} N_{j}^{r} \Delta x_{r} \sigma_{r}^{j} \]  \hspace{2cm} (III.12)

where \( \Delta x_{r} \) is the thickness of region \( r \). The summation over \( r \) continues until a region \( s \) is found such that

\[ \frac{N_{s}^{k} \Delta x_{s}}{N_{s}^{k} \Delta x_{k}} > \epsilon_{\text{het}}. \]  \hspace{2cm} (III.13)

The criterion \( \epsilon_{\text{het}} \) is a user input parameter and has the default value of 0.1.

For cylindrical geometry, the resonance integrals are evaluated only for the central region. All outer regions are homogenized into a single outer region. Denoting the central region with superscript 0 and the homogenized outer region with superscript 1, we have

\[ \Sigma_{p}^{0} = \sum_{m \in 0} \sum_{m} N_{m}^{0} \sigma_{m}^{0} + \frac{\kappa^{2}}{3} \sum_{m} N_{m}^{0} \sigma_{m}^{0} + \Sigma_{e}^{0} \]  \hspace{2cm} (III.14)

where the first summation extends over all isotopes contained in the central region and the second summation is as in Eq. III.7 over all isotopes in the equivalent homogeneous mixture of all cylindrical regions.

The escape cross section for the central region \( \Sigma_{e}^{0} \) is calculated as

\[ \Sigma_{e}^{0} = \Sigma_{e}^{0} \frac{a_{1}(1 - C^{0})}{1 + (a_{2} - 1)C^{0}} \]  \hspace{2cm} (III.15)

where

\[ \Sigma_{e}^{0} = \frac{S^{0}}{4V^{0}} \]  \hspace{2cm} (III.16)

with \( S^{0} \) and \( V^{0} \) the surface area and volume of the central region, \( a_{1} \) and \( a_{2} \) are user supplied with default values of 1.35, and the Dancoff factor \( C^{0} \) is given by

\[ C^{0} = 1 - \gamma - \gamma^{4}(1 - \gamma). \]  \hspace{2cm} (III.17)

In Eq. III.17

\[ \gamma = \frac{\Sigma_{t}^{1}}{\Sigma_{t}^{1} + \Sigma_{e}^{1}} \]  \hspace{2cm} (III.18)
with
\[ \Sigma^1_T = \sum_{m \in 1}^N N^1_m t_m \] (III.19)
and \( V^1 \) is the volume of the homogenized outer regions. The summation in Eq. III.19 extends over all isotopes contained in the outer regions, including the isotope \( i \) if it should be present.

The \( \Delta \) on \( J^*_{x_1} \) in Eq. III.2 refers to either capture or fission. Thus the effective macroscopic fission cross section for the interval \( u_1, u_2 \) can similarly be written as in Eq. III.2
\[ \bar{\Sigma}^1_f = \frac{\sum P \Gamma_{f_i}}{\Delta u E_{o_i}} J^*_{x_1} \] (III.20)
where \( \Gamma_{f_i} \) is the fission width for resonance \( i \).

In the case of the total cross section, we have
\[ \bar{\Sigma}^1_t = \frac{\sum P \Gamma_{t_i}}{\Delta u E_{o_i}} \int_{-\infty}^{\infty} \frac{(\psi_i + a_i x_i)}{\beta_i + \psi_i + a_i x_i + \sum_{i', \#i} (A_{i', \psi}, + B_{i', x_i})} dx_i \]
\[ = \frac{\sum P \Gamma_{t_i}}{\Delta u E_{o_i}} J^*_{x_1} \] (III.21)

Now the resonance integrals can be factored (25) to display a lead term corresponding to the isolated resonance integral (the usual resonance integral as discussed, e.g. by Dresner (26)) and a term due to the overlap of other resonances in the mixture. In particular, \( J^*_{x_1} \) can be rewritten as
\[ J^*_{x_1} = \frac{1}{2} \int_{-\infty}^{\infty} dx_i \frac{\psi_i}{\beta_i + \psi_i + a_i x_i} - \frac{1}{2} \int_{-\infty}^{\infty} dx_i \frac{\psi_i}{\beta_i + \psi_i + a_i x_i} \]
\[ = J^*_{x_1} - \sum_{i', \#i} (A_{i', \psi}, + B_{i', x_i}) \] (III.22)

where the first integral denoted by \( J^*_{x_1} \) is the usual isolated resonance integral and the second denoted by \( O^*_{x_1} \) is the overlap integral due to other single level resonances \( i' \). The zero indicates that resonances are all of one type, that is, all single level.
Eq. III.22 may be similarly factored with $\psi_i + a_i \chi_i$ replacing $\psi_i$ in the numerators of each of the integrals in Eq. III.23. Therefore

$$J^{a,b}_{\ell,1} = \frac{1}{2} \int_{-\infty}^{\infty} dx_i \frac{\psi_i + a_i \chi_i}{\beta_i + \psi_i + a_i \chi_i} - \frac{1}{2} \int_{-\infty}^{\infty} dx_i \frac{\psi_i + a_i \chi_i}{\beta_i + \psi_i + a_i \chi_i}$$

$$\cdot \sum_{i \neq i'} \left( A_{i,i'}^i \psi_i + B_{i,i'}^i \chi_i \right) = J^{a,b}_{\ell,1}(i,i',c). \quad (III.24)$$

Now in the case of multilevel resonances, instead of the expressions given in Eqs. III.3 and III.4 we have

$$\sigma_k = \sigma_0 \left[ \frac{G_{\gamma_k}}{G_{\tau_k}} \right] \left[ \psi_k + b_{\gamma_k} \chi_k \right] \quad (III.25)$$

$$\sigma_{\ell_k} = \sigma_0 \left[ \frac{G_{\tau_k}}{G_{\gamma_k}} \right] \left[ \psi_k + b_{\ell_k} \chi_k \right] \quad (III.26)$$

$$\sigma_{t_k} = \sigma_0 \left[ \frac{G_{\tau_k}}{G_{\tau_k}} \right] \left[ \psi_k + a_{\ell_k} \chi_k \right] \quad (III.27)$$

In Eqs. III.25-III.27 we again set $E = E_0$ and use the shorthand notation $\psi_k = \psi(\omega_k, x_k)$ and $\chi_k = \chi(\omega_k, x_k)$.

The definition of the various coefficients depends upon whether the resonance $k$ is represented by the Adler-Adler or Breit-Wigner forms. In the following, we will assume the flux correction factor $f$ equals 1.

Multilevel Breit-Wigner

$$\sigma_0 = \left( \text{single level Breit-Wigner } \sigma_0 \right) \cdot \left| G_{\tau_k} \right|$$

where the single level Breit-Wigner $\sigma_0$ is defined above

$G_{\tau_k}$ = Breit-Wigner multilevel parameter for the $t_{\ell_k}$ reaction which is $1$ plus the symmetric level-level interference contribution

$G_{\gamma_k}$ = Breit-Wigner multilevel parameter for the radiative capture reaction

$\Gamma_{\gamma_k}/\Gamma_{\tau_k}$

$\Gamma_{t_k}$ = Breit-Wigner multilevel total line width
\[ b_{\gamma_k} = 0 \]

\[ G_{f_k} = \text{Breit-Wigner multilevel parameter for the fission reaction} \]
\[ = \frac{\Gamma_{f_k}}{\Gamma_{\tau_k}} \]

\[ b_{f_k} = 0 \]

\[ a_k = (\text{single level Breit-Wigner } a) + \text{the antisymmetric level-level interference contribution, all divided by } \left| G_{\tau_k} \right|^2 \]

\[ \theta_k = \frac{\Gamma_{\tau_k}}{\Delta_k} \]

\[ x_k = 2(E - E_{\sigma_k})/\Gamma_{\tau_k} \]

**Multilevel Adler-Adler**

\[ \sigma_{\sigma_k} = 2.6039953 \times 10^6 \left[ \frac{A_k + 1}{A_k} \right]^2 \left| \frac{G_{\tau_k}}{2\Gamma_{(s)}} \right|^2 \]

\[ G_{\tau_k} = \sqrt{E_{\sigma_k}} \left[ G_k^T \cos 2\phi_{\ell_k} + H_k^T \sin 2\phi_{\ell_k} \right] \]

\[ G_k^T = \text{Adler-Adler symmetric capture cross section parameter from ENDF/B} \]

\[ H_k^T = \text{Adler-Adler antisymmetric capture cross section parameter from ENDF/B} \]

\[ \phi_{\ell_k} = \text{phase shift} \]

\[ \Gamma_{(s)} = 5\text{-matrix total line width for the Adler-Adler formulation} \]

\[ G_{\gamma_k} = \sqrt{E_{\sigma_k}} \left[ G_k^C \cos 2\phi_{\ell_k} + H_k^C \sin 2\phi_{\ell_k} \right] \]

\[ G_k^C = \text{Adler-Adler symmetric capture cross section parameter from ENDF/B} \]

\[ H_k^C = \text{Adler-Adler antisymmetric capture cross section parameter from ENDF/B} \]

\[ b_{\gamma_k} = -0.5 \left[ \frac{H_k^C \cos 2\phi_{\ell_k} - G_k^C \sin 2\phi_{\ell_k}}{G_{\gamma_k}} \right] \sqrt{E_{\sigma_k}} \]
\[ G_{f_k} = \sqrt{E_{o_k}} \left[ G_{f_k}^F \cos 2\phi_{f_k} + H_{f_k}^F \cos 2\phi_{f_k} \right] \]

\[ G_{f_k}^F = \text{Adler-Adler symmetric fission cross section parameter from ENDF/B} \]

\[ H_{f_k}^F = \text{Adler-Adler antisymmetric fission cross section parameter from ENDF/B} \]

\[ b_{f_k} = -0.5 \left[ \frac{H_{f_k} \cos 2\phi_{f_k} - G_{f_k} \sin 2\phi_{f_k}}{G_{f_k}} \right] \sqrt{E_{o_k}} \]

\[ a_k = -0.5 \left[ \frac{H_{f_k} \cos 2\phi_{f_k} - G_{f_k} \sin 2\phi_{f_k}}{G_{f_k}} \right] \sqrt{E_{o_k}} \]

Using Eqs. III.25-III.27 in Eq. III-1, we have for the case of all Adler-Adler multilevel resonances in the mixture, for example

\[ \overline{\Sigma}_{\gamma_k}^{(s)} = \frac{\Sigma \gamma_k^p}{\Delta uE_{o_k} G_{\gamma_k}^{T_k}} \int_{-\infty}^{\infty} dE \frac{1}{2} \left( \psi_k + b_k \gamma_k X_k \right) \]

\[ = \frac{\Sigma \gamma_k^p}{\Delta uE_{o_k} G_{\gamma_k}^{T_k}} J_{\gamma_k}^{*ml} = \frac{\Sigma \gamma_k^p}{\Delta uE_{o_k} G_{\gamma_k}^{T_k}} S_k J_{\gamma_k}^{*ml} \quad (\text{III.28}) \]

Equation III.28 may be compared with Eq. III.2 and \( S_k = G_{T_k} \left| G_{T_k} \right| \). The ml superscript refers to multilevel. In the case of multilevel Breit-Wigner resonances, \( \gamma_k^{(s)} \) is replaced by the multilevel total line width and \( b_k \gamma_k \) is zero. \( A_k, B_k, \) and \( \beta_k \) are defined as in Eq. III.5 with \( \sigma_{o_k} \) and \( a_k \) defined as appropriate to the multilevel representation involved.

In the case of fission, Eq. III.28 becomes

\[ \overline{\Sigma}_{f_k}^{*ml} = \frac{\Sigma \gamma_k^p G_{f_k}^{(s)}}{\Delta uE_{o_k} G_{f_k}^{T_k}} J_{f_k}^{*ml} \quad (\text{III.29}) \]

where \( J_{f_k}^{*ml} \) is given by the integral of Eq. III.28 but with \( b_{f_k} \) replacing \( b_k \).

For the total cross section
As in the case of the single level resonances, the multilevel resonance integrals may be factored into a lead term and a term due to the overlap of other resonances in the mixture. Thus the integral in Eq.III.28 can be written as

\[
\int_\gamma \psi_k + b_k \chi_k \, dx_k \quad \text{and} \quad \int_\gamma \psi_k + b_k \chi_k \, dx_k \quad \text{can be factored to yield}
\]

\[
\frac{1}{2} \left( \int_\gamma \psi_k + b_k \chi_k \, dx_k \right) - \frac{1}{2} \left( \int_\gamma \psi_k + b_k \chi_k \, dx_k \right) = \int_\gamma \psi_k + b_k \chi_k \, dx_k - \int_\gamma \psi_k + b_k \chi_k \, dx_k
\]

The factored form of Eq.III.29 can be written as

\[
J_{J''} = J_{J'} - \int_\gamma \psi_k + b_k \chi_k \, dx_k
\]

Also, Eq.III.30 may be factored to yield

\[
\int_\gamma \psi_k + b_k \chi_k \, dx_k - \int_\gamma \psi_k + b_k \chi_k \, dx_k = \int_\gamma \psi_k + b_k \chi_k \, dx_k - \int_\gamma \psi_k + b_k \chi_k \, dx_k
\]

So far we have considered the case of a mixture of either all single level (Eqs.III.23-III.24) or all multilevel (Eqs.III.31-III.33) resonances. Two other situations may also arise, namely a single level resonance in the presence of other single and multilevel level resonances, or a multilevel resonance in the presence of other single and multilevel resonances. Each of these cases may be written in factored form to yield a lead integral for the isolated single level (multilevel) resonance, minus integrals resulting from overlap with other single level (multilevel) and other multilevel (single level) resonances.
Thus, for a single level resonance \( i \) we have
\[
J_{x, i}^{*} = J_{x, i} - \alpha_{x, i, 0} - \bar{\alpha}_{x, i, 0} \tag{III.34}
\]
and
\[
J_{t, i}^{*} = J_{t, i} - \alpha_{t, i, 0} - \bar{\alpha}_{t, i, 0} \tag{III.35}
\]
\( J_{x, i} \) and \( \bar{J}_{x, i} \), are given in Eq. III.23 and \( J_{t, i} \) and \( \bar{J}_{t, i} \) are given in Eq. III.29. The second overlap terms which depend upon the single level resonances \( i \) and \( i' \) and upon the multilevel resonances \( k \) can be written explicitly as
\[
O_{x, i, i', k}^{*} = \frac{1}{2} \int_{-\infty}^{\infty} \frac{dx}{\beta_{i} + \psi_{i} + a_{i} \chi_{i} + \sum_{i' \neq i} (A_{i}, \psi_{i}, + B_{i}, \chi_{i})} \int_{-\infty}^{\infty} \frac{\sum_{k} (S_{k} A_{k} \psi_{k} + B_{k} \chi_{k})}{\beta_{i} + \psi_{i} + a_{i} \chi_{i} + \sum_{i' \neq i} (A_{i}, \psi_{i}, + B_{i}, \chi_{i})} \tag{III.36}
\]
and
\[
O_{t, i, i', k}^{*} = \frac{1}{2} \int_{-\infty}^{\infty} \frac{dx}{\beta_{i} + \psi_{i} + a_{i} \chi_{i} + \sum_{i' \neq i} (A_{i}, \psi_{i}, + B_{i}, \chi_{i})} \int_{-\infty}^{\infty} \frac{\sum_{k} (S_{k} A_{k} \psi_{k} + B_{k} \chi_{k})}{\beta_{i} + \psi_{i} + a_{i} \chi_{i} + \sum_{i' \neq i} (A_{i}, \psi_{i}, + B_{i}, \chi_{i})} \tag{III.37}
\]
In Eqs. III.36 and III.37, \( A_{i} \) and \( B_{i} \) are defined in Eq. III.5 and
\[
N_{k} = \frac{N_{k} \sigma_{k}}{\sigma_{i}} \tag{III.38}
\]
\[
A_{k}^{i} = \frac{a_{k} A_{k}}{N_{k} \sigma_{i}} \tag{III.38}
\]
Similarly, for a multilevel resonance \( k \) we have
\[
J_{y, k}^{*} = J_{y, k} - \alpha_{y, k, 0} - \bar{\alpha}_{y, k, 0} \tag{III.39}
\]
\[
J_{f, k}^{*} = J_{f, k} - \alpha_{f, k, 0} - \bar{\alpha}_{f, k, 0} \tag{III.40}
\]
\[
J_{t, k}^{*} = J_{t, k} - \alpha_{t, k, 0} - \bar{\alpha}_{t, k, 0} \tag{III.41}
\]
In Eqs. III.37-III.41 the indices $k$ and $k'$ refer to multilevel resonances and index $i$ refers to single level resonances in the mixture.

\[ J_{k}^{\gamma,ml} \] and \[ O_{k,k',o}^{\gamma,ml} \] are given in Eq. III.31. \[ J_{k}^{f,ml} \] and \[ O_{k,k',o}^{f,ml} \] are the above expressions with $b_f$ replacing $b_{\gamma}$. \[ J_{k}^{t,ml} \] and \[ O_{k,k',o}^{t,ml} \] are given in Eq. III.33. The second overlap terms can be written explicitly as

\[
O_{k,k',i}^{\gamma,ml} \frac{1}{2} \int_{-\infty}^{\infty} dx \frac{\psi_k + b_{\gamma} X_k}{\beta_k + S_k \psi_k + a_k X_k + \sum_{k' \neq k} (S_k A_{k'} \psi_{k'} + B_k X_{k'})} \]

\[
\left[ \frac{\sum_{i} (A_{ik} \psi_i + B_{ik} X_i)}{\beta_k + S_k \psi_k + a_k X_k + \sum_{k' \neq k} (S_k A_{k'} \psi_{k'} + B_k X_{k'})} \right] \]

\[
(III.42)
\]

with \[ O_{k,k',i}^{f,ml} \] as in Eq. III.42 with $b_f$ replacing $b_{\gamma}$, and

\[
O_{k,k',i}^{t,ml} \frac{1}{2} \int_{-\infty}^{\infty} dx \frac{S_k \psi_k + a_k X_k}{\beta_k + S_k \psi_k + a_k X_k + \sum_{k' \neq k} (S_k A_{k'} \psi_{k'} + B_k X_{k'})} \]

\[
\left[ \frac{\sum_{i} (A_{ik} \psi_i + B_{ik} X_i)}{\beta_k + S_k \psi_k + a_k X_k + \sum_{k' \neq k} (S_k A_{k'} \psi_{k'} + B_k X_{k'})} \right] \]

\[
(III.43)
\]

B. Calculation of Isolated Resonance Integrals

Each of the isolated resonance integrals \( J_{i}^{x,\delta,\ell} \), \( J_{i}^{f,\delta,\ell} \), \( J_{k}^{\gamma,ml} \), \( J_{k}^{f,ml} \), and \( J_{k}^{t,ml} \) as given in Eqs. III.23, III.24, III.31, III.32 and III.33 represents a special case of the general resonance integral representation

\[
J(\beta,\theta,a,b) = \frac{1}{2} \int_{-\infty}^{\infty} dx \frac{T\psi + by}{\beta + S\psi + a\chi} \]

\[
(III.44)
\]

In particular for single level resonances $T = S = 1$, and $b = 0$ for capture or fission, and equals $a$ for total. Similarly, for multilevel resonances $b = b_{\gamma}$, $b_f$, or $a$ for capture, fission or total, $T = 1$ for capture and fission, and $T = S$ for total.
Assuming that \( \beta + S\psi + a\chi > 0 \), Equation III.44 can be factored

\[
J(\beta, \theta, a, b) = J(\beta, \theta, 0, 0) + I(\beta, \theta, a) - bM(\beta, \theta, a)
\]  (III.45)

The quantities \( J(\beta, \theta, 0, 0) \), \( I(\beta, \theta, a) \) and \( M(\beta, \theta, a) \) are calculated using the numerical methods described in Section IV of Appendix A involving fixed point Gauss-Jacobi quadrature or asymptotic expressions depending upon the size of \( \beta \).

The user may specify that all resonances for a particular isotope be assigned the infinitely dilute resonance integral limiting value \( n_l(2B) \). In this case, none of the resonances of this isotope will be involved in the calculation of the overlap integrals for any other resonance in the mixture.

C. Calculation of Overlap Integrals

1. Selection of Overlapping Resonances

In the calculation of the various overlap integrals, only those neighboring resonances are included which satisfy the following criterion.

Two "widths" are computed for each resonance \( i \)

\[
W^1_i = \frac{\Gamma_i}{\theta_i} \sqrt{\ln \left[ 2 + \frac{\psi(\theta_i, 0)}{\beta_i} \right]}
\]  (III.49)

and

\[
W^2_i = \frac{\Gamma_i}{2} \sqrt{\frac{\beta_i + 1}{\beta_i}}
\]  (III.50)

where \( \Gamma_i \) is the total line width (or S-matrix total line width for Adler-Adler multilevel resonances) and \( \psi(\theta_i, 0) \) is calculated as in Eq.A.15 of Appendix A. Denoting by \( L_i \) the larger of \( W^1_i \) and \( W^2_i \)

\[
L_i = \max \left[ W^1_i, W^2_i \right]
\]  (III.51)

we include resonance \( i' \) in the overlap integral for resonance \( i \) if
Otherwise resonance $i'$ is ignored.

The code defaults to four neighbors on each side of each resonance as candidates for inclusion in the overlap integrals, but the number of overlap candidates can be specified by the user.

2. Asymptotic Algorithms

The code first evaluates the asymptotic or "large $\beta$" approximations for the various overlap integrals. The integrands of these integrals (Eqs. III.23, III.24, III.31, III.32, III.33, III.36, III.37, III.42 and III.43) consist of products of $\psi$ and $\chi$ functions times a factor of the form

$$\frac{1}{\beta^2 + f}$$

where $f$ represents the energy dependent part of the denominator. If we add and subtract a quantity $\sigma^*$, to be defined below, we can write

$$\frac{1}{\beta^2 + f} = \frac{1}{\beta^2 + \sigma^* - (\sigma^* - f)}$$

$$= \frac{1}{\beta^2 + \sigma^*} \left[ 1 - \frac{1}{\beta^2 + \sigma^*} \left( \frac{\sigma^* - f}{\beta^2 + \sigma^*} \right) \right]$$

$$\approx \frac{1}{\beta^2 + \sigma^*} \left[ 1 + \frac{\sigma^* - f}{\beta^2 + \sigma^*} + \ldots \right]$$

$$\approx \frac{1}{\beta^2 + \sigma^*} + \frac{\sigma^* - f}{(\beta^2 + \sigma^*)^2}$$

(III.54)

As a specific example, consider $O_{i,i',0}^{x,\delta \ell}$ as given in Eq. III.23. Using Eq. III.54 we can write

$$O_{i,i',0}^{x,\delta \ell} \approx \frac{1}{2} \int_{-\infty}^{\infty} dx_i \frac{\sum_{i' \neq i} (A_{i',i,0} + B_{i',i,0})}{\beta_i^2 + \sigma_{i,i',0}^*}$$

$$+ \frac{1}{2} \int_{-\infty}^{\infty} dx_i \left[ \frac{\sigma_{i,i',0}^* - f_{i,i',0}}{\beta_i^2 + \sigma_{i,i',0}^*} \right] \frac{\sum_{i' \neq i} (A_{i,i',0} + B_{i,i',0})}{\left[ \beta_i^2 + \sigma_{i,i',0}^* \right]^2}$$

(III.55)
where
\[ f_{i,i',0} = 2\beta_i (\psi_i + a_i \chi_i) + (\psi_i + a_i \chi_i)^2 + \beta_i \sum_{i \neq i'} (A_i \psi_i + B_i \chi_i) \]
\[ + (\psi_i + a_i \chi_i) \sum_{i \neq i'} (A_i \psi_i + B_i \chi_i) \]
\[ \approx 2\beta_i (\psi_i + a_i \chi_i) + \beta_i \sum_{i \neq i'} (A_i \psi_i + B_i \chi_i). \]  \hspace{1cm} (III.56)

Now if we define
\[ \sigma_{i,i',0} = \frac{\int_{-\infty}^{\infty} dx_i f_{i,i',0} \psi_i \sum_{i \neq i'} (A_i \psi_i + B_i \chi_i)}{\int_{-\infty}^{\infty} dx_i \psi_i \sum_{i \neq i'} (A_i \psi_i + B_i \chi_i)} \] \hspace{1cm} (III.57)

with \( f_{i,i',0} \) given by Eq. III.56, the second order term of Eq. III.55 will vanish and we are left with the approximation
\[ \sigma_{i,i',0} = \frac{1}{2} \int_{-\infty}^{\infty} dx_i e^{\psi_i \sum A_i \psi_i + B_i \chi_i} \beta_i^{2} + \sigma_{i,i',0} \hspace{1cm} \] \hspace{1cm} (III.58)

Similarly, the total overlap integral as given in Eq. III.24 can be written as the sum of two terms
\[ \sigma_{i,i',0} = \sigma_{x}^{2} + \sigma_{y}^{2} \] \hspace{1cm} (III.59)

where \( \sigma_{x}^{2} \) is given in Eq. III.23 and approximated in Eq. III.58 and
\[ \sigma_{y}^{2} \]

Using the same technique as above, we may approximate Eq. III.60 as
\[ \sigma_{i,i',0} = \frac{1}{2} \int_{-\infty}^{\infty} dx_i \frac{a_i \chi_i \sum_{i \neq i'} (A_i \psi_i + B_i \chi_i)}{f_{i,i',0} \beta_i^{2} + \sigma_{i,i',0}^{2}} \] \hspace{1cm} (III.61)
with \( \sigma_{1,i',o}^{**} \) defined as

\[
\sigma_{1,i',o}^{**} = \left[ \int_{-\infty}^{\infty} \text{d}x_i \psi_i \sum_{i'} (A_{i',i} + B_{i',i}) \psi_{i'} \right] \chi_i \chi_{i'}.
\]

This same technique is used to obtain asymptotic expressions for the various other overlap integrals \( \sigma_{k,k',o}^{\gamma,m\ell} \), \( \sigma_{k,k',o}^{\gamma,\lambda \ell} \), etc. where each requires the definition of a corresponding \( \sigma^* \) and \( \sigma^{**} \) appropriate to the specific form of the integrand involved. Note that each of the multilevel overlap integrals, and the single level overlap integral for the total cross section can be written as in Eq. III.58 as the sum of a symmetric term \( OV_1 \) and an antisymmetric term \( OV_2 \).

Once the \( \sigma^* \) and \( \sigma^{**} \) have been evaluated, as described later, the integrals remaining in these asymptotic expressions all involve infinite integrals of products of \( \psi \) and \( \chi \) functions for the resonance being evaluated and for the neighboring resonances included in the overlap calculation. These may be integrated using the following identities:

\[
\int_{-\infty}^{\infty} \text{d}x_i \psi_i \psi_j = \int_{-\infty}^{\infty} \text{d}x_i \psi_i \psi_j
\]

\[
= \pi \frac{\Gamma_i}{\Gamma_i + \Gamma_j} \psi \left[ \frac{E_{i,\gamma} - E_j}{\sqrt{\Delta_i^2 + \Delta_j^2}} \right]
\]

\[
= \pi \frac{\Gamma_i}{\Gamma_i + \Gamma_j} \psi \left[ \theta_{ij}, \chi_{ij} \right]
\]

\[
= \pi \frac{\Gamma_i}{\Gamma_i + \Gamma_j} \psi_{ij}
\]

\[
\int_{-\infty}^{\infty} \text{d}x_i \psi_i \psi_j = 4\pi \frac{\Gamma_i}{\Gamma_i + \Gamma_j} \psi_{ij}
\]

\[
\int_{-\infty}^{\infty} \text{d}x_i \psi_i \chi_j = \pi \frac{\Gamma_i}{\Gamma_i + \Gamma_j} \chi_{ij}
\]

where \( \chi_{ij} \) implies the same notation for \( \chi \) as in the case of Eq. III.63 for \( \psi_{ij} \).
The more compact notation identified in Eq. III.63 is used for Eqs. III.64-III.68.

Making use of Eqs. III.63-III.68 in Eqs. III.58-III.61, and in the analogous integrals for the other cases discussed above, we finally may tabulate the asymptotic overlap integrals as follows.

\[
\begin{align*}
O_{\xi,\delta \ell}^{i,i',0} & \sim \frac{\pi}{2} \sum_{i' \neq i} \frac{\Gamma_{i'}}{\Gamma_{i} + \Gamma_{i'}} (A_{i,i} \chi_{i,i'} + B_{i,i} \chi_{i,i'}) \\
O_{\xi,\delta \ell}^{t,i',0} & = O_{\xi,\delta \ell}^{t,i',0} + \frac{\pi}{2} \sum_{i' \neq i} \frac{\Gamma_{i'}}{\Gamma_{i} + \Gamma_{i'}} (- A_{i,i} \chi_{i,i'} + 4B_{i,i} \chi_{i,i'}) \\
O_{\gamma,ml}^{k,k',0} & \sim \frac{\pi}{2} \sum_{k \neq k'} \frac{\Gamma_{k'}}{\Gamma_{k} + \Gamma_{k'}} (S_{k,k} A_{k,k} \chi_{k,k'} + 4B_{k,k} \chi_{k,k'}) \\
& \quad + \frac{\pi}{2} \sum_{k \neq k'} \frac{\Gamma_{k'}}{\Gamma_{k} + \Gamma_{k'}} (- S_{k,k} A_{k,k} \chi_{k,k'} + 4B_{k,k} \chi_{k,k'}) \\
& = O_{\gamma,ml}^{k,k',0} + O_{\gamma,ml}^{k,k',0}
\end{align*}
\]
\[ O^{x,ml}_{k,k',i} \approx O^{x,ml}_{1,k,k',o} + O^{x,ml}_{2,k,k',o} = O^{x,ml}_{1,k,k',o} + \frac{b_{\gamma_2}}{b_{\gamma_1}} O^{\gamma,ml}_{2,k,k',o} \] (III.72)

\[ O^{t,ml}_{k,k',o} \approx S_k O^{x,ml}_{1,k,k',o} + O^{t,ml}_{2,k,k',o} \]

\[ = S_k O^{x,ml}_{1,k,k',o} + \frac{a_k}{b_{\gamma_1}} O^{\gamma,ml}_{2,k,k',o} \] (III.73)

\[ O^{x,\delta \ell}_{1,1',k} \approx \frac{\sum k_i^{\Gamma_k}}{2 \Gamma_{i+1}} \frac{(S_k A_{ki} \psi_{ik} + B_{ki} \chi_{ik})}{\beta_i^{2+\delta \ell^{*}}_{1,i+1,k}} = O^{x,\delta \ell}_{1,1',k} \] (III.74)

\[ O^{t,\delta \ell}_{1,1',k} = O^{x,\delta \ell}_{1,1',k} + \frac{a_{i} \sum k_i^{\Gamma_k}}{2 \Gamma_{i+1}} \frac{(-S_k A_{ki} \chi_{ik} + 4B_{ki} \psi_{ik})}{\beta_i^{2+\delta \ell^{**}}_{1,i+1,k}} \]

\[ = O^{x,\delta \ell}_{1,1',k} + O^{t,\delta \ell}_{2,1',o} \] (III.75)

\[ O^{\gamma,ml}_{k,k',i} \approx \frac{\sum k_i^{\Gamma_i}}{2 \Gamma_{i+1}} \frac{(A_{ik} \psi_{ki} + B_{ik} \chi_{ki})}{\beta_k^{2+\gamma,ml^{*}_{k,k',i}}} \]

\[ + \frac{\sum k_i^{\Gamma_i}}{2 \Gamma_{i+1}} \frac{(-A_{ik} \chi_{ki} + 4B_{ik} \psi_{ki})}{\beta_k^{2+\gamma,ml^{**}_{k,k',i}}} \]

\[ = O^{x,ml}_{1,k,k',i} + O^{\gamma,ml}_{2,k,k',o} \] (III.76)

\[ O^{f,ml}_{k,k',i} \approx O^{x,ml}_{1,k,k',i} + O^{f,ml}_{2,k,k',i} = O^{x,ml}_{1,k,k',i} + \frac{b_{\gamma_2}}{b_{\gamma_1}} O^{\gamma,ml}_{2,k,k',i} \] (III.77)
In the above, $A_i$ and $B_i$ are defined in Eq. III.5, $A_{ki}$ and $B_{ki}$ are defined in Eq. III.38, and $\psi_{ik}$ and $\chi_{ik}$ are defined by Eq. III.63. Also, we use the indices $i$ and $i'$ to denote single level resonances and $k$ and $k'$ to denote multilevel resonance.

The evaluation of the $\sigma^*$ and $\sigma^{**}$ which appear in Eqs. III.69-III.78 involve infinite integrals of triple products of $\psi$ and $\chi$ functions as can be seen for example by using Eq. III.56 in Eqs. III.57 or III.62. Integrals over triple products of different indices are ignored in this process. That is, for example

\[
\int_{-\infty}^{\infty} \left[ \psi_i \sum_{i' \neq i} A_i, \psi_{i'}, \sum_{i'' \neq i} B_i, \chi_{i''} \right] dx_i
\]

Similarly, the integral

\[
\int_{-\infty}^{\infty} \psi_k \sum_{k' \neq k} S_{k'}, A_{k'}, \psi_{k'} \sum_{i} A_{ik} \psi_i dx_k
\]

will be ignored since it involves the triple index $k$, $k'$, $i$.

As a specific example, we may write out the expression for $\sigma_{i,i',o}^{\Delta \ell^*}$ in detail, with the above approximation, as follows.

\[
\sigma_{i,i',o}^{\Delta \ell^*} \propto \beta_i \int_{-\infty}^{\infty} \psi_i \sum_{i' \neq i} (A_i, \psi_{i'}, + B_i, \chi_i) dx_i
\]

where

\[
0_{k,k',i} \propto S_{k} O_{\gamma,ml} V_{k',i} + \frac{a_k}{b_{\gamma}} O_{\gamma,ml} V_{k',i}.
\]
The denominators in Eq. III.79 and the corresponding expressions for the other $a^*$ and $a^{**}$ are evaluated using Eqs. III.63–III.68. The various integrals of triple products in the numerators are evaluated using the following expressions (25) where we use the notation of Eq. III.63. Also, we use the transformation

\[ \hat{\chi}_k = \frac{1}{2} \chi_k \]  

\[ \int_{-\infty}^{\infty} \psi_k^2 \psi_k^* \chi_k \, dx_k = \sqrt{\frac{\pi}{2}} \frac{\pi}{4} \theta_k \frac{2\Gamma_k'}{k' + i_k'} (I_1 + I_2) \]  

\[ \int_{-\infty}^{\infty} \psi_k^2 \chi_k \, dx_k = \sqrt{\frac{\pi}{2}} \frac{\pi}{4} \theta_k \frac{2\Gamma_k}{k' + i_k'} (I_3 + I_4) \]  

\[ \int_{-\infty}^{\infty} \chi_k^2 \psi_k \, dx_k = \sqrt{\frac{\pi}{2}} \frac{\pi}{4} \theta_k \frac{2\Gamma_k'}{k' + i_k'} (I_1 - I_2) \]  

\[ \int_{-\infty}^{\infty} \chi_k^2 \chi_k \psi_k \, dx_k = \sqrt{\frac{\pi}{2}} \frac{\pi}{4} \theta_k \frac{2\Gamma_k}{k' + i_k'} (I_3 - I_4) \]  

\[ \int_{-\infty}^{\infty} \hat{\chi}_k \hat{x_k} \psi_k \, dx_k = \sqrt{\frac{\pi}{2}} \frac{\pi}{4} \theta_k \frac{2\Gamma_k'}{k' + i_k'} I_2 \]  

\[ \int_{-\infty}^{\infty} \chi_k \psi_k \psi_k \, dx_k = -\sqrt{\frac{\pi}{2}} \frac{\pi}{4} \theta_k \frac{2\Gamma_k'}{k' + i_k'} I_4. \]

The quantities $I_1$ through $I_4$ are given by (25)

\[ I_1 = A_4 \left[ A_5 \psi_k^1 - A_7 \frac{\partial \hat{\chi}_k^1}{\partial x_k^1} - A_8 \frac{3}{2} \psi_k^1 + A_9 \frac{2}{3} \frac{3}{3} \hat{\chi}_k^1 \right] \]  

\[ I_2 = \frac{2}{\sqrt{\pi}} A_3 \left[ \frac{\partial \hat{\chi}_k^1}{\partial x_k^1} - \frac{2}{3} A_2 \frac{3}{3} \hat{\chi}_k^1 \right]. \]
\[
I_3 = A_4 \left[ A_5 \hat{\chi}_{kk} + A_7 \frac{\partial \psi_{kk}}{\partial x_{kk}} - A_8 \frac{\partial^2 \hat{\chi}_{kk}}{\partial x_{kk}^2} - A_9 \frac{\partial^3 \psi_{kk}}{\partial x_{kk}^3} \right] \tag{III.90}
\]
\[
I_4 = -\frac{2}{\sqrt{\pi}} A_3 \left[ \frac{\partial \psi_{kk}}{\partial x_{kk}} - \frac{2}{3} \frac{\partial^3 \psi_{kk}}{\partial x_{kk}^3} \right] \tag{III.91}
\]
where
\[
\frac{\partial \psi_{kk}}{\partial x_{kk}} = \frac{\theta^2_{kk}}{2} \left[ \hat{\chi}_{kk} - x_{kk} \psi_{kk} \right] \tag{III.92}
\]
\[
\frac{\partial \hat{\chi}_{kk}}{\partial x_{kk}} = \frac{\theta^2_{kk}}{2} \left[ 1 - x_{kk} \hat{\chi}_{kk} - \psi_{kk} \right] \tag{III.93}
\]
\[
\frac{\partial^2 \hat{\chi}_{kk}}{\partial x_{kk}^2} = -\frac{\theta^2_{kk}}{2} \left[ \hat{\chi}_{kk} + x_{kk} \frac{\partial \hat{\chi}_{kk}}{\partial x_{kk}} + \frac{\partial \psi_{kk}}{\partial x_{kk}} \right] \tag{III.94}
\]
\[
\frac{\partial^2 \psi_{kk}}{\partial x_{kk}^2} = \frac{\theta^2_{kk}}{2} \left[ \frac{\partial \hat{\chi}_{kk}}{\partial x_{kk}^2} - \psi_{kk} - x_{kk} \frac{\partial \psi_{kk}}{\partial x_{kk}} \right] \tag{III.95}
\]
\[
\frac{\partial^3 \psi_{kk}}{\partial x_{kk}^3} = \frac{\theta^2_{kk}}{2} \left[ \frac{\partial^2 \hat{\chi}_{kk}}{\partial x_{kk}^2} - 2 \frac{\partial \psi_{kk}}{\partial x_{kk}} - x_{kk} \frac{\partial^2 \psi_{kk}}{\partial x_{kk}^2} \right] \tag{III.96}
\]
\[
\frac{\partial^3 \hat{\chi}_{kk}}{\partial x_{kk}^3} = -\frac{\theta^2_{kk}}{2} \left[ 2 \frac{\partial \hat{\chi}_{kk}}{\partial x_{kk}^2} + x_{kk} \frac{\partial \hat{\chi}_{kk}}{\partial x_{kk}^2} + \frac{\partial^2 \psi_{kk}}{\partial x_{kk}^2} \right] \tag{III.97}
\]
and the coefficients \( A_3 \) through \( A_9 \) depend upon the size of \( \theta_k \).

For \( \theta_k \leq 5.5 \sqrt{2} \)

use is made of the rational approximation
\[
\exp^2 \text{erf}(t) = \sum_{i=1}^{3} \frac{a_i}{1 + pt}
\]
with, \( a_1 = 0.3480242; a_2 = -0.0958798; a_3 = 0.7478556; p = 0.47047 \) and
\[
A_3 = \frac{\Gamma_k}{\Theta_k \sqrt{2 (\Gamma_k + \Theta_k)}} \tag{III.98}
\]
\[ A_4 = \frac{1}{p\theta_k} \left( 1 + \frac{\sqrt{2}}{\sqrt{\pi\theta_k}} \right) \]  
\[ \text{(III.99)} \]

\[ A_5 = a_1 + a_2 A_4 + a_3 A_4^2 \]  
\[ \text{(III.100)} \]

\[ A_6 = pA_3 \]  
\[ \text{(III.101)} \]

\[ A_7 = A_4 A_6 (a_1 + 2a_2 A_4 + 3a_3 A_4^2) \]  
\[ \text{(III.102)} \]

\[ A_8 = (A_4 A_6)^2 (a_1 + 3a_2 A_4 + 6a_3 A_4^2) \]  
\[ \text{(III.103)} \]

\[ A_9 = (A_4 A_6)^3 (a_1 + 4a_2 A_4 + 10a_3 A_4^2). \]  
\[ \text{(III.104)} \]

For \( \theta_k > 5.5 \sqrt{2} \):

\[ \frac{\Gamma_k}{\sqrt{2} (\Gamma_k + \Gamma_{k'})}, \text{ as before} \]

\[ A_4 = \frac{1}{\sqrt{\pi} \theta_k} \left( 1 - \left[ 1 - \frac{3\sqrt{2}}{2\theta_k} \right]/\theta_k \right) \]  
\[ \text{(III.105)} \]

\[ A_5 = 1 \]  
\[ \text{(III.106)} \]

\[ A_6 = A_3 \]  
\[ \text{(III.107)} \]

\[ A_7 = \frac{\sqrt{2}}{\theta_k} A_6 \]  
\[ \text{(III.108)} \]

\[ A_8 = A_7^2 \]  
\[ \text{(III.109)} \]

Note that the expression for \( A_4 \) when \( \theta_k > 5.5 \sqrt{2} \) and the break point \( 5.5 \sqrt{2} \) both differ from the values reported in Hwang's original work (c.f. Eq. B.22 of Ref.25). The values used in the code reflect the results of numerical studies aimed at optimizing execution efficiency and minimizing errors in the calculated results.

Now in the evaluation of the quantities \( I_1 \) through \( I_4 \), the \( \psi_{kk'} \) and \( \chi_{kk'} \), as in other parts of MC^2-2 are normally evaluated as described in Section III of Appendix A by a bivariate interpolation in pre-stored tables.

However, if \( |x_{kk',\theta_{kk'}}/2| > 12 \) or \( \theta_{kk',}/2 > 12 \), where \( x_{kk'} \) and \( \theta_{kk'} \) are defined in Eq. III.63, then the following asymptotic expressions are used for \( \psi_{kk'}, \chi_{kk'} \), and their second derivatives.
After computing the asymptotic approximations to the overlap integrals, Eqs. III.69-III.78, the code tests whether these results are adequate or rather if the calculations should be performed using Gauss-Jacobi quadrature and if so, how many quadrature points should be used. The logic used in these tests is shown in Fig. 4. Note that the selection criteria depend upon the ratios of $\beta^2/\alpha^*$, $\beta^2/\alpha^{**}$, and $|\Omega V_2/\Omega V_1|$ for the particular overlap integral being evaluated.

The Gauss-Jacobi quadrature algorithms are described below.

3. Gauss-Jacobi Quadrature Algorithms

The various overlap integrals given in Eqs. III.23, III.24, III.31, III.32, III.33, III.36, III.37, III.42, and III.43 are evaluated using 13, 33, or 61 fixed point Gauss-Jacobi quadrature determined as indicated in Fig. 4.

Since the variable of integration is $x_i$, other resonances such as $i'$ have their $x_i$ transformed as

$$x_i' = \frac{E - E_{0i}'}{\Gamma_{i'}} = \frac{\frac{E - E_{0i}}{\Gamma_i} + \frac{E_{0i}'}{\Gamma_{i'}} - E_{0i}'}{\frac{\Gamma_i}{2}}$$

$$= \frac{x_i}{\Gamma_i} + \frac{E_{0i} - E_{0i}'}{\frac{\Gamma_i'}{2}}$$

The variable of integration is transformed as in the case of the Gauss-Jacobi quadrature for the isolated resonance integrals as described in Section IV of Appendix A. Now, however, since the integration ranges from $-\infty$ to $\infty$, all N Gauss-Jacobi points are used. Also, as discussed in Ref. 25, after transforming the variable of integration as in Eq.A.17 of Appendix A, $a_i/\beta_i$
Fig. 4. Gauss-Jacobi Quadrature Point Selection
is subtracted from the result to provide a better distribution of quadrature abscissae over the distribution of the integrands involved, which are peaked to the left of the origin.

After completing the integrations as indicated above, the asymmetric parts of the multilevel resonance overlap integrals, or of the total overlap integral for single level resonances, may be recomputed depending upon the testing described below.

As a specific example, we rewrite the asymmetric part of the total overlap integral for the case of all single level resonances, Eq.III.60, as

\[
O_{2i,i',0}^{t,\delta \ell} = \frac{1}{2} \sum_{i' \neq i} \int_{-\infty}^{\infty} dx_i \frac{a_i x_i}{\beta_i + \psi_i + a_i x_i} \cdot \frac{A_{i',\psi_{i',0}^{t,\delta \ell}} + B_{i',\chi_i}}{\beta_i + \psi_i + a_i x_i + \sum_{i' \neq i} (A_{i',\psi_{i',0}^{t,\delta \ell}} + B_{i',\chi_i})}
\]

The quantity

\[
SEPTST = \frac{|E_{o_i}^{t} - E_{o_{i'}}^{t}|}{L_i + L_{i'}}
\]  

is computed for each term of the sum in Eq.III.115, where \(L_i\) and \(L_{i'}\) are obtained as indicated in Eqs. 49-51. If \(SEPTST < 2.5\), the value obtained for the Gauss-Jacobi integration of Eq.III.115 for that \(i'\) is used.

However, if \(SEPTST > 2.5\), a special integration procedure described below is used to re-evaluate that term of the sum.

By algebraic manipulation, each term of Eq.III.115 can be written as the sum of two integrals

\[
O_{2i,i',0}^{t,\delta \ell} = \sum_{i' \neq i} \left[ S_{2i,i',0}^{t,\delta \ell} - S_{1i,i',0}^{t,\delta \ell} \right]
\]

where

\[
S_{2i,i',0}^{t,\delta \ell} = \frac{1}{2} \int_{-\infty}^{\infty} dx_i \frac{a_i x_i}{\beta_i} \cdot \frac{A_{i',\psi_{i',0}^{t,\delta \ell}} + B_{i',\chi_i}}{\beta_i + \sum_{i' \neq i} (A_{i',\psi_{i',0}^{t,\delta \ell}} + B_{i',\chi_i})}
\]  

and
$s_{i,i',o} = \frac{1}{2} \int_{-\infty}^{\infty} dx_i \frac{a_i x_i (\psi_i + a_i x_i) (A_i, \psi_i, + B_i, x_i)}{\beta_i \left[ \beta_i + \psi_i + a_i x_i + \sum_{i', \neq i} (A_{i'}, \psi_{i'}, + B_{i'}, x_{i'}) \right]}.

2 \frac{\beta_i + \psi_i + a_i x_i + \sum_{i', \neq i} (A_{i'}, \psi_{i'}, + B_{i'}, x_{i'})}{\beta_i + \psi_i + a_i x_i}

\left[ \beta_i + \psi_i + a_i x_i + \sum_{i', \neq i} (A_{i'}, \psi_{i'}, + B_{i'}, x_{i'}) \right] \right]. \tag{III.119}

For $F_{i,i',o}^{t,\delta \ell}$, an asymptotic algorithm similar to that described in Section C.2 is first tried. That is, we approximate $F_{i,i',o}^{t,\delta \ell}$ as

$F_{i,i',o}^{t,\delta \ell} \approx \frac{1}{2} \int_{-\infty}^{\infty} dx_i \frac{a_i x_i \left[ A_i, \psi_i, + B_i, x_i \right]}{\beta_i + \delta \ell^{***}} \tag{III.120}

where

$\delta \ell^{***} = \int_{-\infty}^{\infty} dx_i \frac{x_i \left[ A_i, \psi_i, + B_i, x_i \right]}{\beta_i + \delta \ell^{***}} \int_{-\infty}^{\infty} dx_i \frac{x_i \left[ A_i, \psi_i, + B_i, x_i \right]}{\beta_i + \delta \ell^{***}}. \tag{III.121}

Products of triple indices are ignored in Eq.III.121 and Eq.III.120 is evaluated using Eq.III.121 and the various Eqs.III.63-III.68 and Eqs.III.82-III.108 as for the case of the earlier $\sigma^*$ and $\sigma^{**}$.

A criterion $T_4$ is then evaluated, namely

$T_4 = \frac{\beta_i^2}{\delta \ell^{***}} \tag{III.122}$

If $T_4 > 0.6$ or if $T < -3.0$ the asymptotic expression above is used for $F_{i,i',o}^{t,\delta \ell}$. However, if not, the criterion $T_5$ is evaluated as

$T_5 = \frac{L_i}{L_{i'}} \tag{III.123}$

If $SEPTST \leq 3.5$ and $T_5 \geq 1.0$, then the code reverts to the use of the original Gauss-Jacobi quadrature of Eq.III.115. However, if not, then $F_{i,i',o}^{t,\delta \ell}$ is finally approximated by
This procedure is similarly used on all the other overlap integrals having an asymmetric part, that is a part proportional to $\chi$. 

\[ F_{i,i',0} = \frac{a_i}{2 \beta_i} \cdot \left\{ \begin{array}{c} E_{i'1} - E_{i1} \end{array} \right\} \cdot \int_{-\infty}^{\infty} dx_i \frac{\lambda_i \psi_i + B_i \chi_i}{\beta_i + \lambda_i \psi_i + B_i \chi_i} \]

\[ = \frac{1}{2 \beta_i} \cdot \left\{ \begin{array}{c} E_{i'1} - E_{i1} \end{array} \right\} \cdot \int_{-\infty}^{\infty} dx_i \frac{\psi_i + a_i \chi_i}{\beta_i + \psi_i + a_i \chi_i} \]

\[ = \frac{a_i}{\beta_i} \cdot \left\{ \begin{array}{c} E_{i'1} - E_{i1} \end{array} \right\} \cdot \frac{1}{\Gamma_i} J(\beta_i, \theta_i, a_i, a_i). \] (III.124)
IV. CALCULATION OF UNRESOLVED RESONANCE INTEGRALS

A. General Formulation

The algorithms involved in the unresolved resonance integral calculation developed by R. Hwang assume the narrow resonance approximation and account for interference scattering, the effects of accidental overlap with resonances in other spin sequences, and the effects of self-overlap with resonances of the same spin sequence. The single level Breit-Wigner representation is used for the resonance cross sections.

The effective macroscopic capture cross section for material \( m \) within an arbitrary energy interval \( E_2 - E_1 \) can be written as

\[
\bar{\Sigma}_c^{m}(E^*) = \frac{1}{E_2 - E_1} \int_{E_1}^{E_2} \frac{N^m \sigma_c^{m}(E) dE}{\Sigma_t(E)}
\]

where \( E^* \) is an energy point within the interval \( E_2 - E_1 \). Eq. IV.1 is equivalent to Eq. III.1. \( N^m \) is the atom density of material \( m \), \( \sigma_c^{m} \) is the microscopic capture cross section for material \( m \), \( \Sigma_t \) is the total macroscopic cross section for the mixture, and as in the case of the resolved resonance integral calculations we assume that the narrow resonance approximation is valid. In order to satisfy the statistical criteria described below we assume no significant attenuation of flux in the energy interval \( E_2 - E_1 \) and a constant collision density.

\( \sigma_c^{m} \) and \( \Sigma_t \) correspond to sums over contributing resonances belonging to various spin sequences, that is, resonances having a particular angular momentum and channel spin. If we separate the total cross section in Eq. IV.1 into a resonant part \( \Sigma_r(E) \) and a remaining non-resonant part \( \Sigma_p \), we can rewrite Eq. IV.1 as

\[
\bar{\Sigma}_c^{m}(E^*) = \frac{1}{E_2 - E_1} \int_{E_1}^{E_2} \frac{N^m \sum_{si} \sigma_c^{m}(E) dE}{\sum_{msi} \sum_{ri} \Sigma_r^{m}(E) + \Sigma_p}
\]

In Eq. IV.2, \( s \) represents a particular spin sequence and \( i \) represents the resonances in that sequence. The sums in the numerator of the upper integral ranges only over those sequences belonging to material \( m \) while the other sums are over all materials.
Now the interval $E_2 - E_1$ may be replaced by the average spacing of the resonances of the particular sequence being considered, $\langle D \rangle$, times the number of resonances contained within the interval, $N_s$. Also, on the assumption that a large number of resonances exist in the interval, we may replace $\frac{1}{N_s} \sum_i f(\Gamma_n^i)$ by an integration over the chi-squared distribution with $\mu$ degrees of freedom as indicated in Eq. A.30 of Appendix A. This latter step corresponds to providing a statistical average over the distribution functions of the resonance parameters. Thus, as an example, we may write

$$\lim_{\Delta E \to \infty} \frac{1}{\Delta E} \sum_i f(\Gamma_n^i) = \frac{1}{\langle D \rangle} \int_0^\infty P_\mu(x)f(x\Gamma_n(E^*))dx = \frac{1}{\langle D \rangle} \langle x \rangle_{E^*} \quad (IV.3)$$

where $x$ corresponds to the ratio of neutron width at energy $E$ to mean neutron width at $E^*$, $\Gamma_n(E^*)$ is the mean neutron width at energy $E^*$, and $\mu$ is the number of entrance channels for neutrons of the particular spin sequence under consideration. $P_\mu$ is the chi-squared distribution of order $\mu$ given in Eq. A.31 of Appendix A. The fission width would be similarly averaged with perhaps a different number of exit channels as appropriate to the data involved. The angular brackets $\langle \rangle$ will be used to designate the expectation value due to the statistical integration.

The mean neutron width at $E^*$ for neutrons of angular momentum $\ell$ and total channel spin $J$ is given by

$$\Gamma_n(E^*)_{\ell,J} = \frac{\Gamma^0_n(E^*)_{\ell,J} \sqrt{E^*}}{V_\ell R, J} \quad (IV.4)$$

where $\Gamma^0_n(E^*)_{\ell,J}$ is the reduced neutron width at energy $E^*$, $V_\ell$ is the penetration factor for neutrons of angular momentum $\ell$, and $\mu_{\ell,J}$ is the number of entrance channels for neutrons of the $\ell,J$ sequence.

$$V_o = 1$$

$$V_1 = \frac{n^2}{1 + n^2}$$

$$V_2 = \frac{n^4}{9 + 3n^2 + n^4} \quad (IV.5)$$

$$n = \frac{R}{\lambda^*}$$

where $R$ is the channel radius and $\lambda^*$ is the reduced neutron wavelength at energy $E^*$. 
Resonances in different spin sequences are assumed to be completely uncorrelated whereas resonances in a given spin sequence are assumed to be distributed according to the Dyson two-level correlation function

\[ \Omega(y) = 1 - (\xi(y))^2 + \frac{\delta \xi(y)}{y} \sin(y) \]  

(IV.6)

where

\[ y = \frac{\pi |E_{o_k} - E_{o_k'}|}{\langle D \rangle} \]  

(IV.7)

\[ \xi(y) = \frac{\sin|y|}{y} \]  

(IV.8)

\[ \sin(y) = -\int_0^\infty \frac{\sin t}{t} \, dt \]  

(IV.9)

Eqs. III.3 and III.4 express the resolved resonance capture and total cross sections in terms of the symmetric and antisymmetric Doppler broadened line shapes \( \psi \) and \( \chi \). Eq. III.3 is still appropriate for the unresolved region but the low energy limit form of Eq. III.4 must be rewritten for use here as

\[ \sigma = \cos^2 \delta \left[ \frac{\sigma}{\cos^2 \delta} \frac{\sigma}{\chi} + \sigma \frac{\psi}{\psi} + \sigma_a \frac{a}{\chi} \right] \]  

(IV.10)

where \( \delta \) is the phase angle for angular momentum \( L \) given by

\[ \delta_0 = m \]

\[ \delta_1 = m - \arctan m \]

\[ \delta_2 = m - \arctan \left( \frac{3m}{3 - m^2} \right) \]  

(IV.11)

\[ m = \frac{R}{\lambda^*} \]

R is the effective scattering radius and \( \lambda^* \) is the reduced neutron wavelength at energy \( E^* \). \( \psi \) and \( \chi \) are the usual shorthand notation for \( \psi(\theta, \chi) \) and \( \chi(\theta, \chi) \).

In Eq. IV.10, the interference factor \( a \) is given by

\[ a = \frac{1}{2} \tan(2\delta) \]  

(IV.12)
If we express Eq. IV.2 in terms of the $\psi$ and $\chi$ functions, perform the statistical average over the distribution functions for the resonance parameters, and factor the resulting equation in a manner typified by Eq. III.23, we may finally write for the expectation value for a given spin sequence

$$\frac{\cos 2\delta}{\langle D_k \rangle} \left( \sum_{i \neq k}^{\gamma_k} \left( \langle D_k \rangle \langle \gamma_{i} J(\beta_i, \theta_i, a_i, 0) \rangle - O_{\gamma_i} \right) \right) \cdot S + \sum_{i \neq k}^{\gamma_k} r_{\gamma_{ki}}. \quad (IV.13)$$

In Eq. IV.13, $J$ is defined in Eqs. III.44-III.48 and $\beta_k$ is defined as in Eq. III.5 except divided by $\cos 2\delta$. $S$ represents the first-order correction for the accidental overlap with the uncorrelated resonances in spin sequences $i \neq k$ given by

$$S = 1 - \sum_{i \neq k}^{\gamma_k} \left[ \frac{1}{\langle D_i \rangle} \left( \langle \gamma_{i} J(\beta_i, \theta_i, a_i, 1) \rangle - O_{\gamma_i} \right) \right]. \quad (IV.14)$$

The $r_{\gamma_{ki}}$ represent the higher order corrections for the accidental overlap effect which, to second order is approximately given by

$$r_{\gamma_{ki}} \approx \left( \langle \gamma_{k} \rangle \langle D_k \rangle \frac{1}{\langle D_i \rangle} \left( \langle \gamma_{i} J(\beta_i, \theta_i, a_i, 1) \rangle - O_{\gamma_i} \right) \right). \quad (IV.15)$$

$$\langle \gamma_{k} \rangle = \left( \frac{\gamma_{k}}{2\beta_k} \int_{-\infty}^{\infty} \frac{\psi^2(\theta_k, x_k) dx_k}{\beta_k + \psi(\theta_k, x_k)} \right). \quad (IV.16)$$

$MC^2 - 2$ assumes that $r_{\gamma_{ki}}$ in Eq. IV.13 is negligible.

$O_{\gamma_k}$ represents the capture self-overlap term for resonances of the same spin sequence $k$ and is approximated by

$$O_{\gamma_k} \approx \frac{1}{\langle D_k \rangle} \left( \langle \gamma_{k} \rangle \frac{1}{2} \int_{-\infty}^{\infty} \frac{\psi_k (0, x_k) dx_k}{\beta_k + \psi_k} \right). \quad (IV.17)$$

In Eq. IV.17 the resonances $k$ and $k'$ all belong to the same spin sequence $k$. $\Omega(\delta)$ is the probability of finding a resonance $k'$ at a distance $\delta = E_{k'} - E_{k}$ from a given resonance $k$ as given in Eq. IV.6, $\psi_k$ is a shorthand notation referring to $\psi(\theta_k, x_k)$, and $A_k$ is defined in Eq. III.5. Note that the contribution from the asymmetric line shape function $\chi$ is ignored for the self-overlap calculation. $O_{\gamma_i}$ in Eq. IV.14 is given by Eq. IV.17 where $\Gamma_{\gamma_{ki}}$ replaces $\Gamma_{\gamma_{ki}}$. $t_1$ replaces $t_1$.
In deriving Eq.IV.13, it has been explicitly assumed that products of more than two $\psi$ or $\chi$ functions can be neglected. This is the so-called "nearest neighbor" approximation.\textsuperscript{28} As a simple example, consider

\[
\frac{\sigma^1}{\sigma^1 + \sigma^2 + \sigma^3 + \sigma_p} = \frac{\sigma_1^2}{\sigma^1 + \sigma} \quad \frac{\sigma^1}{\sigma^1 + \sigma_p} \quad \frac{\sigma^1}{\sigma^1 + \sigma} \quad \frac{\sigma^2 + \sigma^3}{\sigma^1 + \sigma^2 + \sigma^3 + \sigma_p}
\]

\[
= \frac{\sigma^1}{\sigma^1 + \sigma} - \frac{\sigma^1}{\sigma^1 + \sigma_p} \left( \frac{\sigma^2}{\sigma^1 + \sigma} - \frac{\sigma^2}{\sigma^2 + \sigma_p} \right) \quad \frac{\sigma^1}{\sigma^1 + \sigma} \quad \frac{\sigma^2 + \sigma^3}{\sigma^1 + \sigma^2 + \sigma^3 + \sigma_p}
\]

\[
\approx \frac{\sigma^1}{\sigma^1 + \sigma} \left( 1 - \frac{\sigma^2}{\sigma^1 + \sigma_p} - \frac{\sigma^3}{\sigma^1 + \sigma_p} \right)
\]

We shall also later use the fact that Eq.IV.18 can be approximated by

\[
\frac{\sigma^1}{\sigma^1 + \sigma^2 + \sigma^3 + \sigma_p} \approx \frac{\sigma^1}{\sigma^1 + \sigma} \left( 1 - \frac{\sigma^2}{\sigma^1 + \sigma_p} \right) \quad \frac{\sigma^1}{\sigma^1 + \sigma} \quad \frac{\sigma^2 + \sigma^3}{\sigma^1 + \sigma^2 + \sigma^3 + \sigma_p}
\]

where again we have neglected triple products. Eq.IV.19 makes use of the general first order approximation

\[
1 - \sum \bar{B}_i \approx \prod_i (1 - B_i)
\]

The expression corresponding to Eq.IV.13 for fission simply requires replacing $\Gamma_\gamma$ with $\Gamma_f$, so that $0_f$, $r_f$, and $\langle \tau_f \rangle$ become respectively $0_f$, $r_f$, and $\langle \tau_f \rangle$. In the case of the total reaction, $\Gamma_f$ replaces $\Gamma_k$, and $J(\theta_k, \phi_k, a_k, \alpha_k)$ is used in Eq.IV.13. Also, in this case the factor $\cos^2 \beta_k$ does not appear in Eq.IV.13.

Since the $J$ integrals and other related integrals can be readily evaluated as described in Section B of Chapter III with the statistical averaging accomplished as specified in Section V Appendix A, the main computational effort is related to the evaluation of the self-overlap integrals.
As in the case of the resolved resonances, Eq.IV.13 is evaluated for a homogeneous mixture, and for heterogeneous slab geometries or cylindrical geometries with the value used for $\Sigma_p$ and hence for $\beta$ determined as specified in Eqs.III.16-III.20.

B. Evaluation of the Self-Overlap Term

In order to evaluate Eq.IV.17, we note that

$$\int_{-\infty}^{\infty} \frac{\psi_k}{\beta_k + \psi_k} \frac{A_k \psi_k'}{\beta_k' + \psi_k'} dx_k =$$

$$\int_{-\infty}^{\infty} \frac{\psi_k}{\beta_k + \psi_k} \left\{ \frac{\psi_k'}{\beta_k' + \psi_k'} - \frac{A_k \psi_k \psi_k'}{(\beta_k' + \psi_k')^2} + \ldots \right\}$$  \hspace{1cm} (IV.21)

provided the resulting integrals are uniformly convergent. In Eq.IV.21, $A_k = 1/A_k'$. Substituting Eq.IV.21 into Eq.IV.17, Hwang has shown\textsuperscript{25} that

$$O_{k} = K_1 - K_2 + \ldots$$  \hspace{1cm} (IV.22)

where $K_1 >> K_2$ if the self-shielding effect is relatively weak.

$$K_1 = \frac{1}{\langle D_k \rangle} \left\langle \Gamma_{k} \right\rangle \left\langle J_{k} \right\rangle - L_1$$  \hspace{1cm} (IV.23)

$$L_1 = \frac{1}{\langle D_k \rangle} \int_{-\infty}^{\infty} W\left(\frac{\delta}{\langle D_k \rangle}\right) \frac{d\delta}{\langle D_k \rangle} \cdot \left\langle \frac{\Gamma_{k}}{2} \frac{\psi_k}{\beta_k + \psi_k} \right\rangle \left\langle \frac{\psi_k'}{\beta_k' + \psi_k'} \right\rangle dx_k$$  \hspace{1cm} (IV.24)

$$K_2 = -r_{\gamma_{kk}'} - L_2$$  \hspace{1cm} (IV.25)

where $r_{\gamma_{kk}'}$ is given by Eqs.IV.15 and IV.16 and

$$L_2 = -\frac{1}{\langle D_k \rangle} \int_{-\infty}^{\infty} W\left(\frac{\delta}{\langle D_k \rangle}\right) \frac{d\delta}{\langle D_k \rangle} \int_{-\infty}^{\infty} \left\langle \frac{\Gamma_{k}}{2} \frac{\psi_k^2}{\beta_k (\beta_k + \psi_k)} \right\rangle \left\langle \frac{\psi_k'}{\beta_k' (\beta_k' + \psi_k')} \right\rangle dx_k$$  \hspace{1cm} (IV.26)
In Eq. IV.24 and IV.25

\[ \Omega \left( \frac{\delta}{\langle D_k \rangle} \right) = 1 - \Omega \left( \frac{\delta}{\langle D_k \rangle} \right) \]  \hspace{1cm} (IV.27)

and in Eq. IV.26

\[ \frac{\partial}{\partial \beta_k} \left( \frac{\psi_k}{\beta_k + \psi_k} \right) = \frac{\psi_k}{(\beta_k + \psi_k)^2} \]  \hspace{1cm} (IV.28)

The computational effort now is centered on the evaluation of the term \( L_1 \) since \( L_2 \) can easily be obtained once \( L_1 \) is known.

1. Evaluation of \( L_1 \)

Using the Fourier transform technique, Hwang has shown that Eq. IV.24 can be written in the form

\[ L_1 = \frac{1}{2 \langle D_k \rangle} \int_{-\infty}^{\infty} \sqrt{2\pi} \omega(\xi) \left\langle \Gamma_{t_k^1} \left( \frac{\Gamma_{t_k^2}}{2} \xi \right) \right\rangle_k \]

\[ \cdot \left\langle \Gamma_{t_k^1} \left( \frac{\Gamma_{t_k^2}}{2} \right) P_k \left( \frac{\Gamma_{t_k^2}}{2} \xi \right) \right\rangle_k d\xi \]  \hspace{1cm} (IV.29)

where \( P_k \) is the Fourier transform

\[ P_k(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{\psi_k \exp(i\xi x_k)}{\beta_k + \psi_k} dx_k = F \left\{ \frac{\psi_k}{\beta_k + \psi_k} \right\} \]  \hspace{1cm} (IV.30)

and \( \omega(\xi) \), the Fourier transform of the Dyson function, is given

\[ \omega(\xi) = \frac{\langle D_k \rangle}{\sqrt{2\pi}} \left\{ 1 - \left| \frac{\langle D_k \rangle \xi}{\pi} \right| + \left| \frac{\langle D_k \rangle \xi}{2\pi} \right| \ln \left[ 1 + \left| \frac{\langle D_k \rangle \xi}{\pi} \right| \right] \right\}; \]

\[ \left| \frac{\langle D_k \rangle \xi}{2\pi} \right| \leq 1 \]

\[ = \frac{\langle D_k \rangle}{\sqrt{2\pi}} \left\{ -1 + \left| \frac{\langle D_k \rangle \xi}{2\pi} \right| \ln \left[ \left| \frac{\langle D_k \rangle \xi}{\pi} \right| + 1 \right] \right\}; \]

\[ \left| \frac{\langle D_k \rangle \xi}{2\pi} \right| > 1 \]  \hspace{1cm} (IV.31)
As usual, in Eq. IV.29 the quantities inside the angular brackets are the statistically averaged values over the appropriate chi-squared distribution functions of the resonance parameters, and the resonances \( k \) and \( k' \) belong to the same spin sequence.

Now we make a change of variable to convert Eq. IV.29 into a form amenable to Gauss-Hermite quadrature. If we let

\[
\eta = \alpha \xi
\]

\[
\alpha = \sqrt{\frac{\langle D_k \rangle}{\pi}} + \frac{\Delta^2}{2} + \gamma^2
\]

\[
\gamma = \left\langle \frac{\beta_k + 1}{\beta_k} \right\rangle
\]

and multiplying the integral in Eq. IV.29 by \( \exp(-\eta^2) \cdot \exp(\eta^2) \), Eq. IV.29 can be converted into the equivalent form

\[
L_1 = \frac{1}{2 \langle D_k \rangle^2} \frac{1}{\alpha} \int_{-\infty}^{\infty} e^{-\eta^2} \left\{ \sqrt{2\pi} \omega \left( \frac{\eta}{\alpha} \right) \left\langle \frac{\Delta^2 \eta^2}{4\alpha^2} \right\rangle_p \left( \frac{\Gamma_{t_k} \eta}{2\alpha} \right) \right\}_k
\]

\[
\cdot \left\langle \frac{\Gamma_{t_{k'}}}{2} \right\rangle_p \left( \frac{\Gamma_{t_k} \eta}{2\alpha} \right) \left\langle \frac{\langle D_k \rangle^2 \gamma^2}{\pi^2 \alpha^2 + \gamma^2} \right\rangle \eta^2 \right\} \frac{d\eta}{\alpha} \quad \text{(IV.33)}
\]

Eq. IV.33 is of the form

\[
\int_{-\infty}^{\infty} e^{-y^2} f(y) dy = \sum_{i=1}^{N} a_i f(y_i) + R_N \quad \text{(IV.34)}
\]

where \( a_i \) and \( y_i \) are the weights and zeros of the Hermite polynomial and Eq. IV.34 corresponds to the usual Gauss-Hermite quadrature with the remainder term \( R_N \). Since \( p_k \) and \( \omega \) are each symmetric, only a sum over the positive zeros \( y_i \) is required to evaluate Eq. IV.33. The code uses \( N = 10 \) for the quadrature. Specifically, with \( N = 10 \) we assume

\[
L_1 = \frac{1}{2 \langle D_k \rangle^2} \frac{2}{\alpha} \sum_{i=1}^{N/2} a_i \sqrt{2\pi} \omega \left( \frac{\eta_i}{\alpha} \right) \left\langle \frac{\Gamma_{t_k} \eta_i}{4\alpha^2} \right\rangle_p \left( \frac{\Gamma_{t_k} \eta_i}{2\alpha} \right) \right\}_k
\]
The evaluation of Eq. IV.35 depends upon the availability of the Fourier transforms $P_k(\Gamma, \xi/2)$. Two algorithms are used depending upon the size of $\beta_k$ relative to $\psi(\theta_k, 0)$. The large $\beta$ approximation or asymptotic algorithms provide significant computational economy as compared with the non-asymptotic algorithms. Since $\beta_k$ is usually large compared to $\psi(\theta_k, 0)$ for many of the unresolved resonances, the large $\beta$ approximation is frequently invoked for realistic problems with subsequent savings in execution time.

a. **Asymptotic Algorithms for $L_1$**

If $(\beta_k + \psi(\theta_k, 0))/\psi(\theta_k, 0) \geq 2.5$, $P_k$ may be approximated by

$$P_k\left(\frac{\Gamma t_k}{2}\right) \approx \sqrt{\frac{\pi}{2}} \exp \left\{- \frac{\Delta^2}{4} \xi^2 - \frac{\Gamma t_k}{2} |\xi|\right\} \cdot Q_k(\xi)/(\beta_k + \rho) + \ldots \quad (IV.36)$$

where $\Delta$ is the Doppler line width as defined below Eq. III.4 with $E_i$ replaced by $E*$.

$$Q_k(\xi) = 1 + \frac{\rho - U}{\beta_k + \rho} \quad (IV.37)$$

$$U_k = \frac{\theta_k \sqrt{\pi}}{2 \sqrt{2}} \left[ \exp \left(\frac{\Delta |\xi|}{2 \sqrt{2}} + \frac{\theta_k}{\sqrt{2}}\right)^2 \text{Erfc} \left(\frac{\Delta |\xi|}{2 \sqrt{2}} + \frac{\theta_k}{\sqrt{2}}\right) \right.$$  
$$+ \exp \left(\frac{\Delta^2 \xi^2}{8}\right) \text{Erf} \left(\frac{\Delta |\xi|}{2 \sqrt{2}}\right) \right] \quad (IV.38)$$

$$\rho = \frac{1}{2} \psi(\sqrt{2} \theta_k, 0) \quad (IV.39)$$

and Erfc and Erf are respectively the complementary error function and the error function which are evaluated as specified for Eq.A.15 of Appendix A.

The asymptotic evaluation of $L_1$ is then completed with the variable change of Eq. IV.32 and substitution of Eq. IV.36 into Eq. IV.35.
b. Non-Asymptotic Algorithms for $L_1$

When \((\beta_k + \psi(\theta_k, 0))/\psi(\theta_k, 0) < 2.5\), the more elaborate algorithms described below must be used to obtain the $P_k$ for use in the solution of Eq.IV.35. 

\[ P_k \left( \frac{\Gamma t_k}{2} \right) \text{ is the unique solution of the integral equation } \]

\[ \beta_k P_k \left( \frac{\Gamma t_k}{2} \right) + \frac{1}{4} \Gamma t_k \int_{-\infty}^{\infty} e^{-\frac{\Delta^2}{4} (\xi - t)^2} - \frac{\Gamma t_k}{2} |\xi - t| P_k \left( \frac{\Gamma t_k}{2} \right) dt = \frac{\Delta^2 \xi^2}{4} - \frac{\Gamma t_k |\xi|}{2} \text{ (IV.40)} \]

Making the substitutions $y = \alpha \xi$ and $x = \alpha t$ and multiplying the integral by $\exp(-x^2) \cdot \exp(x^2)$, Eq.IV.40 may be cast into the form suitable for Gauss-Hermite quadrature

\[ \frac{\Delta^2 y^2}{4\alpha^2} \beta_k P_k \left( \frac{\Gamma t_k}{2\alpha} \right) + \frac{1}{4} \frac{\Gamma t_k}{\alpha} \int_{-\infty}^{\infty} e^{-x^2} \cdot \frac{\Delta^2 y x}{4 \alpha^2} - \frac{\Delta^2 x^2}{4 \alpha^2} - \frac{\Gamma t_k}{2} |y-x| |x| + x^2 P_k \left( \frac{\Gamma t_k}{2\alpha} \right) dx = \frac{\Gamma t_k |y|}{2 \alpha} \text{ (IV.41)} \]

The integral in Eq.IV.41 can again be written as a ten point Gauss-Hermite quadrature, so that at each mesh point $y_i$ we have

\[ \frac{\Delta^2 y^2}{4\alpha^2} \beta_k P_k \left( \frac{\Gamma t_k}{2\alpha} \right) + \frac{1}{4} \frac{\Gamma t_k}{\alpha} \sum_{i=1}^{10} a_j e^{-x^2} \frac{\Delta^2 y_i x_i}{\alpha^2} - \frac{\Delta^2 x_i^2}{4 \alpha^2} - \frac{\Gamma t_k}{2} |y_i-x_i| |x_j| + x_j^2 P_k \left( \frac{\Gamma t_k}{2\alpha} \right) dx = \frac{\Gamma t_k |y_i|}{2 \alpha} \text{ (IV.42)} \]

Equation IV.42 can be looked at as a system of 10 equations in the ten unknowns

\[ P_k \left( \frac{\Gamma t_k y_i}{2\alpha} \right) \text{.} \]

Thus we may write the matrix equation

\[ A P = B \text{ (IV.43)} \]
so that the desired $P$ may be obtained by inversion of the $A$ matrix

$$P = A^{-1}B.$$  \hspace{1cm} (IV.44)

Eqs. IV.42 are normalized by dividing each row of the $A$ matrix by the respective diagonal element, namely

$$N_{i}^{o} = \frac{\Delta^2 y_i^2}{4\alpha^2} \left\{ \frac{\Gamma_{t_k}}{e^{\frac{\Delta^2 y_i^2}{4\alpha^2}}} \right\}, \hspace{1cm} (IV.45)$$

Therefore

$$B = \sqrt{\frac{\pi}{2}} e^{-\frac{\Delta^2 y_i^2}{4\alpha^2}} N_{i}^{o}. \hspace{1cm} (IV.46)$$

$$A_{ii} = 1 \hspace{1cm} (IV.47)$$

$$A_{ij} = \left\{ \frac{\Gamma_{t_k} a_j}{4\alpha} \frac{\Delta^2 y_i^2 y_j}{2\alpha^2} - \frac{\Gamma_{t_k} |y_i - y_j|}{2\alpha} \right\} \left( \frac{\Delta^2 x_i^2}{e^{4\alpha^2}} \frac{\langle D_k \rangle^2 x_i^2}{\pi^2 \alpha^2} + \frac{\gamma^2 x_i^2}{2\alpha^2} \right) N_i^o. \hspace{1cm} (IV.48)$$

In Eq. IV.48 we have made use of the identity

$$\frac{\Delta^2 x_i^2}{e^{\frac{\Delta^2 x_i^2}{2\alpha^2}}} = \frac{\langle D_k \rangle^2 x_i^2}{\pi^2 \alpha^2} + \frac{\gamma^2 x_i^2}{2\alpha^2} \hspace{1cm} (IV.49)$$

with $\alpha$ and $\gamma$ defined as before in Eqs. IV.32.

The inversion of the 10 x 10 matrix $A$ can be considerably simplified and the execution time thereby significantly reduced by partitioning $A$ into four sub-matrixes and recognizing the fact that $A_{ij} = A_{ji}$ as is obvious from Eq. IV.48. If we let $D$ represent the inverse of $A$, we can write

$$AA^{-1} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{bmatrix} = I \hspace{1cm} (IV.50)$$

where $I$ is the 10 x 10 identity matrix and each of the sub-matrixes is 5 x 5.
By algebraic manipulation of the equations represented by Eq.IV.50, we can easily show that

\[
\begin{align*}
D_{11} & = (A_{11} - A_{12} A_{11}^{-1} A_{12})^{-1} \\
D_{12} & = -A_{11}^{-1} A_{12} D_{11} \\
D_{22} & = D_{11} \\
D_{21} & = D_{12}
\end{align*}
\]

where we have made use of the fact that \(A_{11} = A_{22}\) and \(A_{12} = A_{21}\).

Thus the inversion of the 10 x 10 \(A\) matrix can be accomplished by the much faster inversion of two 5 x 5 matrices as shown in Eqs.IV.51.

Finally, taking advantage of the fact that \(P_k\) is symmetric, we need be concerned only with the positive Gauss-Hermite quadrature points so that we may obtain the upper half of the \(P\) vector from \((D_{11} D_{12}) B\).

The non-asymptotic evaluation of \(L_1\) is then completed using the \(P_k\) obtained as above in Eq.IV.35.

2. Evaluation of \(L_2\)

Using the same technique as was used to convert Eq.IV.24 into the form of Eq.IV.29 for \(L_1\), Hwang has converted Eq.IV.26 into the form

\[
L_2 = -\frac{1}{2 \langle D_k \rangle^2} \int_{-\infty}^{\infty} \sqrt{2\pi} \omega(\xi) \left\langle \Gamma_k \left\{ -\frac{\Delta^2 \xi^2}{4} - \frac{\Gamma_{tk}}{2} \right\} e^{\frac{\pi}{\beta_k}} \right\rangle_k \cdot \left\langle \frac{\Gamma_{tk'}}{2} \frac{\partial}{\partial \beta_k} \frac{\partial}{\partial \beta_k} p_k \left( \Gamma_{tk'} \xi \right) \right\rangle_{k'} d\xi .
\]

Making the variable changes indicated in Eqs.IV.32 and multiplying the integral by \(\exp(-\eta^2)\exp(\eta^2)\) as for the case of \(L_1\), Eq.IV.52 can be converted to the equivalent form
Eq. IV.53 as before can be evaluated using Gauss-Hermite quadrature. Note that after obtaining $L_1$ as described earlier, the only new quantity needed to obtain $L_2$ is $R_k$.

As for $L_1$, two algorithms are used to obtain $R_k$ depending upon the size of $\beta_k$ relative to $\psi(\theta_k,0)$.

a. **Asymptotic Algorithms for $L_2$**

As for $L_1$, a fast, large $\beta$ approximation is used to obtain $R_k$ if $(\beta_k + \psi(\theta_k,0))|\psi(\theta_k,0)| > 2.5$. Specifically,

$$R_k \left( \frac{\Gamma_{t_k}}{2} \right) \approx \sqrt{\frac{\pi}{2}} \beta_k \exp \left[ -\frac{\Delta^2\xi^2}{4} - \frac{\Gamma_{t_k} |\xi|}{2} \right] \cdot \frac{1 + 2[\rho - U_k(\xi)]/(\beta_k + \rho)}{(\beta_k + \rho)^2}$$

(IV.55)

where $U_k$ and $\rho$ are given in Eqs. IV.38 and IV.39.

b. **Non-Asymptotic Algorithms for $L_2$**

When $(\beta_k + \psi(\theta_k,0))/|\psi(\theta_k,0)| < 2.5$, $R_k$ is obtained in a manner similar to that used for obtaining $P_k$ in the non-asymptotic case.

In order to obtain $R_k$, we differentiate Eq. IV.41 with respect to $\beta_k$ to obtain a new matrix equation similar to Eq. IV.43, namely

$$AR = \mathbf{V}$$

(IV.56)

where $A$ is the matrix defined in Eqs. IV.47 and IV.48 and

$$V_I = \frac{\beta_k p_k \left( \frac{\Gamma_{t_k} y_1}{2\alpha} \right)^2}{p_k}$$

(IV.57)
with $N^0_1$ the previously defined normalization factor given in Eq.IV.45.

Thus we have

$$R = A^{-1}_1 V.$$  \hspace{1cm} (IV.58)

Since $A^{-1}$ has already been obtained for use in computing $L_1, L_2$ is also available with little additional computational effort.

C. Evaluation of Unresolved Resonance Cross Sections

As stated previously, MC"-2 neglects the higher order corrections for the accidental overlap so that, for example Eq.IV.13 becomes

$$\frac{1}{D_k} \left\langle \Gamma_k, J^*_k \right\rangle \sim \frac{1}{\cos 2\delta_k} \left\{ \frac{1}{D_k} \left\langle \Gamma_k, J(\beta_k, \theta_k, a_k, a_k') \right\rangle - O_{\gamma_k} \right\} \cdot S \hspace{1cm} (IV.59)$$

where $S$ is defined by Eq.IV.14 and the evaluation of the overlap term $O_{\gamma_k}$ has been discussed in Section B above.

If we define the flux correction factor $f$ as

$$f = 1 - \sum_k \left[ \frac{1}{D_k} \left\langle \Gamma_{t_k}, J(\beta_k, \theta_k, a_k, a_k') \right\rangle - O_{t_k} \right] \hspace{1cm} (IV.60)$$

where $f$ is just Eq.IV.14 except that the sum extends over all spin sequences, we may write the effective unresolved resonance capture cross section for a given spin sequence $k$ as

$$\overline{\sigma}_{c_k} = \frac{\sigma_p \left\langle \Gamma_k, J^*_k \right\rangle}{\langle D_k, f \rangle}. \hspace{1cm} (IV.61)$$

If we accept the approximation given in Eq.IV.20, $\overline{\sigma}_{c_k}$ depends to first order only on the resonances of sequence $k$ since all other terms cancel in the ratio $S/f$. Thus

$$S \sim \prod_{i \neq k} \left\{ 1 - \left[ \frac{1}{D_i} \left\langle \Gamma_{t_i}, J(\beta_i, \theta_i, a_i, a_i') \right\rangle - O_{t_i} \right] \right\} \hspace{1cm} (IV.62)$$

and

$$f \sim \prod_k \left\{ 1 - \left[ \frac{1}{D_k} \left\langle \Gamma_{t_k}, J(\beta_k, \theta_k, a_k, a_k') \right\rangle - O_{t_k} \right] \right\} \hspace{1cm} (IV.63)$$

so that
with similar expressions for the fission and total cross sections where \( \Gamma_{\gamma_k} \) is replaced by \( \Gamma_{f_k} \) and \( \Gamma_{t_k} \) respectively.

The unresolved cross sections at each library specified \( E^* \) energy are finally obtained by summing the partial contributions such as given by Eq. IV.64 over all spin sequences. Thus the unresolved cross section for process \( x \) (capture, fission or total), material \( m \) at energy point \( E^* \) is given by

\[
\overline{\sigma}_x^m(E^*) = \sum_{k \in m} \overline{\sigma}_x^m(E^*)
\]

where the sum ranges over all sequences belonging to material \( m \).

D. Unresolved Resonance Integrals and Resolved-Unresolved Resonance Interaction

Since the \( E^* \) points for which the average unresolved resonance parameters are supplied in the library vary from isotope to isotope of each material, the code generates a fixed energy grid onto which the resonance integrals as given by Eq.IV.59 are linearly interpolated. The user may specify the energy grid, or the code will generate the grid using the following algorithm.

The first grid point corresponds to the energy of the top of the highest energy broad group. For points 2 through 25, the successive mesh point energies are in the ratio \( \exp(-0.25) \); for points 26 through 125 in the ratio \( \exp(-0.05) \); for points 126 through 149 in the ratio \( \exp(-0.25) \); and finally mesh point 150 corresponds to \( E_{\text{MIN}} \), the energy at the top of the thermal group. If \( E_{\text{MIN}} \) is encountered before mesh point 150, the grid terminates with point \( E_{\text{MIN}} \) and fewer than 150 points are in the fixed energy grid. Finally, the fixed grid is truncated so that only those points remain which fall within the unresolved \( E^* \) points of any of the isotopes in the problem under investigation.

If there is more than one \( E^* \) point between any of the fixed energy grid points, the unresolved resonance integrals are averaged over the several \( E^* \) points so that there is a single average resonance integral at a single average energy \( E^* \) between any two fixed energy grid points. These average resonance integrals as well as the flux correction factors \( f \) are then linearly interpolated onto the fixed grid.

Figure 5 schematically represents the energy structure if we denote the fixed energy grid points by \( \text{ESR}_i \) with corresponding midpoint energies \( E_i \).

In the case where resolved and unresolved resonances are present in the same energy region, the code accounts for interaction effects in the following way.
If resolved resonances $j$ have energies lying with energies $E_i$ and $E_{i-1}$ in Fig 5, then the unresolved resonance integral at mesh point \( \text{ESF}_i \) is modified to

\[
\frac{1}{\langle D_k \rangle} \left( \frac{\Gamma_{\text{ESF}}}{\gamma_k} \right) \left\{ 1 - \frac{1}{E_i - E_{i-1}} \sum_j J^*_{\ell_i} \right\}
\]  

where the sum in Eq.IV.66 includes all resolved resonances in the energy range $E_i - E_{i-1}$ and $J^*_{\ell_i}$ is given by Eq.III.24. If the resolved resonances are multilevel resonances, the $J^*_{\ell_i}$ is replaced by the appropriate multilevel expression given by Eq.III.33. Similar corrections are made to the unresolved fission and total resonance integrals.

The resolved resonance integrals for resonances $i$ in the energy range $E_i - E_{i-1}$ are similarly modified to

\[
\frac{J^*_{\ell_i}}{\xi_{i}} \left( \frac{f}{E_{i}^{\text{ESF}}} \right)
\]  

where $f$ is given by Eq.IV.63 and the value corresponding to grid point \( \text{ESF}_i \), $\xi_{i}$ is given by Eq.III.23, and $E_{i}^{\text{ESF}}$ is the energy of resolved resonance $i$.

Corresponding expressions for multilevel resolved resonance integrals are used where appropriate.

For resolved resonances falling within the end points and first corresponding midpoint energies, such as the range \( \text{ESF}_i - E_1 \) for example, the $f$ is the value corresponding to the last grid point.

E. Ultra-Fine-Group Unresolved Resonance Cross Sections

The ultra-fine-group spectrum calculation described in Chapter II and the hyper-fine-group RABANL calculation described in Chapter V make use of group averaged unresolved resonance cross sections. These cross sections are derived by assuming a constant weighting function in the ultra-fine-group so that

\[
\sigma^g_{x} = \frac{1}{E_{g-1} - E_{g}} \int_{E_{g}}^{E_{g-1}} \sigma^m_{x}(E) dE
\]

\[
(IV.68)
\]
Fig. 5. Unresolved Resonance Energy Grid.
and $\bar{\sigma}^m(E)_x$ is defined by Eq.IV.65. Future releases of the ENDF/B data files will provide information to specify the functional form of $\bar{\sigma}^m(E)_x$ versus $E$. Since such information is not available with ENDF/B-IV, the code MC$^2$-2 assumes that $\ln \bar{\sigma}^m(E)_x$ is linear in $\ln E$,

$$
\frac{\bar{\sigma}^m(E)_x}{\sigma^m(E)_n} = \left( \frac{E}{E^*_n} \right)^{A_n} \frac{\bar{\sigma}^m(E^*_n)}{\sigma^m(E^*_n)}
$$

(IV.69)

$$
A_n \equiv \frac{\ln \left( \frac{\sigma^m(E^*_n+1)}{\sigma^m(E^*_n)} \right)}{\ln \left( \frac{E^*_n+1}{E^*_n} \right)}
$$

The averaging of Eq.IV.68 using the $\ln - \ln$ interpolation of Eq.IV.69 is performed analytically in the same manner as used in the MC$^2$ code.\(^{(10)}\)
V. RABANL, HYPER-FINE GROUP INTEGRAL TRANSPORT THEORY
NEUTRON SLOWING DOWN

A. Introduction

The RABANL algorithms provide rigorous resolved resonance cross sections and are intended for use in the lower energy ranges for which the narrow resonance approximation of the $MC^2$ module CSC006 is not valid. The methods used in RABANL are based on the earlier work of Kier and Robba in the RABBLE code (5) and the improvements afforded for slab geometry by Olson in the RABID code (6). The present coding represents an improvement over these earlier codes with regard to accuracy and numerical stability, and also provides a fully variable dimensioned and CCCC compatible package which can be used in a standalone mode, (as with RABBLE or RABID), or in conjunction with a full $MC^2$ execution. In the latter case, elastic scattering sources as well as inelastic, $(n,2n)$, and fission sources are supplied by the ultra-fine-group $MC^2$ calculation. In either mode of operation, RABANL uses the standard $MC^2$ library as derived from ENDF/B data. Thus, e.g., resonance parameters are library supplied as opposed to being provided by the code user as is the case for the earlier codes. The user may also optionally include unresolved resonance cross sections derived from the $MC^2$ module CSC005 in the RABANL calculation as described below.

RABANL may be used for homogeneous one region calculations or for multi-region cylindrical or slab heterogeneous geometries. In the latter cases, the spatial flux distribution is obtained using integral transport theory methods involving calculation of cylindrical or slab collision probabilities.

Section B discusses the algorithms used in computing the elastic slowing down sources. Section C discusses the calculation of the collision rates and fluxes for both homogeneous one region and for multi-region problems. The algorithms used for the calculation of the cross sections are presented in Section D. Finally, in Section E, the calculation of the edited broad group fluxes and cross sections is described.

B. Calculation of Elastic Slowing-Down Sources

In order to accurately calculate the neutron slowing down in the presence of rapidly varying resonance cross sections, the hyper-fine-group (hfg) width used in the calculation must be extremely narrow. By the same token the hfg width should be small compared with the maximum lethargy gained per collision with the heaviest of the nuclides in the mixture so that the assumption of only one collision per group is valid.

The code determines the hfg width relative to the resolved resonance Doppler width $\Delta$

where

$$\Delta = \left[ \frac{4kT_E}{A} \right]^{\frac{1}{2}} \quad (V.1)$$
for temperature $T$, energy $E$, mass $A$, and with the Boltzmann constant $k$ equal to $8.61708 \times 10^{-5}$ eV/degree Kelvin. In particular

$$\Delta u_{J}^{\text{hfg}} = \frac{\Delta'}{NE_J}$$

(V.2)

for the hfg width appropriate to broad group $J$ where $E_J$ is the upper energy of broad group $J$, $N$ is specified by the user on card type 14 of data set A.MCC2 with a default value of 4, and $\Delta$ is obtained from Eq.V.1 using $T = 293$ degrees Kelvin, $E = E_J$, and $A = 250$. The hfg width is generally broad group dependent. The user may however specify that a fixed hfg width be used for the entire problem. In that case, $E_J$ corresponds to the upper energy of the highest broad group in the problem.

In any case, the code requires that Eq.V.2 yield a width not greater than 0.001. $\Delta u_{J}^{\text{hfg}}$ is then finally adjusted to correspond to an integral sub-multiple of the ultra-fine group (ufg) width. This adjustment may result in a lethargy width somewhat larger than 0.001. Thus, for example, for the current $\Delta u_{\text{ufg}}$ of 1/120, the largest possible $\Delta u_{J}^{\text{hfg}}$ is 0.00141667. For a broad group with upper energy of 275.36 eV, for example, $\Delta u_{J}^{\text{hfg}}$ is 0.00030864. A nucleus of mass 250 could elastically scatter neutrons a maximum lethargy width of 0.016 which corresponds to about 11.3 times the largest hyper-fine group width. Lighter nuclei of course can scatter down a greater lethargy span and hence would contain more hyper-fine groups in their scattering band. For example, a nucleus of mass 23 contains about 62.8 of the maximum width hyper-fine groups within its scattering lethargy band.

The probability per unit lethargy that a neutron is scattered from lethargy $u'$ to lethargy $u$ by a nucleus of mass ratio $A$ is given by

$$P(u' \rightarrow u) = \begin{cases} \frac{1}{1-\alpha} e^{-(u-u')}, & u \geq u' \geq u - \varepsilon \\ 0, & u' < u - \varepsilon \end{cases}$$

(V.3)

where

$$\alpha = \left[ \frac{A-1}{A+1} \right]^2$$

(V.4)

$$\varepsilon = \ln(1/\alpha)$$

(V.5)

and $A$ is the ratio of target nuclide mass to the mass of the neutron. Note that for hydrogen, the code uses the actual $A (\approx 0.99917)$ rather than the approximation $A = 1.0$.

In particular, the probability of scattering down $\ell$ hfg each of width $\Delta u$ into the group having lower lethargy $u_0$ is given by
Equation V.6 must be corrected for scattering into the lowest energetically possible hfg as indicated below.

The scattering band \( \varepsilon \) is adjusted by making small changes to the mass \( \Lambda \) so that

\[
L = \varepsilon / \Lambda u
\]  

is an integer. Thus a given hfg may scatter down into the next \( L \) hfg.

The probability of scattering down into the lowest hfg is given by

\[
P_{\text{lowest}} \Delta u = \frac{1}{1-\alpha} \int_{u_0}^{u_0+\Delta u} du \int_{u_0}^{u_0-\varepsilon+\Delta u} du' e^{-(u - u')} \]

\[
= \frac{(1 - e^{-\Delta u})^2}{1 - \alpha} e^{-(\ell - 1)\Delta u}
\]

\[
= p_1 \Delta u e^{-(\ell - 1)\Delta u} \]  

(V.6)

The ingroup scattering is given by

\[
P_s \Delta u = \frac{1}{1-\alpha} \int_{u_0}^{u_0+\Delta u} du \int_{u_0}^{u} du' e^{-(u - u')}
\]

\[
= \frac{1}{1-\alpha} (\Delta u - 1 + e^{-\Delta u}) \]  

(V.9)

Now if \( \ell \) is set equal to \( L \) in Eq.V.6, we obtain

\[
P_L \Delta u = \frac{\alpha}{1-\alpha} (e^{\Delta u} - 2 + e^{-\Delta u})
\]  

(V.10)

where we make use of the fact that

\[
\alpha = e^{-L\Delta u}
\]  

(V.11)
By comparing Eqs. V.8, V.9, and V.10, we see that

$$P_{\text{lowest}} \Delta u = P_L \Delta u - \alpha P_s \Delta u \quad (V.12)$$

If we denote the hfg flux per unit lethargy in hfg k by $\phi_k$ and the macroscopic scattering cross section for that group by $\Sigma_{sk}$, the source of neutrons per unit lethargy into group k due to elastic scattering-in from all energetically possible lower lethargy hfg is given by

$$S_{\phi_k} = \frac{1}{L} \sum_{\ell=1}^{L} \Sigma_{sk-\ell} \phi_{k-\ell} P_{\ell} \Delta u \cdot e^{\ell \Delta u} - \alpha \Sigma_{sk-L} \phi_{k-L} P_{s} \quad (V.13)$$

where $P_{\ell}$ and $P_{s}$ are obtained from Eqs. V.6 and V.9, respectively. Similarly, the ingroup or self-scattering source of neutrons per unit lethargy is given by

$$S_{\phi_k} = \Sigma_{sk} \phi_k P_{s} \quad (V.14)$$

In the case of a mixture of various mass nuclides, the previous equations will have a contribution from each of the constituents of the composition in question. In particular, for a heterogeneous problem these equations will have contributions from the constituents appropriate to the particular spatial mesh involved.

Note that in the previous equations, $\Delta u$, $P_{\ell}$, and $P_{s}$ have not contained a subscript relating to hfg number. This is appropriate so long as the hfg width is a constant. Since in the normal problem $\Delta u$ changes from broad group to broad group, $P_{\ell}$ and $P_{s}$ become broad group dependent quantities.

The direct evaluation of $S_{\phi_k}$ for each hfg using the summation in Eq. V.13 would be too time consuming since hundreds, and for light nuclides thousands, of lower lethargy hfg contribute to the scattering-in source for each hfg. By noting from Eq. V.6 that

$$P_{\ell} = e^{-\Delta u} P_{\ell-1} \quad (V.15)$$

and making use of Eq. V.11, one can show that Eq. V.13 may be rewritten in the form

$$S_{\phi_k} = e^{-\Delta u} S_{\phi_{k-1}} - \left( P_{1} - e^{-\Delta u} P_{s} \right) \phi \Sigma_{s} k_{L-1} = P_{1} \phi \Sigma_{s} k_{L} + P_{s} \phi \Sigma_{s} k_{L} - \alpha P_{s} \phi \Sigma_{s} k_{L} \quad (V.16)$$
Thus, the scattering source into hfg k requires only the source into the previous hfg \( S_{k-1} \), and the scattering rates \( \Sigma_s \) for hyper-fine groups \( k-1, k-L, \) and \( k-L-1 \).

When a variable hfg lethargy width is used, the lower lethargy scattering rates required in Eq. V.16 may occur in a broad group having a different hfg width from that of the receptor group k. In that case, the required \( \Sigma_s \) is in general obtained by a three point interpolation formula, namely

\[
f(x_o + ph) = \frac{p(p-1)}{2} f_{-1} + (1-p^2) f_o + \frac{p(p+1)}{2} f_1
\]

(V.17)

where the scattering rates \( f_{-1}, f_o, \) and \( f_1 \) are assigned to a lethargy at the center of the hfg involved. If the scattering source occurs within the first or last hfg of a broad group having a different hfg width from that of the receptor group, then the two point formula

\[
f(x_o + ph) = (1-p)f_o + pf_1
\]

(V.18)

is used for interpolation.

RABANL has provision for storing all energetically reachable lower lethargy scattering rates if the user specifies sufficient core storage. If this is not the case however, the code will store averages of the scattering rates over several hfg as necessary to accommodate the available storage. Results using averaged scattering rates will of course be less accurate than if all required hfg can be core contained. However, in practical problems, only slight changes have been observed in the resultant broad group cross sections if hfg averaging is used.

If scattering rates required in Eq. V.16 occur at energies above the top of the RABANL energy range, they are obtained in two ways depending upon whether RABANL is being run as a standalone or if the full MC\(^2\)-2 calculation is being made. In the former case, the code assumes \( \phi = 1.0 \) for all energies above the top of the RABANL energy range and takes \( \Sigma_s \) to be constant and equal to the homogenized hard sphere potential scattering cross sections for the materials in the composition involved. If the full MC\(^2\)-2 problem is run, the scattering rates \( \Sigma_s \) are provided to RABANL for all energetically reachable ultra-fine groups above the top of the RABANL energy range in a data set SRATES. RABANL assumes that \( \Sigma_s \) is constant within any ufg in obtaining the necessary \( \Sigma_s \) for use in Eq. V.16. If data set SRATES is saved from a previous MC\(^2\)-2 calculation, then a standalone RABANL calculation will similarly use these ufg \( \Sigma_s \) rather than the potential scattering cross sections and flat unit flux above the top of the RABANL calculation.
The source into the first, lowest lethargy hfg also depends upon whether RABANL is being run as a standalone code without access to a previously supplied data set SRATES, or rather if such data are available. If no SRATES data are available, from Eq.V.13 with $\phi=1.0$ and $\Sigma_s=\Sigma$ for all groups, one can show that

$$S_{o1} = \sum_p \left( 1 - e^{-\Delta u} \frac{1}{\Delta u} - \alpha_p \right)$$

(V.19)

where $\Delta u$ is the hfg lethargy width of the first hfg in the RABANL energy range. As before, for a mixture of materials, Eq.V.19 receives a contribution from each of the constituents with appropriate $\Sigma_p$, $\alpha$, and $P_s$ for each.

When data set SRATES is available, the source into hfg number 1 is derived by directly performing the sum in Eq.V.13 and assuming that $\Sigma_s\phi$ is constant within each of the hfg above the top of the RABANL energy range.

In order to minimize numerical roundoff problems, Eq.V.13 is used to obtain $S_o$ for the first hfg of each broad group rather than using the Eq.V.16 recursion relationship throughout all hfg in the problem. This has been found to be essential for heavily absorbing compositions for which exclusive use of Eq.V.16 for all hfg has led to the generation of negative sources.

If ingroup scattering is omitted, on user option, then $P_s=0$ and Eq.V.16 becomes

$$S_{o} = e^{-\Delta u} S_{o_{k-1}} - \alpha P_1 \left( \Sigma_s \phi \right)_{k-1} + P_1 \left( \Sigma_s \phi \right)_{k-1}$$

(V.20)

In this case, the $P_1$ as defined in Eq.V.16 must be altered in order to conserve neutrons. In particular, one can show that

$$\sum_{\ell=1}^{L} P_{\ell} - \alpha P_s + P_s = 1.0$$

(V.21)

using Eqs.V.6, V.9, and V.11. That is the sum of the scattering-in source (corrected for scattering from the highest hfg) plus the ingroup self-scattering is normalized to unity. On the other hand if $P_s=0$, then one finds using Eq.V.6 that

$$\sum_{\ell=1}^{L} P_{\ell} \Delta u = 1 - e^{-\Delta u}$$

(V.22)

Hence if ingroup scattering is deleted so that Eq.V.20 is pertinent, then to force normalization of all scattering to unity, $P_1$ as defined in Eq.V.6 must be divided by $1 - e^{-\Delta u}$ so that...
The reason why the user might choose to accept this more approximate treatment is to reduce running time in the case of heterogeneous problems as discussed later. For homogeneous problems, there is no running time advantage in deleting the self-scattering.

C. Calculation of Collision Rates

1. One Region (Homogeneous) Problems

   From neutron balance, the collision rate in a particular hfg k, $CR_k$, is given by
   
   $$CR_k = P_n \left\{ S_{\alpha_k} + S_{s_k} \right\}$$
   
   where $P_n$ is the non-leakage probability, and $S_{\alpha_k}$ and $S_{s_k}$ are respectively the scattering-in and self-scattering sources. Using Eq.V.14, Eq.V.24 can be rewritten as
   
   $$CR_k = P_n \left\{ \frac{\Sigma_{\alpha_k}}{P_s} + (\Sigma_\phi)_k \right\}$$
   
   $$= P_n \left\{ \frac{\sum_{\alpha_k} S_{s_k}}{\Sigma_{t_k}} \right\}$$
   
   $$= P_n \left\{ S_{\alpha_k} + R_k \cdot CR_k \right\}$$

   where $\Sigma_{t_k}$ is the macroscopic total cross section for hfg k,

   $$\Sigma_{t_k} = \frac{\sum_{\alpha_k} P_s}{S_{s_k}}$$
   
   $$R_k = \frac{\sum_{t_k}}{S_{t_k}}$$

   and from neutron balance, $CR_k = \Sigma_{t_k}$.

   Solving then for $CR_k$, we have

   $$CR_k = \frac{P_n \alpha_k}{1 - P_n R_k}$$
For the special case of an infinite medium, \( P_{n\ell_k} = 1.0 \). As discussed earlier, \( P_s \) will depend upon hfg for the case in which the hfg widths are variable. The hfg index has been omitted here for simplicity.

The non-leakage probability \( P_{n\ell_k} \) is taken to be

\[
P_{n\ell_k} = \frac{\Sigma_{t_k}}{\Sigma_{t_k} + D_k B^2}
\]

where again \( \Sigma_{t_k} \) is the hfg k total macroscopic cross section for the mixture,

\[
D_k = \frac{1}{3\Sigma_{tr_k}}
\]

and \( \Sigma_{tr_k} \) is the macroscopic transport cross section for the mixture where we assume

\[
\Sigma_{tr_k} = \sum_{i=1}^{M} n_i \sigma_{t_k}^i (\sigma_{t_k}^i - \mu_i \sigma_{s_k}^i).
\]

In Eq.V.29 the sum extends over all isotopes in the mixture, each with atom density \( N_i \) and microscopic total and scattering cross sections given by \( \sigma_{t_k}^i \) and \( \sigma_{s_k}^i \) respectively. \( \mu_i \) is \( 2/3A^i \) where \( A^i \) is the ratio of nuclide i mass to neutron mass. The buckling, \( B^2 \), is user specified on the A.MCC2 type 09 card.

The calculation of the \( S_{\ell_k} \) has been discussed earlier for the case of \( \sigma_{\ell_k} \) elastic slowing down. In addition to the elastic scattering sources, neutrons can also appear in a hfg due to inelastic and \((n,2n)\) scattering or to fissions at energies above the top of the RABANL energy range, or due to external sources specified by the user on the A.MCC2 type 08 cards. The former are referred to as fixed source neutrons in that they do not depend upon the RABANL fluxes, while the latter are referred to as external sources. The fixed sources are supplied on data set SRATES which is generated by an MC^2-2 ufg calculation. These sources, as in the case of the external sources are specified at an ufg level. RABANL creates equivalent hfg values for these ufg data by a linearization algorithm as specified below.
Suppose ufg data are available for ufg numbers 1 to NG where \( Y_I \) is the ufg datum for ufg \( I \). Defining

\[
\Delta_1 = Y_2 - Y_1
\]

\[
\Delta_I = \frac{Y_{I+1} - Y_I}{2}, \ I = 2, \ NG-1
\]

\[
\Delta_{NG} = Y_{NG} - Y_{NG-1}
\]

then the value assigned to a hfg \( j \) lying within ufg \( I \), assuming there are exactly \( N \) hfg per ufg, is given by

\[
y_j = (Y_I - \Delta_I/2) + f_j \Delta_I
\]

where

\[
f_j = \frac{2j - 1}{2N}, \ j = 1,2, \ldots, N
\]  

An example is shown in Fig. 6 for the case of \( N = 5 \) and \( NG = 4 \). The dashed line represents the linearized hfg histogram equivalent to the solid line ufg histogram.

The fixed sources as supplied on data set SRATES are given for each isotope in the mixture. RABANL homogenizes these sources according to the atom densities of the materials contained in the mixture. If we denote the homogenized hfg fixed sources as \( S_{\text{fix}} \), and the external hfg sources as \( S_{\text{ext}} \), Eq. V.26 is modified to

\[
CR_k = \frac{P_n \ell_k}{1 - P_n R_k} S_{\text{fix}}_k + S_{\text{ext}}_k
\]

where

\[
S_{\text{fix}}_k = S_{\text{fix}} + S_{\text{ext}}_k
\]

From Eq. V.32 and the macroscopic total cross section in hfg \( k \), we have

then the hfg \( k \) flux per unit lethargy

\[
\phi_k = \frac{CR_k}{\Sigma t_k}
\]  

The calculation of the \( \phi_k \) thus proceeds hfg by hfg: the elastic slowing down source is calculated for the hfg in question using the methods in Section B; this source is augmented by \( S_{\text{fix}} \) and \( S_{\text{ext}} \) and the collision rate is calculated as shown above; the hfg flux is then obtained from Eq. V.34 and the scattering rate \( (\Sigma s) \phi \) is stored for use in later slowing down source calculations as required in Eq. V.16.
Fig. 6. Linearization of Ultra-Fine-Group Data.
RABANL also provides for calculation of cross sections of foils immersed in the flux of the homogeneous composition. The foil material is assumed to have a negligible influence on the spectrum. The expressions for the collision rate in the foil and hence the flux in the foil are presented at the end of Section C.2.a.

2. **Multi-region (Heterogeneous) Problems**

The integral transport form of the Boltzmann equation can be written in general terms as

\[ \phi(\vec{r}, u) = \iiint d\vec{r}' \int_0^u du' \Sigma_s(u') \phi(\vec{r}', u') P(u' \to u) T(u, \vec{r}' \to \vec{r}) \]

\[ = \iiint d\vec{r}' S(u, \vec{r}') T(u, \vec{r}' \to \vec{r}) \quad \text{(V.35)} \]

where \( \phi(\vec{r}, u) \) is the flux per unit lethargy at space point \( \vec{r} \), \( \Sigma_s(u') \) is the scattering cross section at lethargy \( u' \), \( P(u' \to u) \) is the probability of a lethargy change of \( u' \) to \( u \) due to the scattering event at \( \vec{r}' \), \( S(u, \vec{r}') \) is the source of neutrons of lethargy \( u \) at space point \( \vec{r}' \), and \( T(u, \vec{r}' \to \vec{r}) \) is the transport kernel giving the probability that neutrons of lethargy \( u \) at space point \( \vec{r}' \) will reach space point \( \vec{r} \) without suffering a collision. \( P(u' \to u) \) is defined in Eq. V.3. The transport kernel depends upon the geometry of the problem since it involves the geometric distance \( |\vec{r} - \vec{r}'| \), namely

\[ T(u, \vec{r}' \to \vec{r}) = \exp\left[ -\Sigma_t(u, \vec{r}') |\vec{r} - \vec{r}'| \right] \frac{1}{4\pi |\vec{r} - \vec{r}'|^2} \quad \text{(V.36)} \]

RABANL provides solutions for multi-region slab or cylindrical geometries as described below.

a. **Slab Geometry**

In the case of infinite slab geometry, with reference to Fig. 7, the spatial integral in Eq. V.35 can be expressed as

\[ \int d\vec{r}' \Sigma_s(u') \phi(\vec{r}', u') \frac{\exp\left[ -\Sigma_t(u, \vec{r}') |\vec{r} - \vec{r}'| \right]}{4\pi |\vec{r} - \vec{r}'|^2} \]

\[ = \int dx' \Sigma_s(u') \phi(x', u') \int_0^\infty 2\pi \rho d\rho \frac{\exp\left[ -\Sigma_t(u, x') \left\{ \rho^2 + |x-x'|^2 \right\}^{1/2} \right]}{4\pi \left\{ \rho^2 + |x-x'|^2 \right\}} \]

\[ = \frac{1}{2} \int dx' \Sigma_s(u') \phi(x', u') \int_1^\infty \frac{\exp\left[ -\Sigma_t(u, x') |x-x'| \right]}{t} \]

\[ = \frac{1}{2} \int dx' \Sigma_s(u') \phi(x', u') E_1\{\Sigma_t(u, x') |x-x'| \} \quad \text{(V.37)} \]
Fig. 7. Slab Geometry Coordinates.
where $E_1$ is the exponential integral defined in Eq.A.37 of Appendix A. The $t$ used in transforming the variable of integration in Eq.V.37 is $1/\cos \theta$ where $\theta$ is shown in Fig. 7.

The flux is therefore given by

$$\phi(x,u) = \frac{1}{2} \int dx' \int_0^u \Sigma_s(u') \phi(x',u') P(u' \rightarrow u) E_1 \left\{ \Sigma_t(u,x') | x-x' | \right\}$$

(V.38)

Now since the current is $\phi \cos \theta$, from the definition of the exponential integrals, the current is given by

$$\vec{J}(x,u) = \frac{1}{2} \int dx' \int_0^u \Sigma_s(u') \phi(x',u') P(u' \rightarrow u) E_2 \left\{ \Sigma_t(u,x') | x-x' | \right\}$$

(V.39)

If now the continuous-lethargy expressions in Eqs.V.38 and V.39 are transformed into the equivalent hyper-fine multigroup form, Eq.V.39 can be written as

$$\vec{J}_k(x) = \frac{1}{2} \int dx' S_k(x') E_2 \left\{ \Sigma_{t_k}(x') | x-x' | \right\}$$

(V.40)

where $\vec{J}_k(x)$ is the hfg $k$ current at $x$, $S_k(x')$ is the hfg $k$ source at $x'$, and $\Sigma_{t_k}(x')$ is the total macroscopic cross section for hfg $k$ and spatial point $x'$. The calculation of the $S_k$ has been described earlier in Section B, and $S_k$ contains the source into hfg $k$ due to slowing down from all other hfg plus the ingroup or self-scatter source for hfg $k$

$$S_k(x') = S_{o_k}(x') + S_{s_k}(x')$$

(V.41)

Noting that the optical thickness $\tau_k$ is given by $\Sigma_{t_k} x$, the current at $\tau_k$ mean free paths beyond a slab of optical thickness $\tau_k$ is given by

$$\vec{J}_k(\tau_k, \tau_k) = \frac{1}{2} \int_0^{\tau_k} dx' \left[ S_{o_k}(x') + S_{s_k}(x') \right] E_2(\tau_k + \Sigma_{t_k} x')$$

(V.42)

where $\Sigma_{t_k}$ is the total macroscopic cross section in the slab for hfg $k$.

Assuming that the self-scatter source and the in-scattered source have the same dependence on $x'$ and assuming that the spatial source per unit length in the slab is given by a flat component plus a linearly varying component
\[ S_k(x') = \frac{1}{t_1} \left[ \frac{S_k}{t_1} + \frac{\Delta S_k}{t_1} (t_1/2 - x') \right] \]  

(Eq. V.43)

as shown in Fig. 8, Eq. V.42 may be rewritten as

\[ \dot{J}_k(\tau_k, \tau_{k_1}) = \frac{S_k}{2t_1} \int_0^{t_1} dx' E_2(\tau_k + \tau_{k_1} x') \]

\[ - \frac{\Delta S}{2t_1^2} \int_0^{t_1} dx' x' E_2(\tau_k + \tau_{k_1} x') \]

\[ + \frac{\Delta S}{4t_1} \int_0^{t_1} dx' E_2(\tau_k + \tau_{k_1} x') \]  

(Eq. V.44)

The first and last integrals of Eq. V.44 are easily evaluated using Eq. A.60 of Appendix A. The second integral may be evaluated by noting that

\[ \int x^m E_n(ax + b) dx = - \sum_{i=0}^{m} \frac{m!}{(m-i)!} \frac{x^{m-i}}{a^{i+1}} E_n+i+1(ax + b). \]  

(Eq. V.45)

Finally, one may show that the current

\[ \dot{J}_k(\tau_k, \tau_{k_1}) = \frac{S_k}{2t_1} \left[ E_3(\tau_k) - E_3(\tau_k + \tau_{k_1}) \right] \]

\[ + \frac{\Delta S}{2t_1} \left\{ E_3(\tau_k) + E_3(\tau_k + \tau_{k_1}) \right\} \left[ 2 - \frac{1}{t_1} \left[ E_4(\tau_k) - E_4(\tau_k + \tau_{k_1}) \right] \right\} \]  

(Eq. V.46)

Now the collision rate in a slab is the difference between the uncollided current into the slab and the uncollided current out of the slab. Thus the collision rate in a slab of optical thickness \( \tau_{k_2} \) due to the source in a slab of optical thickness \( \tau_{k_1} \), when slabs 1 and 2 are separated by \( \tau_k \) mean free paths is, using the notation of Eq. V.46

\[ \dot{C}_{k_2}^{(1 \rightarrow 2)} = \dot{J}_k(\tau_k, \tau_{k_1}) - \dot{J}_k(\tau_k + \tau_{k_2}, \tau_{k_1}). \]  

(Eq. V.47)

The arrow above \( \dot{C} \) in Eq. V.47 implies that slab 2 lies to the right of slab 1.

Now if there exists an infinite array of unit cells each made up of a number of slab mesh intervals, then the collision rate in all type 2 slabs which lie to the right of the type 1 slabs is given by the infinite sum

\[ \dot{C}_{\infty}^{(1 \rightarrow 2)} = \sum_{m=0}^{\infty} \left[ \dot{J}_k(\tau_k + mh, \tau_{k_1}) - \dot{J}(\tau_k + \tau_{k_2} + mh, \tau_{k_1}) \right] \]  

(Eq. V.48)
Fig. 8. Slab Geometry Optical Distance
where \( h \) is the optical thickness of the unit cell.

Since neutrons proceed both to the right and to the left, the total collision rate in slab \( j \) due to sources in slab \( i \) is given by

\[
CR_\infty (i \rightarrow j) = CR_\infty (i \rightarrow j) + CR_\infty (j \rightarrow i) \tag{V.49}
\]

where the arrows above the CR denote the direction of neutron motion. Appendix A describes the numerical methods used in evaluating the infinite sums of \( E_n \) functions involved in obtaining Eq.V.49.

Thus, for the neutron source \( S_i \) in mesh interval \( i \), the collision probability from region \( i \) to \( k \) and \( hfg \) \( k \) is given by

\[
C_{i \rightarrow k} = CR_\infty (i \rightarrow j)/S_{i \rightarrow k} \tag{V.50}
\]

The unit cell may have either periodic or reflective boundary conditions as specified by the user. Thus if a four mesh interval cell having compositions ordered as ABCD is specified to have periodic boundary conditions, the infinite lattice will have the compositions \( \ldots ABCDABC \ldots \). If instead reflective boundary conditions are specified, the infinite lattice will correspond to \( \ldots DCBABC \ldots \).

We will now drop the \( hfg \) index to simplify the notation. If the unit cell consists of \( N \) slab mesh intervals, then the collision probability can be represented by an \( N \times N \) square matrix \( C \). Similarly, the collision rate, the scattering-in sources, and the self-scattering sources are all \( N \) dimensional vectors, and are represented by \( CR, S_0, \) and \( S_s \) respectively.

Using matrix arithmetic then one has from neutron balance

\[
CR = C \left[ S_0 + S_s \right] \tag{V.51}
\]

Again, as for the case of the homogeneous one region calculation, the \( S_0 \) are augmented by the fixed and external sources as in Eq.V.33 so that we rewrite Eq.V.51 as

\[
CR = C \left[ S_e + S_s \right] \tag{V.52}
\]

where \( S_e \) is the \( N \) dimensional vector representation of Eq.V.30. Now from Eqs.V.25 and V.34, we can replace the self-scattering source \( S_s \) by

\[
S_s = R \cdot CR \tag{V.53}
\]
In matrix notation, \( R \) will be a square, \( NxN \) diagonal matrix with elements given by Eq.V.25 for each slab mesh interval. Thus we have

\[
CR = C \left[ S_t + R CR \right]
\]

Solving Eq.V.54 for \( CR \) we have

\[
[I - C R] CR = C S_t
\]

and hence

\[
CR = [I - C R]^{-1} C S_t
\]

(V.55)

where \( I \) is the unit matrix.

Note that the solution of Eq.V.55 requires the inversion of an \( NxN \) matrix. Also, if self-scattering is ignored so that \( R \) is the null matrix, then Eq.V.54 reduces to

\[
CR = C S_t, \text{ if } P_s = 0.
\]

(V.56)

Now to this point, the algorithms for the slab geometry problem have referred to infinite geometry. If however the user choose to specify a buckling and permit leakage from each mesh interval, the code calculates the non-leakage probabilities as in Eq.V.27. Expressing these in the form of a square \( NxN \) diagonal matrix \( P_{NL} \) where each diagonal element is the non-leakage probability for the particular mesh interval, we may rewrite Eq.V.54 as

\[
CR = C P_{NL} \left[ S_t + R CR \right].
\]

Again, solving for \( CR \), we have in place of Eq.V.55

\[
CR = [I - C P_{NL} R]^{-1} C P_{NL} S_t
\]

(V.58)

and if self-scattering is omitted,

\[
CR = C P_{NL} S_t, \text{ if } P_s = 0.
\]

(V.59)

Thus, as noted earlier, the execution time is reduced if the user chooses to omit the self-scattering contribution because the matrix inversion is eliminated.

The calculation of the spatially integrated hfg flux per unit lethargy \( \phi(i) \) where \( i \) denotes spatial mesh interval proceeds as for the homogeneous case, hfg by hfg: the elastic slowing down sources are calculated for each spatial mesh interval; these sources are augmented by the linearized fixed and external sources; the collision probability is calculated as in Eq.V.50 where however the self-scatter source is not included in \( S_i \); the collision
rate is computed using Eq. V.55 or V.56 as appropriate; the hfg spatially integrated flux for each mesh interval is calculated using Eq.V.34; the scattering rates $\Sigma_s\phi$ are computed and stored for use in calculating lower energy slowing sources.

As mentioned above, in computing the collision probability as in Eq.V.50, the self-scattering source is not included since the hfg $k$ flux is not yet available. Since the self-scattering contribution is always a very small part of the total source in a hfg, the alternative procedure requiring an iteration procedure to compute the true collision probability is not justified.

As in the case of the homogeneous calculation, the slab geometry problem provides for the calculation of foil cross sections. The code calculates the cross section for each foil specified at the interface between each spatial mesh interval and that immediately to its right. A foil is also place at the rightmost boundary of the unit cell.

The same procedure is used for the foil calculations as indicated above for the calculation of the collision rates in the slab mesh intervals. Thus, for example, by analogy with Eq.V.48, the collision rate in a foil due to the sources in all intervals $i$ in the infinite lattice lying to the left of the foil is given by

$$CR_i(foil) = \sum_{m=0}^{\infty} \left[ F(\tau_{mh}, \tau_i) - F(\tau_{f+mh}, \tau_i) \right]$$  \hspace{1cm} (V.60)

where the arrows indicate that the current is right directed. The foil with optical thickness $\tau_f$ is separated from the interval of optical thickness $\tau_i$ by the distance $\tau_{mh}$ where again $h$ is the unit cell optical thickness. Similar contributions to the collision rate are provided by the left directed currents which when add to Eq.V.60 yield the total collision rate $CR_{\infty}(foil)$.

Since the collision rate in the foil is given by

$$CR_{\infty}(foil) = \int_{\text{foil}} \phi(x) \Sigma_{tf} \, dx = \bar{\phi}_{\text{foil}} \tau_f$$  \hspace{1cm} (V.61)

where $\Sigma_{tf}$ is the total foil macroscopic cross section, the average flux in the foil can be written as

$$\bar{\phi}_{\text{foil}} \tau_f = \frac{CR_{\infty}(foil)}{\tau_f}$$  \hspace{1cm} (V.62)

Now for a homogeneous one region problem, the current into the left surface of a foil due to all sources to the left is given by Eq.V.40 as

$$J_L = \frac{1}{2} \int_0^\infty dx' S E_2(\Sigma_t x')$$

$$= \frac{S}{4\Sigma_t}$$  \hspace{1cm} (V.63)
where \( S \) is the space independent source of neutrons in the homogenous mixture and \( \Sigma_t \) is the macroscopic total cross section. Similarly, the current at the right surface of the foil due to the region to the left of the foil is given by:

\[
\hat{J}_R = \frac{1}{2} \int_0^{\infty} dx' S(E_x S(x' \tau_f))
\]

\[
= \frac{S}{2\Sigma_t} E_3(\tau_f) \tag{V.64}
\]

Hence the collision rate in the foil due to the incident flux from the left half space is:

\[
CR_\infty(\text{foil}) = \hat{J}_L - \hat{J}_R = \frac{S}{2\Sigma_t} \left[0.5 - E_3(\tau_f)\right] . \tag{V.65}
\]

Since the same contribution is provided by the incident flux from the right half space, the total collision rate then is given by:

\[
CR_\infty(\text{foil}) = \frac{S}{\Sigma_t} \left[0.5 - E_3(\tau_f)\right] . \tag{V.66}
\]

Finally, Eq. V.66 in Eq.V.62 yields the average flux in the foil.

\[\text{b. Cylindrical Geometry}\]

RABANL makes the same approximation as does the RABBLE(5) code in the case of cylindrical geometry. Namely, the flux at the surface of any cylindrical mesh interval is assumed to be isotropic so that neutron currents at an interface vary as the cosine of the incident angle (the so called cosine current approximation). In this case, the collision rate in an interval need be related only to the neutron currents impinging on its inner and outer surfaces so that, the collision rate is dependent only upon the adjacent mesh intervals.

Following the notation of Ref. 5, let:

\[
J^+_{i} = \text{the current impinging on the inner surface of the (i + 1)th cylindrical interval (in the increasing radial direction)}
\]

\[
J^-_{i} = \text{the current impinging on the outer surface of the ith interval (in the decreasing radial direction)}
\]

\[
F^+_{i} = \text{the probability of escape through the outer surface of interval i due to a flat volume source}
\]

\[
F^-_{i} = \text{the probability of escape through the inner surface of interval i due to a flat volume source}
\]
\[ T^O_i \] = the transmission probability from the inner to the outer surface of interval \( i \)

\[ T^I_i \] = the transmission probability from the outer to the inner surface of interval \( i \)

\[ T^{II}_i \] = the transmission probability from the outer to the outer surface of interval \( i \).

If mesh interval 1 is the center interval and if isotropic return is assumed as the outer boundary condition for the cylindrical unit cell (the so-called white boundary condition), then by neutron balance we have for an \( N \) cylindrical mesh interval unit cell

\[ J^+_i = \begin{cases} T^O_i J^+_i + P^+_i S^+_i & i = 1 \\ T^O_i J^+_i & i = 2, N \end{cases} \quad (V.67) \]

\[ J^-_i = \begin{cases} T^O_i J^-_i + P^-_i S^-_i & i = 1, N-1 \\ J^+_i & i = N \end{cases} \quad (V.68) \]

If we define the column vector \( J \) having 2\( N \) elements \( J^+_1, J^-_1, J^+_2, J^-_2, \ldots, J^-_N \) and the column vector \( P_S \) having 2\( N \) elements \( P^+_1 S^+_1, P^+_2 S^+_2, P^-_2 S^-_2, P^+_3 S^+_3, P^-_3 S^-_3, \ldots, P^-_N S^-_N, P^+_N S^+_N \) \( 0 \), then the 2\( N \) Eqs. V.67 plus V.68 may be represented in matrix notation as

\[ T J = P_S \quad (V.69) \]

where \( T \) is a 2\( N \)+2\( N \) square matrix whose elements involve the \( T^O_i, T^I_i \), and \( T^{II}_i \).

The set of Eqs. V.69 may be solved for the \( J^+_i \) and \( J^-_i \) either by inverting the \( T \) matrix, or equivalently by the method of forward elimination, backward substitution. RABANL uses the latter procedure.

Having solved for the \( J^+_i \) and \( J^-_i \), the collision rates for each interval \( i \) can be obtained from neutron balance as

\[ CR_i = \begin{cases} S^-_1 + J^-_1 - J^+_1 & i = 1 \\ S^-_1 + J^-_i - J^+_i + J^+_i - J^-_{i-1} - J^-_{i-1} & i = 2, N \end{cases} \quad (V.70) \]

The above procedure is used if self-scattering is ignored. If this approximation is not made, the code first must compute the collision probabilities. In order to compute the collision probabilities \( C_{ij} \), RABANL proceeds as indicated above by setting \( S^+_i = 1 \), setting all other \( S^-_j = 0 \), and solving for
This procedure is repeated for each interval \( i \) to complete the evaluation of the \( C_{ij} \).

Having obtained the \( C_{ij} \), the collision rates are calculated as indicated above for slab geometries using Eq. V.55 which requires a matrix inversion. Note that infinite geometry is assumed for the cylindrical geometry option so that the non-leakage probability is always 1.0.

The \( T^{0I} \) and \( T^{00} \) are obtained as described in Section VII of Appendix A. The other quantities needed in the evaluation of the CR can be expressed in terms of these transmission probabilities as shown in Ref. 5. In particular, define

\[
x_i = \frac{r_{i-1}}{r_i}
\]

where \( r_0 = 0 \) and

\[
z_i = \sum t_i (r_i - r_{i-1})
\]

where \( r_i \) is the outer radius of mesh interval \( i \) and \( \sum t_i \) is the total macroscopic cross section in interval \( i \). Then

\[
T^{0I}_i = x_i T^{0I}_i
\]

\[
p_i^- = \frac{x_i (1 - T^{0I}_i)}{2z_i (1 + x_i)}
\]

\[
p_i^+ = \frac{1 - T^{00}_i - T^{10}_i}{2z_i (1 + x_i)}
\]

The foil capability described earlier for homogeneous or slab geometry problems is not provided in the case of cylindrical cells.

D. Calculation of Hyper-fine Group Cross Sections

The cross sections for a particular material in a given hfg are made up of both smooth and resonance contributions. The smooth data are available at an ufg detail from the library as provided by ETOE-2. At user option, as specified on card type 02 of data set A.STP015, the contribution from ufg unresolved resonance cross sections as prepared by the modules CSC004 and CSC008 will be added to the other library provided smooth data. These ufg smooth data are linearized as in the case of the fixed and external sources using the algorithms given in Eqs. V.30 and V.31 to generate the hfg cross sections to be added to the resolved resonance cross sections.
The contributions due to the resolved resonances are computed in RABANL during the sweep down through the hfg. The code will accept Breit-Wigner single level resonance parameters, or multilevel parameters in either the Adler-Adler or Breit-Wigner representations. The resolved resonance cross sections for a given hfg are evaluated at the energy corresponding to the average lethargy of the hfg.

1. **Resonance Selection**

Due to the large number of hfg, the calculation of the resonance cross sections in each due to all resolved resonance in the problem mixture may be rather time consuming. The user has the option of specifying a resolved resonance selection criterion using the type 14 card of data set A.MCC2. An intermediate group is specified corresponding to an integral number of ufg, with the default number being two. The contribution of any resonance falling within the intermediate group is automatically included in each hfg contained in the intermediate group in question. Those resonances lying outside the intermediate group, whose resonant total cross sections at the intermediate group boundary equal or exceed the criterion specified on the type 14 card, are also included for all hfg contained in the intermediate group. The default for this criterion is 0.05. All other resonances are ignored for that intermediate group. In calculating the total resonant cross sections during the selection process, the resonances are Doppler broadened using the temperature of the hottest composition in the problem.

By specifying a criterion of 0.0 on the type 14 card, the user may include the contributions of all resonances in each of the hfg in the calculation. This option, which is the most rigorous is also the most time consuming.

2. **Resolved Resonance Algorithms**

a. **Single Level Breit-Wigner**

Single level Breit-Wigner s-wave resonance scattering, capture, and fission cross sections are respectively evaluated using the expressions

\[
\sigma_s^s(E) = \sigma_s^0 \left\{ \frac{\Gamma_s^r}{\Gamma_s^t} \psi(\xi, x) + \left[ \frac{\sigma_p g_{J=0}^r}{\sigma_o t} \right] \left( \begin{array}{c} \chi(\xi, x) \end{array} \right) \right\}
\]

\[
= \sigma_s^0 \left\{ \frac{\Gamma_s^r}{\Gamma_s^t} \psi(\xi, x) + a^s \chi(\xi, x) \right\}
\]  

(V.77)
In the above,

\[ \sigma^S_c(E) = \sigma^S_o \left[ \frac{|E_o|}{E} \right]^{1/2} \frac{\Gamma^S}{\Gamma_t} \psi(\xi, x) \]  

\[ \sigma^S_f(E) = \sigma^S_o \left[ \frac{|E_o|}{E} \right]^{1/2} \frac{\Gamma^f}{\Gamma_t} \psi(\xi, x) . \]  

\( \sigma^S_o \) = the peak cross section of the s-wave resonance  
\( E_o \) = the resonance energy in eV  
\( A \) = the mass number of the target nucleus  
\( \varepsilon_J \) = \( \frac{2J+1}{2(2J+1)} \) where \( J \) is the total spin of the compound nucleus and \( I \) is the spin of the target nucleus  
\( \Gamma^S_t \) = the s-wave total line width  
\( \Gamma^S_\gamma \) = the s-wave radiation line width  
\( \Gamma^S_f \) = the s-wave fission line width  
\( \Gamma^S_n = \Gamma^S_t - \Gamma^S_\gamma - \Gamma^S_f \)  
\( E \) = the laboratory neutron energy in eV corresponding to the average lethargy for the hfg in question  
\( \omega_p \) = the target nucleus potential scattering cross section  
\( \psi(\xi, x) \) = the Doppler-broadened symmetric line shape function  
\( \chi(\xi, x) \) = the Doppler-broadened anti-symmetric line shape function  
\( W(z) \) = the error function for complex arguments  
\( \exp(-z^2) \operatorname{erfc}(-iz) \) where \( z = x + iy \)
\[ \xi = \Gamma_t^p / \Delta \text{ and } \Delta \text{ is defined in Eq. V.1 with } E \text{ defined above and } \\
\text{with the Boltzmann constant equal to } 8.6168 \times 10^{-5} \text{ eV/degree} \\
\text{Kelvin} \\
x = 2(E - E_o) / \Gamma_t^p. \]

The \( \psi \) and \( \chi \) functions are obtained from bivariate interpolation in prestored tables as described in Section III of Appendix A.

Single level Breit-Wigner p-wave resonance scattering, capture, and fission cross sections are, respectively evaluated using the expressions

\[
\sigma_s^p(E) = \sigma_o^p \frac{\Gamma_t^p}{\Gamma_n^p} \left\{ \psi(\xi, x) + \frac{\Gamma_t^p}{2E_o} \chi(\xi, x) + \left[ \frac{\Gamma_t^p}{2E_o} \right]^2 \left[ 1 - \psi(\xi, x) \right] \right\} \tag{V.80}
\]

\[
\sigma_c^p(E) = \sigma_o^p \left[ \frac{|E_o|}{E} \right]^{\frac{1}{2}} \frac{\Gamma_t^p}{\Gamma_t^p} \left[ \psi(\xi, x) + \frac{\Gamma_t^p}{4E_o} \chi(\xi, x) \right] \tag{V.81}
\]

\[
\sigma_f^p(E) = \sigma_o^p \left[ \frac{|E_o|}{E} \right]^{\frac{1}{2}} \frac{\Gamma_t^p}{\Gamma_t^p} \left[ \psi(\xi, x) + \frac{\Gamma_t^p}{4E_o} \chi(\xi, x) \right]. \tag{V.82}
\]

In the above,

\( \sigma_o^p \) = the peak cross section of the p-wave resonance evaluated as before but using the parameters for the p-wave resonance

\( \Gamma_t^p \) = the p-wave total line width

\( \Gamma_n^p = \Gamma_t^p - \Gamma_r^p - \Gamma_f^p \)

\( \Gamma_r^p \) = the p-wave radiation line width

\( \Gamma_f^p \) = the p-wave fission line width

\( \xi = \Gamma_t^p / \Delta \)

\( x = 2(E - E_o) / \Gamma_t^p \).

b. **Multilevel Breit-Wigner**

Multilevel Breit-Wigner s-wave resonance scattering, capture, and fission cross sections are, respectively evaluated using the expressions
\[ \sigma_{s,bw}(E) = \frac{\sigma_{o}^{bw}}{|g_{t}^{bw}|} \left\{ g_{t}^{bw} \psi(\xi,x) + |g_{t}^{bw}| a^{bw} \chi(\xi,x) - G_{t}^{bw} \psi(\xi,x) - G_{f}^{bw} \psi(\xi) \right\} \]  
(V.83)

\[ \sigma_{c,bw}(E) = \sigma_{o}^{bw} \frac{G_{p}^{bw}}{|g_{t}^{bw}|} \left[ \frac{|E_{o}|}{E} \right]^{\frac{1}{2}} \psi(\xi,x) \]  
(V.84)

\[ \sigma_{f,bw}(E) = \sigma_{o}^{bw} \frac{G_{f}^{bw}}{|g_{t}^{bw}|} \left[ \frac{|E_{o}|}{E} \right]^{\frac{1}{2}} \psi(\xi,x) \]  
(V.85)

In the above:

\[ \sigma_{o}^{bw} = \sigma_{o}^{S} g_{t} \] where \( \sigma_{o}^{S} \) is defined below Eq. V.79.

\[ g_{t}^{bw} = \text{Breit-Wigner multilevel symmetric parameter for the total reaction which is 1 plus the symmetric level-level interference contribution} \]

\[ a^{bw} = a^{S} \text{ as defined in Eq. V.77 plus the asymmetric level-level interference contribution, all divided by } g_{t} \]

\[ G_{t}^{bw} = \text{Breit-Wigner multilevel symmetric parameter for the radiative capture reaction} \]

\[ = \frac{\Gamma_{t}^{S}}{\Gamma_{t}^{bw}} \]

\[ \Gamma_{t}^{bw} = \text{the Breit-Wigner multilevel total line width} \]

\[ G_{f}^{bw} = \text{Breit-Wigner multilevel symmetric parameter for the fission reaction} \]

\[ = \frac{\Gamma_{f}^{S}}{\Gamma_{t}^{lw}} \]

\[ x = \frac{2(E - E_{o})}{\Gamma_{t}^{bw}} \]

\[ \xi = \frac{\Gamma_{t}^{bw}}{\Delta}. \]

Multilevel Breit-Wigner p-wave resonance scattering, capture, and fission cross sections are, respectively evaluated using the single level expressions given by Eqs. V.80, V.81 and V.82 where \( \sigma_{o}^{p} \) is replaced by \( \sigma_{o}^{bw} \), \( \Gamma_{o}^{p} \) is replaced by \( \Gamma_{t}^{bw} \), \( \Gamma_{p}^{p} \) is replaced by \( \Gamma_{p}^{bw} \), \( \Gamma_{t}^{p} \) is replaced by \( \Gamma_{t}^{bw} \), \( \Gamma_{f}^{p} \) is replaced by \( \Gamma_{f}^{bw} \), \( \Gamma_{t}^{bw} \) and \( \Gamma_{n}^{p} \) is replaced by \( \Gamma_{t}^{bw}(1 - G_{t}^{bw} - G_{f}^{bw}) \).
c. Multilevel Adler-Adler

Multilevel Adler-Adler resonance scattering, capture, and fission cross sections are, respectively evaluated using the expressions

\[ c_{s}^{aa} = \left[ \frac{|E_{0}|}{E} \right]^{\frac{1}{2}} \frac{c_{o}^{aa}}{c_{t}^{aa}} \left\{ c_{t}^{aa} \psi(\xi,x) + |c_{t}^{aa}| a^{aa} \chi(\xi,x) \right\} \]

\[ c_{c}^{aa}(E) = \frac{c_{c}^{aa}}{c_{t}^{aa}} \left[ \frac{|E_{0}|}{E} \right]^{\frac{1}{2}} \{ \psi(\xi,x) + b \chi(\xi,x) \} \]  

\[ c_{f}^{aa}(E) = \frac{c_{f}^{aa}}{c_{t}^{aa}} \left[ \frac{|E_{0}|}{E} \right]^{\frac{1}{2}} \{ \psi(\xi,x) + b \chi(\xi,x) \} \]  

In the above

\[ c_{o}^{aa} = 2.6039953 \times 10^{6} \left( \frac{A+1}{A} \right)^{2} \frac{|c_{t}^{aa}|}{2t_{t}^{aa}} \]

\[ c_{t}^{aa} = \sqrt{|E_{0}|} \left[ G^{T} \cos 2\phi_{\ell} + H^{T} \sin 2\phi_{\ell} \right] \]

\[ G^{T} = \text{Adler-Adler symmetric total cross section parameter from ENDF/B} \]

\[ H^{T} = \text{Adler-Adler antisymmetric total cross section parameter from ENDF/B} \]

\[ \phi_{\ell} = \text{phase shift} \]

\[ t_{t}^{aa} = \text{S-matrix total line width for the Adler-Adler formulation} \]

\[ a^{aa} = -0.5 \left( \frac{H^{T} \cos 2\phi_{\ell} - G^{T} \sin 2\phi_{\ell}}{|c_{t}^{aa}|} \right) \sqrt{|E_{0}|} \]

\[ c_{\gamma}^{aa} = \sqrt{|E_{0}|} \left[ G^{c} \cos 2\phi_{\ell} + H^{c} \sin 2\phi_{\ell} \right] \]

\[ G^{c} = \text{Adler-Adler symmetric capture cross section parameter from ENDF/B} \]

\[ H^{c} = \text{Adler-Adler antisymmetric capture cross section parameter from ENDF/B} \]
The various G and H parameters as obtained from ENDF/B are assumed to include the factor $2g_J/\sqrt{E_0}$. Thus the factor $g_J$ does not appear explicitly in the expression for $\sigma_{\text{aa}}$.

### E. Broad Group Edits

The hfg spatially integrated fluxes per unit lethargy as calculated from Eq. V.34 are summed over the corresponding ufg to obtain the ufg fluxes and these in turn are summed over the broad group involved to obtain the broad group fluxes. Thus the broad group J flux in mesh interval i is given by

$$\phi^b_g(i) = \sum_j \phi^u_j(i) \Delta u.$$  \hspace{1cm} (V.89)

where the sum over hfg j extends over all hfg contained in bg J. The code edits the broad group fluxes per unit volume by dividing each of the $\phi^b_g(i)$ by the corresponding mesh interval volume.

Each spatial region is made up of one or more spatial mesh intervals each of which contains the same mixture of isotopes. The region R integrated bg fluxes are obtained by summing Eq. V.89 to yield

$$\phi^b_g(R) = \sum_i \phi^b_g(i)$$  \hspace{1cm} (V.90)

where the sum over i extends over all mesh intervals contained in region R.

The broad group, region dependent microscopic capture, fission, and scattering cross sections for each material m are obtained by dividing the reaction rate by the integrated flux. Therefore
where \( x \) corresponds to capture, fission, or scattering. \( \sigma_x^m(i) \) is the microscopic cross section for material \( m \) in mesh interval \( i \) and hfg \( j \) evaluated as described in Section D above. The sums over \( j \) and \( i \) as above extend over all hfg contained in bg \( J \) and all mesh intervals contained in region \( R \).

Now in order to calculate the scattering cross section from broad group \( J \) to broad group \( K \), we require the probability of scattering from each hfg \( j \) in bg \( J \) to bg \( K \).

If we let \( u_j \) be the lower lethargy of hfg \( j \) in bg \( J \), \( \Delta u_j \) be the lethargy width of hfg \( j \), \( U_K \) be the lower lethargy of bg \( K \), and \( \Delta U_K \) be the lethargy width of bg \( K \), then the probability of scattering by material \( m \) from hfg \( j \) into bg \( K \), if all parts of bg \( K \) can be reached by scattering from hfg \( j \), is given by

\[
P^m(j \rightarrow K) \Delta u_j = \frac{1}{1-\alpha^m} \int_{U_K}^{U_K+\Delta U_K} du \int_{u_j}^{u_j+\Delta u_j} du' e^{-(u-u')} = \frac{\Delta u_j}{1-\alpha^m} \left\{ \frac{e^{u_j-U_K}}{1-e^{-U_K}} \right\} \quad (V.92)
\]

In the case of the lowest broad group, say bg \( L \) which can be reached by scattering from hfg \( J \), since not all parts of bg \( L \) may be energetically reachable by scattering from hfg \( j \),

\[
P^m(j \rightarrow L) = \frac{1}{1-\alpha^m} \int_{U_j}^{u_j+\Delta u_j} du' \int_{u_j}^{u_j+\Delta u_j} du e^{-(u-u')} = \frac{\Delta u_j}{1-\alpha^m} e^{u_j-U_L} \frac{\alpha^m \Delta u_j}{1-\alpha^m} \quad (V.93)
\]

In Eqs. V.92 and V.93, contributions are made from each of the materials in the mixture.

Using Eqs. V.92 or V.93 as appropriate, the scattering from broad group \( J \) to broad group \( K \) for material \( m \) in region \( R \) is given by

\[
\sigma_{J \rightarrow K}^m(R) = \frac{\sum_i \sum_j \sigma_x^m(i) \phi_j(i) P^m(j \rightarrow K)}{\phi_{bg}^b(R)} \quad (V.94)
\]

where the sums over \( i \) and \( j \) are as above.
For foil materials, the capture, fission, and scattering cross sections are obtained as in Eq. V.91 where now the fluxes used are the averaged fluxes in each foil as given by Eq. V.62.

In addition to the region dependent cross sections, the code also edits quantities needed to calculate cell averaged macroscopic cross sections.

The all volume-averaged atom densities for each material \( m \) are computed as

\[
N_m^m(C) = \frac{\sum_R n^m(R) V(R)}{\sum_R V(R)}
\]

(V.95)

where \( n^m(R) \) is the atom density of material \( m \) in the composition contained in region \( R \) and \( V(R) \) is the volume of region \( R \). The sums extend over all regions in the cell.

Spatial self-shielding factors are computed for each broad group \( J \) and material \( m \) as

\[
F_J^m = \frac{\sum_R n^m(R) \phi_{bJ}^m(R) V(R)}{N_m^m(C) \sum_R \phi_{bJ}^m(R) V(R)}
\]

(V.96)

The product of \( N_m^m(C) \) and \( F_J^m \) represents the effective cell averaged atom density for use in creating effective cell averaged macroscopic cross sections. The consistent cell averaged microscopic cross sections for use with the effective atom densities \( N_m^m(C)F_J^m \) are given by

\[
\bar{\sigma}_{J, m}^m(C) = \frac{\sum_R \phi_{bJ}^m(R) \sigma_{J, m}^m(R) n^m(R) V(R)}{\sum_R \phi_{bJ}^m(R) n^m(R) V(R)}
\]

(V.97)

Thus the effective cell averaged macroscopic cross sections can be obtained from the product \( N_m^m(C)F_J^m \bar{\sigma}_{J, m}^m(C) \). Equation V.97 is used for capture, fission, scattering, and for transfer between broad groups.
VI. A GUIDE TO USER APPLICATION

A. **Standard Path STP015**

STP015 is a path driver of the ARC System which invokes the following modules to provide the MC$^2$-2 capability.

- **CSI010 (Area 4)**
  - Processes BCD input from files A.MCC2 and A.NIP

- **CSC004 (Area 5)**
  - Performs the unresolved resonance calculation

- **CSC005 (Area 6)**
  - Performs the resolved resonance calculation

- **CSC006 (Area 65)**
  - Calculates $\Sigma_p$ and performs resolved-unresolved resonance overlap calculations

- **CSC008 (Area 7)**
  - Calculates homogenized ultra-fine-group (ufg) cross sections, elastic scattering matrices, and moderating parameters

- **CSC009 (Area 8)**
  - Calculates the ufg real spectrum using multigroup and continuous slowing down (CSD) algorithms, obtains a critical buckling, and prepares broad group (bg) cross sections

- **CSC010 (Area 9)**
  - Calculates the bg fundamental mode real and adjoint spectra and obtains a critical buckling.

- **CSC011 (RABANL)**
  - Performs a hyper-fine-group (hfg) integral transport calculation and prepares rigorous resolved resonance cross sections

- **CSE009**
  - Edits broad group cross sections from data set ISOTXS

- **CSE007**
  - Prepares a single or double precision ARC System XS.ISO data set from the CCCC data set ISOTXS

- **CSE012**
  - Edits data set XS.ISO
The flow through the code as shown in the flow diagram, Fig. 9, is controlled by standard path STP015 in conjunction with the user supplied data in the A.STP015 BCD data set (Appendix B). As can be seen, the various code areas may be selectively included or excluded on user option. As a specific example, the user may select only CS1010 and RABANL, thereby effecting the equivalent of a RABBLE(5) or RABID(6) standalone calculation. Similarly if only module CSE012 is selected, a standalone XS.ISO editor capability is effect. Also e.g., if data sets related to the unresolved resonance calculation CSC004 are saved, a subsequent related execution of STP015 could reduce execution time by eliminating execution of this module.

A listing of the path STP015 is provided in Fig. 10.

B. Job Control Language Procedure ARCSP015

The Job Control Language procedure ARCSP015 is listed in Fig. 11. The procedure is consistent with IBM JCL conventions and with release 3.1 of the Attached Support Processor (ASP). The data set blocking is oriented toward use with 3330 magnetic disks.

The symbolic parameters used for the various datasets, their default values, usage, and corresponding DDNAME are given within the listing of the procedure. In addition, the contents of each of the datasets is given on comment cards in the procedure.

The parameters FULLBLK, HALFBLK, and UNITS which are used in many of the datasets are defined with the other symbolic parameters. The block size defaults of 12280 and 6136 for FULLBLK and HALFBLK are consistent with use of 3330 disks, and with the fact that IBM allocates space for buffers in blocks of 2K contiguous bytes (256 real*8 words). In the case of unformatted Fortran data sets (double buffered by default), the number of bytes of core required for buffers is given by 2*BLKSIZE+8 where BLKSIZE is given on the DD card and is rounded up to the nearest double word boundary. Thus, for example in the case of FULLBLK, 24576 bytes would be allocated for buffer space which corresponds to exactly 12, 2K blocks. This is only 8 bytes more than is required for the two buffers. The use of very closely an integral number of 2K byte blocks avoids the problem of possible core fragmentation when data sets are written, closed (rewound) and then read again several times during a run.

The use of SASCR and BATCHDSK for the UNIT parameter throughout the procedure correspond to ANL conventions for generic names corresponding to the class of units involved. SASCR is used to designate permanently resident disk packs for scratch data. BATCHDSK corresponds to both permanently resident and setup disk packs and is used for those files which may be saved on user option for later use. The default names for parameters MCC2F1, MCC2F2, ..., MCC2F8 correspond to the eight MC2-2 library files currently in use. The PRELIB and POSTLIB parameters used in the STEPLIB DD statement are provided to simplify concatenation of program library data sets. They default to empty partitioned data sets.

Through use of the catalogued procedure, the amount of JCL which must be provided by the user is vastly decreased. In particular, Fig. 12 lists the minimal JCL required to execute a problem using the catalogued procedure ARCSP015. Further illustrations of the use of this procedure and of the symbolic parameters are given in Section D, Sample Problem Input.
Fig. 9. MC²-2 Module Flow Diagram
STP015 is a standard path driver of the ARC system which
controls the MCC-2 cross section preparation capability.

Modules invoked by STP015

CSCI010 MCC-2 input processor
CSC004 MCC-2/SDX unresolved resonance calculation
CSC005 MCC-2/SDX resolved resonance calculation
CSC006 resolved-unresolved resonance overlap
CSC008 MCC-2 ultra-fine-group macroscopic data
processor
CSC009 MCC-2 ultra-fine-group spectrum calculation
and broad group collapse
CSC010 broad-group pl spectrum calculation
CSC011 hyper-fine-group integral transport spectrum
calculation
CSE009 editor of file ISOTXS
CSE007 ISOTXS to XS.ISO format conversion
CSE012 editor of file XS.ISO
NUE003 SIMPLOTTER line printer graphics

DECLARE ALL LITERAL VARIABLES TO BE DOUBLE PRECISION

C

C DOUBLE PRECISION DSNANE,CSI010,CSCI04,CSCI05,CSCI06,NUE003,
C CSCI08,CSCI09,CSCI10,CSE009,STP015,APATH,CSE007,
C CSE009,CSCI10,CSE009,CSCI010/6HSTP015/,APATH/8HA.STP015/,
C CSCI011/6HCSCI011/,UNREG/6HNREG/,
C CSCI012/6HCSCI012/

C

C DIMENSION NSTAND(6),PREC(2),DSNAME(89)
C COMMON /OUTPUT/NOUT

C

C SET LITERAL VARIABLES IN DATA STATEMENTS

C DATA CSI010/6HCSI010/,CSCI04/6HCSCI04/,CSCI05/6HCSCI05/,
C CSCI06/6HCSCI06/,CSCI08/6HCSCI08/,CSCI09/6HCSCI09/,
C CSCI10/6HCSCI10/,CSE009/6HCSE009/,STP015/6HSTP015/,
C NUE003/6HNUE003/,CSE007/6HCSE007/,APATH/8HA.STP015/,
C XSISO/6HXS.ISO/,CSCI011/6HCSCI011/,UNREG/6HNREG/,
C CSE012/6HCSCI012/

C DATA PREC/6HDDOUBLE,6HSINGLE/
C DATA DSNANE/
C 16HA.MCC2,6HA.NIP,8HA.STP015,6HATNUAT,6HBC,6HBGRES,
C 26HGEOM1,6HGRPORD,6HISOTXS,6HLORENZ,6HMACTOT,6HMCC2F1,
C 36HMCC2F2,6HMCC2F3,6HMCC2F4,6HMCC2F5,6HMCC2F6,6HMCC2F7,
C 46HMCC2F8,6HMCTOT,6HOLDGS,6HOPTICL,6HPLOTIT,6HPRBCHI,
C 56HPRBSPC,6HRESINT,6HSCR001,6HSCR002,6HSCR003,6HSCR004,
C 6HSCR005,6HSIGMAP,6HSMSIGS,6HSPECTR,6HSPECXS,6HSRATES,
C 76HUNREG,6HUNRES,6HXS.ISO,6HXSISO2,6HIRESCS,

Fig. 10. MC^2-2 Path Driver Listing
Fig. 10. MC\(^2\)-2 Path Driver Listing (Contd.)
WRITE (NOUT, 1200) PREC(ID01+1), PREC(2-ID01), PREC(2-ID01) 
ID01 = NSTAND(6) 
130 CONTINUE

C INVOKE AREA 4
C IF (TDO4.EQ.0) CALL LINK(CSI010)
C INVOKE AREA 5
C IF (TDO5.EQ.0) CALL LINK(CSC004)
C INVOKE AREA 6
C IF (TDO6.EQ.0) CALL LINK(CSC005)
C INVOKE AREA 6.5
C IF (TDO5.EQ.0.OR.TDO6.EQ.0) CALL LINK(CSC006)
C INVOKE AREA 7
C IF (TDO7.EQ.0) CALL LINK(CSC008)
C INVOKE AREA 8
C IF (TDO8.EQ.0) CALL LINK(CSC009)
C INVOKE AREA 9
C IF (TDO9.EQ.0) CALL LINK(CSC010)
C IF (TDO10 .NE. 1) GO TO 120
C IF (IUNREG.LE.0) CALL SNIFF(UNREG,IUNREG,12)
C INVOKE AREA 10
C CALL LINK(CSC017)
C 120 CONTINUE

C EDIT BROAD GROUP CROSS SECTIONS
C IF (TDO10.EQ.0) CALL LINK(CSE009)
C PREPARE A DOUBLE PRECISION OR SINGLE PRECISION VERSION OF 
C DATA SET XS.ISO ACCORDING TO WHETHER ID011 IS 0 OR 1, RESPECTIVELY 
C IF (ID011.EQ.0.OR.ID011.EQ.1) CALL LINK(CSE007,ID011)
C EDIT DATA SET XS.ISO

Fig. 10. MC²–2 Path Driver Listing (Contd.)
IF (IDO13 .NE. 0) CALL LINK (CSE012)

C
C INVOKE THE SIMPLOTTER PRINTER GRAPHICS PACKAGE
C

CALL LINK (NUE003, I0)
500 CONTINUE
1000 FORMAT (A8, 2I5/(I615))
1100 FORMAT (6X, 11I6)
1200 FORMAT (1H0, 129 (1H*)/1H 1H*, 3X, A6, 46H PRECISION CROSS SECTIONS MAY 1 NOT BE ADDED TO , A6, 45H PRECISION XS.ISO. NEW DATA ARE PROCESSED 2IN , A6, 11H PRECISION.. 4X, 1H*/1H , 129 (1H*))
RETURN
END

Fig. 10. MC2-2 Path Driver Listing (Contd.)
PARAMETER | DEFAULT VALUE | USAGE |
---|---|---|
PATH | STP015 | PROGRAM NAME |
TIMLIM | (600,0) | STEP TIME LIMIT |
REGN | 700K | STEP REGION SIZE |
MODLIB1 | C116.B09202.MODLIB | FIRST REAL LIBRARY |
MODLIB2 | C116.ARC.MODLIB | ARC SYSTEM LIBRARY |
PRELIB | SYS1.DUMMYLIB | FIRST STEP LIBRARY |
POSTLIB | SYS1.DUMMYLIB | LAST STEP LIBRARY |
DEST | A | OUTPUT DEST. (PRINTER) |
DMPDEST | F | ROUTE DUMP TO FICHE |

Fig. 11. MC2-2 JCL Procedure
// GRPORD &GRPORD DSN FOR FILE GRPORD 18
// GRPDSP (NEW,DELETE) DISPOSITION OF GRPORD 18
// GRPJCL ,UNIT=(SASCR,SEP=(DUMMY1,DUMMY2)) GRPORD UNIT & VOL 18
// ISOTXS &ISOTXS DSN FOR FILE ISOTXS 19
// ISODSP (NEW,DELETE) DISPOSITION OF ISOTXS 19
// ISOJCL ,UNIT=SASCR ISOJCL UNIT AND VOLUME 19
// ISOCYL 1 NO. CYL FOR X SECTIONS 19,50
// XSBLK2 6447 X SECTION BLOCKING 19,50
// MCC2F1 C116.MCC2F1.MEV14.V4 LIBRARY FILE 1 DSN 22
// MCC2F2 C116.MCC2F2 LIBRARY FILE 2 DSN 23
// MCC2F5 C116.MCC2F5.MEV14.V4 LIBRARY FILE 5 DSN 26
// MCC2VOL LIBRARY VOLUME 22-29
// OLDSGS NULLFILE RESTART ELASTIC MATRICES 31
// OLDSVOL NULLFILE VOLUME FOR OLDSGS 31
// SMSIGS 6SMSIGS PROBLEM ELASTIC MATRICES 43
// SCATBLK 12280 BLKSIZE FOR SMSIGS 43
// SCATDSP (NEW,DELETE) DISPOSITION OF SMSIGS 43
// SCATJCL ,SUBALLOC=(CYL,(20,3),DUMMY2) SMSIGS UNIT,SPACE & VOL 43
// SPECTR &SPECTR DSN FOR SPECTRUM FILE 44
// SPECDSP (NEW,DELETE) DISPOSITION OF SPECTRUM 44
// SPECJCL ,UNIT=SASCR SPECTRUM UNIT AND VOLUME 44
// MICRXS1 &MICRXS1 XS.ISO FILE 1 DSN 49
// XSBKL1 3156 BLOCKING FOR 6MICRXS1 49
// MICRXS2 6MICRXS2 XS.ISO FILE 2 DSN 50
// MICRDS2 (NEW,DELETE) DISPOSITION OF XS.ISO 49-50
// MICRVol ------ VOLUME OF FILE XS.ISO 49-50
// ATNUAT &ATNUAT DSN FOR FILE ATNUAT 14
// RESINT 8RESINT DSN FOR FILE RESINT 36
// UNRES 8UNRES DSN FOR FILE UNRES 48

THE FOLLOWING THREE PARAMETERS ARE APPLICABLE TO THE THREE
RESONANCE FILES ATNUAT, RESINT AND UNRES

RESBLK 12280 FILE BLKSIZE 14,36,48
RESDSP (NEW,DELETE) FILE DISPOSITION 14,36,48
RESJCL ,UNIT=SASCR FILE UNIT AND VOLUME 14,36,48

THE FOLLOWING THREE PARAMETERS DEFINE UNIT AND BLKSIZE FOR A
VARIETY OF FILES

FULLBLK 12280 FULL TRACK BLOCKING
HALFBLK 6136 HALF TRACK BLOCKING
UNITS BATCHDSK GENERIC UNIT NAME
UNITSCR SASCR GENERIC SCRATCH UNIT

---

Fig. 11. M2-2 JCL Procedure (Contd.)
Fig. 11. MC\textsuperscript{2}-2 JCL Procedure (Contd.)
DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&XSBLK2)

BROAD GROUP CROSS SECTION FILE IN CCCC FORMAT ISOTXS

DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)

LORENTZIAN J-INTEGRALS FOR WIDE RESONANCES

MACROSCOPIC TOTAL CROSS SECTION

FILE 1 OF MCC-2 LIBRARY

FILE 2 OF MCC-2 LIBRARY

FILE 3 OF MCC-2 LIBRARY

FILE 4 OF MCC-2 LIBRARY

FILE 5 OF MCC-2 LIBRARY

FILE 6 OF MCC-2 LIBRARY

FILE 7 OF MCC-2 LIBRARY

FILE 8 OF MCC-2 LIBRARY

MICROSCOPIC TOTAL CROSS SECTIONS

MICROSCOPIC SCATTERING MATRICES SAVED FROM PREVIOUS EXECUTION FOR RESTART PURPOSES

Fig. 11. MC^2-2 JCL Procedure (Contd.)
OPTICAL THICKNESS DATA
FT33F001 DD DSN=&PLOTIT,UNIT=&UNITSCR,SPACE=(TRK,(1,1)), DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)

SPMIMPUTER DATA FILE
FT34F001 DD DSN=&PRBCHT,UNIT=&UNITSCR,SPACE=(CYL,(1,1)), DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)

FISSION SPECTRUM DATA
FT35F001 DD DSN=&PRBPSPC,UNIT=&UNITSCR,SPACE=(TRK,(1,1)), DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)

MCC-2 GENERAL PROBLEM SPECIFICATIONS
FT36F001 DD DSN=&RESINT, DISP=&RESDSP&RESJCL, DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&RESBLK), SPACE=(CYL,(1,1))

RESOLVED RESONANCE J-INTEGRALS
FT37F001 DD DSN=&SCR001, SUBALLOC=(CYL,(1,1),DUMMY1), DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)

SCRATCH DATA
FT38F001 DD DSN=&SCR002, SUBALLOC=(CYL,(1,1),DUMMY1), DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)

SCRATCH DATA
FT39F001 DD DSN=&SCR003, SUBALLOC=(CYL,(23,1),DUMMY1), DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)

SCRATCH DATA
FT40F001 DD DSN=&SCR004, SUBALLOC=(CYL,(1,1),DUMMY1), DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)

SCRATCH DATA
FT41F001 DD DSN=&SCR005, SUBALLOC=(CYL,(1,1),DUMMY1), DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)

SCRATCH DATA
FT42F001 DD DSN=GSCRO0~, SUBALLOC=(CYL,(1,1),DUMMY1), DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)

SCRATCH DATA
FT43F001 DD DSN=&SMSIGS, DISP=&SCATDSP&SCATJCL, DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&SCATBLK)

MICROSCOPIC ELASTIC SCATTERING MATRICES
FT44F001 DD DSN=&SPECSTR, DISP=&SPECDSP&SPECJCL, SPACE=(TRK,(1,1)), DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)

ULTRA-FINE-GROUP FLUX AND CURRENT SPECTRA
FT45F001 DD DSN=&SPECXS, UNIT=&UNITSCR, SPACE=(CYL,(1,1)), DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)

ULTRA-FINE-GROUP MACROSCOPIC CROSS SECTIONS AND MODERATING PARAMETERS
FT46F001 DD DSN=&SRA'IES, UNIT=&UNITSCR, SPACE=(TRK,(1,1)), DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)

SCATTERING COLLISION DENSITY AND EXTERNAL SOURCE FOR INTEGRAL TRANSPORT CALCULATION
FT47F001 DD DSN=&UNREG,UNIT=&UNITSCR,SPACE=(CYL,(1,1))

Fig. 11. MC\textsuperscript{2}-2 JCL Procedure (Contd.)
DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&FULLBLK)

UNRESOLVED MICROSCOPIC ULTRA-FINE-GROUP CROSS SECTIONS

//FT48F001 DD DSN=&UNRES,
// DISP=&RESDSP&RESJCL,
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&RESBLK),
// SPACE=(CYL,(1,1))

UNRESOLVED RESONANCE CROSS SECTION-ESTAR PAIRS

//FT49P001 DD DSN=&MICRXS1,
// UNIT=&UNITS,VOL=(,RETAIN,SER=&MICRVOL),
// DISP=&MICRDSP,SPACE=(TRK,(1,1))

FILE 1 CP BROAD GROUP XS.ISO CROSS SECTION FILE

//FT50F001 DD DSN=&MICRXS2,
// UNIT=&UNITS,VOL=(,RETAIN,SER=&MICRVOL),
// DISP=&MICRDSP,SPACE=(CYL,(ISOCYL,1))

FILE 2 OF BROAD GROUP XS.ISO CROSS SECTION FILE

//FT51F001 DD DSN=&IRESCS,UNIT=&UNITSCR,SPACE=(CYL,(ISOCYL,1))

BROAD GROUP INTEGRAL TRANSPORT RESONANCE CROSS SECTIONS

//FT52F001 DD DSN=&BIGXS1,SUBALLOC=(CYL,(2,1),DUMMY2),
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)

//FT53P001 DD DSN=&BIGXS2,SUBALLOC=(CYL,(2,1),DUMMY2),
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)

//FT54P001 DD DSN=&BIGXS3,SUBALLOC=(CYL,(2,1),DUMMY2),
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)

//FT55P001 DD DSN=&BIGXS4,SUBALLOC=(CYL,(2,1),DUMMY2),
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)

//FT56P001 DD DSN=&BIGXS5,SUBALLOC=(CYL,(2,1),DUMMY2),
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)

//FT57P001 DD DSN=&BIGXS6,SUBALLOC=(CYL,(2,1),DUMMY2),
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)

//FT58P001 DD DSN=&BIGXS7,SUBALLOC=(CYL,(2,1),DUMMY2),
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)

//FT59P001 DD DSN=&BIGXS8,SUBALLOC=(CYL,(2,1),DUMMY2),
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)

//FT60P001 DD DSN=&BIGXS9,SUBALLOC=(CYL,(2,1),DUMMY2),
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)

//FT61P001 DD DSN=&BIGXSA,SUBALLOC=(CYL,(2,1),DUMMY2),
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)

//FT62P001 DD DSN=&BIGXSZ,SPACE=(CYL,(0,1)),UNIT=&UNITSCR,
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)

//FT63P001 DD DSN=&BIGXSC,SPACE=(CYL,(0,1)),UNIT=&UNITSCR,
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)

//FT64P001 DD DSN=&BIGXSD,SPACE=(CYL,(0,1)),UNIT=&UNITSCR,
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFBLK)

Fig. 11. MC²-2 JCL Procedure (Contd.)
Fig. 11. \( M^2-2 \) JCL Procedure (Contd.)
C. Problem Specification

The user input to the MC²-2 code is supplied on various card types from the BCD data sets A.STP015, A.MCC2, A.NIP, ACS009, and ACSE12. These data sets are described in the listings given in Appendix B. Table III summarizes the use of the various BCD data sets. This first release of MC²-2 lacks a full heterogeneous treatment in that heterogeneous broad group cross sections are not yet generated by CSC009.

The input data deck for the execution of MC²-2 follows the general ARC System format as described on pages 42-45 of Reference 1. A data set initialization block (DSIB) given the block name "OLD" is used if any data sets are to be used which were generated in previous jobs. In the case of the eight MC²-2 library files (MCC2F1-MCC2F8), the path driver STP015 has been written so that these files need not be named in a DSIB. The format of these library files which are normally written by the ETOE-2 code are given in Appendix C. One common use of the DSIB with MC²-2 is the addition of material cross sections to an existing XS.ISO file by the module CSE007. In this case the card DATASET=XS.ISO appears in the dataset initialization block.

The DSIB, if any, is followed in the input deck by a data block given the name STP015. This block may include the path dependent data set A.STP015 and the data sets A.MCC2, A.NIP, ACS009, and ACSE12. These data sets are discussed below in greater detail and examples of BCD input data are given in Section D, Sample Problems.

The BCD input processor has been written with particular attention to easing the burden on the user when preparing problem input. By using defaults, many of the card types may be omitted for a given problem. Thus for example, as a minimum for homogeneous problems, only type 06 cards of data set A.MCC2 need be supplied if the defaults supplied are acceptable to the user. Similarly, for heterogeneous problems, as a minimum one type 03 card of data set A.MCC2 and the type 06, 14, and 15 cards of data set A.NIP need be supplied.

In order to ease user specification work load, eleven prestored broad group structures are available on option in MC²-2. These structures are selected as indicated on card type 03, cols. 31-36. If any type 05 or type 07 cards are supplied, the card type 03 selection, if any, is ignored. Similarly, if an old XS.ISO data set is included in the DSIB as discussed above, the card type 03 selection is ignored. If card type 03 is not supplied or if cols. 31-36 are blank and no type 05 or 07 cards are supplied, a built in default structure will be used.

In order to ease user specification work load, eleven prestored broad group structures are available on option in MC²-2. These structures are selected as indicated on card type 03, cols. 31-36. If any type 05 or type 07 cards are supplied, the card type 03 selection, if any, is ignored. Similarly, if an old XS.ISO data set is included in the DSIB as discussed above, the card type 03 selection is ignored. If card type 03 is not supplied or if cols. 31-36 are blank and no type 05 or 07 cards are supplied, a built in default structure will be used.

The group structures for each of the eleven sets are given in Table IV which lists the broad group lethargy widths and upper energy boundaries. The upper energy of all of the sets is 10 MeV except for set USS226 which has an upper energy of 14.190675 MeV. Note that the last group for the BOND26 and the last two groups for the HANS16 sets have been changed relative to the original structures. This was required due to the fact that the current MC²-2 library has a lower energy of 0.41399 eV. Also, the third from the last group in the sets USS212 and USS226 was altered slightly in order to fall on an integral multiple of an MC²-2 ultra fine group.
# TABLE III. BCD Input Data Sets

<table>
<thead>
<tr>
<th>Data Set Name</th>
<th>Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>A.STP015</td>
<td>Needed only if various of the code Areas 4 - 9 are to be omitted, if RABANL is to be executed, if broad group cross sections are not to be edited, if data set XS.ISO is not to be written, or if XS.ISO is to be edited.</td>
</tr>
<tr>
<td>A.MCC2</td>
<td>Always present unless only data set XS.ISO and/or ISOTXS is to be edited.</td>
</tr>
<tr>
<td>A.NIP</td>
<td>Needed only if a heterogeneous problem is involved.</td>
</tr>
<tr>
<td>ACSE12</td>
<td>Needed only if data set XS.ISO is to be edited, and then only if a non-standard edit is desired.</td>
</tr>
<tr>
<td>ACS009</td>
<td>Needed only if data set ISOTXS is to be edited, and then only if a non-standard edit is desired.</td>
</tr>
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</tbody>
</table>

*USS226 is the same as USS212 except that an additional 14 groups with Δu = 0.025 are added above group 1 up to an upper energy of 14.190675 MeV.*
<table>
<thead>
<tr>
<th>Group</th>
<th>Lethargy Width</th>
<th>Group</th>
<th>Lethargy Width</th>
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</table>
D. Sample Problems

A number of examples of typical MC²-2 problems will be given in this section along with a listing of the user supplied BCD data.

1. Homogeneous Reference Problem

The user input deck is shown in Fig. 13.

This problem creates the XS.ISO data set having the data set names C116.BXXXXX.XSISOFl and C116.BXXXXX.XSISOF2 for files 1 and 2 respectively as specified in the symbolic parameters MICRXS1 and MICRXS2. The data set will be catalogued as specified in the symbolic parameter MICRDSP. No data set initialization block is specified.

The type 01 card of data set A.STP015 is set to execute Areas 4, 5, 6, 6.5, 7, 8, and 9, to edit the broad group cross sections, and to create a double precision XS.ISO data set. This could also have been accomplished by supplying a card with only 01 in columns 1 and 2. Also, these same choices could have been selected by omitting the DATASET=A.STP015 card and the type 01 card which follows it since the standard defaults are used.

The data set A.MCC2 type 01 cards provide title information desired by the user.

The type 02 card specifies a BPOINTER main core container of 25000 real*8 words.

The type 03 card uses defaults for all fields except for columns 7-12 and 31-36 in which a consistent P1 fundamental mode calculation and the standard ANL27 broad group structure are specified.

The type 06 cards specify the five isotopes in the problem along with their atom densities. The problem material names were omitted from columns 19-24 and will default to the names given in columns 13-18. Also, the temperatures all default to 300 degrees K and all cross sections will be added to the output cross section data set.

The type 16 card specifies that the fission spectrum of PU2394 be used for all fissionable nuclides.

The type 22 cards classify the problem isotopes and assign values for MeV/fission for U-2384 and PU2394.

2. Hyper-fine Group Homogeneous Integral Transport Problem

The user input deck is shown in Fig. 14.

This problem corresponds to a standalone RABID(6) calculation for the homogeneous composition given in the previous example.
The type 01 card of data set A.STP015 is set to execute only the input processor Area 4 and the RABANL module.

As in example 1, a container of 25000 real*8 words is specified on card type 02 of data set A.MCC2.

The same type 06 cards are used as in example 1.

A fixed buckling of 0.0011466 is specified on the type 09 card.

The type 14 card specifies 3354.4 eV as the upper energy for the calculation with all other fields on that card using the default values specified.

The mixture temperature is specified as 300 degrees K on the type 21 card.

3. Hyper-fine Group Heterogeneous Integral Transport Problem

The user input deck is shown in Fig. 15.

This problem corresponds to a standalone RABI(6) calculation for a six slab region heterogeneous problem.

As in example 2, the data set A.STP015 type 01 card is set to execute only Area 4 and RABANL.

A larger container of 30000 real*8 words is specified on the data set A.MCC2 type 02 card. Since this is the default, the type 02 card could have been omitted.

The type 03 card again specifies the ANL27 broad group structure and 1 in column 42 indicates slab geometry.

No data set A.MCC2 type 06 cards are supplied so that the mixture composition will be derived from the data set A.NIP input.

The upper energy of the problem is specified to be 275.36425 electron volts on the type 14 card.

The type 15 cards define two foils.

The type 21 card assigns a temperature of 293 degrees K to each of the compositions defined in the data set A.NIP type 14 cards.

The data set A.NIP type 04 card indicates that the left and right cell boundaries have reflective boundary conditions.

The A.NIP type 06 cards define the dimensions of the three regions in the problem. Because of the reflective boundary conditions, both regions MATX and CLAD 1 will have double the thicknesses as given on the type 06 cards.

The three compositions MATX, U308, and CLADA are defined on the type 14 cards.
The composition - region assignments are made on the type 15 cards.

E. Error Messages

Error messages issued by various subroutines of the modules of MC\textsuperscript{2}-2 are listed in Table V. The subroutines are presented alphabetically within each module, and the error messages for each subroutine are listed in numerical order.

The convention used is that fatal errors are negative, while non-fatal errors are positive.

As a general rule, fatal errors will not halt execution until the particular module involved has been completed. This will not be true in those cases in which the error results in some subsequent computer system error such as a divide check, core region violation, etc.

Also included are the error messages issued by the ANL version of the CCCC compatible I/O routine REED/RITE.\textsuperscript{(2)}
Figure 12
Minimum JCL Execution Deck

//MINJCL JOB (FXXXXX,20,,MM),'YOUR CHOICE',MSGLEVEL=1,CLASS=A,
// ACCOUNTING INFORMATION
// EXEC ARCSPO15
//SYSIN DD *
PROBLEM INPUT DATA
/*

Figure 13
Input for Sample Problem 1

//SAMPLE1 JOB (FXXXXX,20,,05),'YOUR CHOICE',MSGLEVEL=1,CLASS=A,
// ACCOUNTING INFORMATION
// EXEC ARCSPO15,
// MICRXS1='C116.BXXXXX.XSISOF1',
// MICRXS2='C116.BXXXXX.XSISOF2',
// MICRDS2='(NEW,CATLG)'
//SYSIN DD *
BLOCK=STP015
DATASET=A.STP015
01 0 0 0 0 0 0 0 0 0
DATASET=A.MCC2
01 25000
02 3
03 ANL27
06 U-2384 .006383
06 PU2394 .001086
06 NA23 4 .01041
06 O-16 4 .01419
06 FE 4 .01814
16 PU2394
22 U-2384 2 201.8150613
22 PU2394 1 215.7333414
22 NA23 4 6
22 O-16 4 0
22 FE 4 5
/*
Figure 14
Input for Sample Problem 2

//SAMPLE2 JOB (FXXXXX,20,,05), 'YOUR CHOICE', MSGLEVEL=1, CLASS=C,
// REGION=550K
ACCOUNTING INFORMATION
// EXEC ARCSPO15
// SYSIN DD *
BLOCK=STP015
DATASET=A.STP015
01 0 1 1 1 1 1 1 1 -1 1
DATASET=A.MCC2
01 01 01 END

FIVE ISOTOPE HOMOGENEOUS REFERENCE PROBLEM
STANDALONE HYPER-FINE-GROUP INTEGRAL TRANSPORT (RABANL)
CALCULATION
BPOINTER CONTAINER IS SET TO 25000 WORDS
STANDARD ANL27 BROAD GROUP STRUCTURE
FIXED BUCKLING IS SET TO .0011466
TOP ENERGY OF PROBLEM IS SET TO 3354.4 ELECTRON VOLTS
MIXTURE TEMPERATURE IS SET TO 300 DEGREES KELVIN

25000

ANL27
06 U-2384 .006383
06 PU2394 .001086
06 NA23 4 .01041
06 O-16 4 .01419
06 FE 4 .01814
09 .0011466
14 3354.4
21 300.0
/*
Figure 15
Input for Sample Problem 3

//SAMPLE3 JOB (FXXXXX,20,,08),'YOUR CHOICE',MSGLEVEL=1,CLASS=C, REGION=650K
ACCOUNTING INFORMATION
// EXEC ARCSP015
// SYSIN DD *
BLOCK=STP015
DATASET=A.STP015

01 0 1 1 1 1 1 1 1
DATASET=A.MCC2

01 ************************************************************
01 * ENDF/B-IV DATA *
01 * SIX REGION HETEROGENEOUS PROBLEM *
01 * STANDALONE HYPER-FINE-GROUP INTEGRAL TRANSPORT (RABANL) *
01 * CALCULATION *
01 * BPOINTER CONTAINER IS SET TO 30000 WORDS *
01 * STANDARD ANL27 BROAD GROUP STRUCTURE *
01 * TOP ENERGY OF PROBLEM IS SET TO 275.36426 EV *
01 * ALL COMPOSITION TEMPERATURES SET TO 293 DEGREES K *
01 ************************************************************
02 30000
03
14 275.36425
15 FOILA U-2354 .00003 .00036
15 FOILB PU2394 .00015 PU2414 .000025 .00044
21 MATX 293. U308 293. CLADA 293.
DATASET=A.NIP

04 10 10
06 MATX 0.0 0.286 1
06 U308 0.286 0.921 1
06 CLAD 0.921 0.959 1
14 MATX MO 4 0.00005 0-16 4 0.00025 FE 4 0.04474
14 MATX NI 4 0.005479 CR 4 0.01257 MN55 4 0.00101
14 U308 U-2354 0.0000336 U-2384 0.01572 0-16 4 0.04201
14 CLADA NI 4 0.009832 CR 4 0.01939 MN55 4 0.00147
14 CLADA MO 4 0.000075 0-16 4 0.00038 FE 4 0.06811
15 MATX MATX
15 U308 U308
15 CLADA CLAD 1
/*
TABLE V. MC²-2 Error Messages

<table>
<thead>
<tr>
<th>Subroutine CARD05</th>
<th>Error Messages</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fatal Error -10100</td>
<td>CARD PRESUMED TO BE TYPE 05 NOT FOUND</td>
</tr>
<tr>
<td>Fatal Error -10200</td>
<td>THE FIRST GROUP NUMBER AND UPPER ENERGY OF THAT GROUP MUST BE GIVEN ON THE FIRST TYPE 05 CARD</td>
</tr>
<tr>
<td>Fatal Error -10300</td>
<td>BROAD GROUP ENERGIES MUST ALL BE SPECIFIED</td>
</tr>
<tr>
<td>Fatal Error -10400</td>
<td>THE HIGHEST ENERGY BROAD GROUP IN THE PROBLEM MAY NOT LIE ABOVE THE HIGHEST ENERGY IN THE LIBRARY</td>
</tr>
<tr>
<td>Fatal Error -10500</td>
<td>ALL GROUPS MUST BE SPECIFIED</td>
</tr>
<tr>
<td>Fatal Error -10600</td>
<td>BROAD GROUP ENERGIES MUST ALL BE UNIQUE</td>
</tr>
<tr>
<td>Fatal Error -10700</td>
<td>THE SPECIFIED BROAD GROUP STRUCTURE EXTENDS BELOW THE BOTTOM OF THE LIBRARY GROUP STRUCTURE</td>
</tr>
<tr>
<td>Fatal Error -10800</td>
<td>IF ONLY ONE UPPER ENERGY IS GIVEN, IT MUST CORRESPOND TO GROUP 1</td>
</tr>
<tr>
<td>Fatal Error -10900</td>
<td>THE HIGHEST BROAD GROUP SPECIFIED LIES BELOW THE LOWEST ENERGY IN THE LIBRARY</td>
</tr>
<tr>
<td>Fatal Error -11000</td>
<td>THE ADJUSTED BROAD GROUP ENERGY BOUNDARIES MUST ALL BE UNIQUE.</td>
</tr>
</tbody>
</table>

Subroutine CARD06

| Fatal Error -10100 | CARD PRESUMED TO BE TYPE 06 NOT FOUND                                         |
| Fatal Error -10200 | EACH MATERIAL MUST CORRESPOND TO SOME LIBRARY MATERIAL                       |
| Fatal Error -10400 | MATERIAL NAMES MUST BE NON-BLANK                                              |

Subroutine CARD07

| Fatal Error -10100 | CARD PRESUMED TO BE TYPE 07 NOT FOUND                                         |
| Fatal Error -10200 | LETHARGY WIDTHS SPECIFIED ON TYPE 07 CARDS MUST BE GREATER THAN ZERO         |
| Fatal Error -10300 | FINAL BROAD GROUP NUMBERS IN COLS. 31-36 ON TYPE 07 CARDS MUST BE .GE. INITIAL BROAD GROUP NUMBERS GIVEN IN COLS. 25-30 |
Fatal Error -10400. FINAL BROAD GROUP NUMBERS IN COLS. 55-60 ON TYPE 07 CARDS MUST BE .GE. INITIAL BROAD GROUP NUMBERS GIVEN IN COLS. 49-54

Fatal Error -10500. THE FIRST BROAD GROUP NUMBER MUST BE 1

Fatal Error -10600. THE BROAD GROUP NUMBERS MUST ALL BE SPECIFIED

Fatal Error -10700. THERE MAY BE NO MORE BROAD GROUPS THAN THERE ARE ULTRA FINE GROUPS IN THE LIBRARY

Fatal Error -10800. THE PRESTORED BROAD GROUP STRUCTURE SELECTED IS NOT CONSISTENT WITH THE LIBRARY ENERGY STRUCTURE

Fatal Error -10900. THE PRESTORED BROAD GROUP STRUCTURE SELECTED IS NOT CONSISTENT WITH THE LIBRARY ENERGY STRUCTURE

Subroutine CARD08

Fatal Error -10100. CARD PRESUMED TO BE TYPE 08 NOT FOUND

Fatal Error -10200. LOWER ENERGY BROAD GROUP NUMBER IN COLS. 31-36 ON TYPE 08 CARDS MUST BE .GE. HIGHER ENERGY BROAD GROUP NUMBER IN COLS. 25-30

Fatal Error -10300. LOWER ENERGY BROAD GROUP NUMBERS IN COLS. 55-60 ON TYPE 08 CARDS MUST BE .GE. HIGHER ENERGY BROAD GROUP NUMBERS IN COLS. 49-54

Fatal Error -10400. MATERIAL SPECIFIED IN COLS. 25-30 ON TYPE 08 CARD DOES NOT CORRESPOND TO ANY FISSION SPECTRUM MATERIAL NAME ON DATA SET MCC2F7

Fatal Error -10500. ONLY INITIAL ENERGY INDEPENDENT FISSION SPECTRA MAY BE SPECIFIED ON TYPE 08 CARDS

Fatal Error -10600. MATERIAL SPECIFIED IN COLS. 25-30 ON TYPE 08 CARD DOES NOT CORRESPOND TO ANY PROBLEM MATERIAL

Subroutine CARD09

Fatal Error -10100. CARD PRESUMED TO BE TYPE 09 NOT FOUND

Fatal Error -10200. THE ULTRA FINE GROUP NUMBER IN COLS. 55-60 ON TYPE 09 CARDS MUST BE GREATER THAN OR EQUAL TO THE ULTRA FINE GROUP NUMBER IN COLS. 49-54

Fatal Error -10300. CARD PRESUMED TO BE TYPE 09 NOT FOUND
TABLE V. Contd.

CSI010 (AREA 4) Contd.

Subroutine CARD09 (contd.)

Fatal Error -10400. 
THE ULTRA FINE GROUP NUMBERS IN COLS. 49-54 ON TYPE 
09 CARDS MUST BE .GT.0

Fatal Error -10500. 
THE ULTRA FINE GROUP NUMBER IN COLS. 55-60 ON TYPE 
09 CARDS MUST BE GREATER THAN OR EQUAL TO THE ULTRA 
FINE GROUP NUMBER IN COLS. 49-54

Error 10600. 
THE CONVERGENCE CRITERION ON THE TYPE 09 CARD 
MUST BE .GE. 0.

Fatal Error -10700. 
BUCKLING ITERATION IS NOT POSSIBLE FOR AN 
INHOMOGENEOUS SOURCE PROBLEM

Fatal Error -10800. 
BUCKLING ITERATION IS NOT ALLOWED FOR GROUP DEPENDENT 
BUCKLINGS

Fatal Error -10900. 
BUCKLING ITERATION IS NOT ALLOWED FOR INHOMOGENEOUS 
SOURCE PROBLEMS

Subroutine CARD10

Fatal Error -10100. 
CARD PRESUMED TO BE TYPE 10 NOT FOUND

Fatal Error -10200. 
NUCLIDE IDENTIFICATION LABELS ON TYPE 10 CARDS 
MUST CORRESPOND TO SOME PROBLEM MATERIAL

Subroutine CARD11

Fatal Error -10100. 
CARD PRESUMED TO BE TYPE 11 NOT FOUND

Fatal Error -10200. 
NUCLIDE IDENTIFICATION LABELS ON TYPE 11 CARDS 
MUST CORRESPOND TO SOME PROBLEM MATERIAL

Subroutine CARD12

Fatal Error -10100. 
CARD PRESUMED TO BE TYPE 12 NOT FOUND

Fatal Error -10200. 
MATERIAL NAMES MUST BE NON-BLANK

Error 10300. 
MATERIALS SPECIFIED ON TYPE 12 CARDS MUST BE PRESENT 
IN THE PIN REGION

Error 10400. 
MATERIALS SPECIFIED ON TYPE 12 CARDS MUST BE 
RESONANCE MATERIALS

Fatal Error -10500. 
ALL MATERIALS SPECIFIED ON TYPE 12 CARDS MUST 
CORRESPOND TO SOME PROBLEM MATERIAL

Fatal Error -10600. 
CARD PRESUMED TO BE TYPE 12 NOT FOUND
TABLE V. Contd.

CSI010 (AREA 4) Contd.

Subroutine CARD12 (contd.)

Fatal Error -10700. MATERIAL NAMES MUST BE NON-BLANK
Fatal Error -10800. CARD PRESUMED TO BE TYPE 12 NOT FOUND
Fatal Error -10900. MATERIAL NAMES MUST BE NON-BLANK
Error 11000. ONLY ONE TYPE 12 CARD MAY BE SUPPLIED FOR A GIVEN MATERIAL WITH COLS. 13-18 BLANK
Fatal Error -11100. ALL REGIONS REFERRED TO IN COLS. 14-24, 31-36, 43-48, 55-60, AND 67-72 ON TYPE 12 CARDS MUST CORRESPOND TO SOME REGION ON THE DATA SET A.NIP TYPE 06 CARDS
Fatal Error -11200. ALL MATERIALS REFERRED TO ON TYPE 12 CARDS MUST CORRESPOND TO SOME PROBLEM MATERIAL
Fatal Error -11300. ALL REGIONS REFERRED TO IN COLS. 13-18, 25-30, 37-42, 49-54, AND 61-66 ON TYPE 12 CARDS MUST CORRESPOND TO SOME REGION DEFINED ON THE DATA SET A.NIP TYPE 06 CARDS
Fatal Error -11400. NO REGION REFERRED TO IN COLS. 19-24, 31-36, 43-48, 55-60, OR 67-72 ON TYPE 12 CARDS MAY ALSO BE REFERRED TO IN COLS. 13-18, 25-30, 37-42, 49-57, OR 61-66

Subroutine CARD14

Fatal Error -10100. CARD PRESUMED TO BE TYPE 14 NOT FOUND
Fatal Error -10300. THE ENERGY SPECIFIED IN COLS. 13-25 OF CARD TYPE 14 OR THE DEFAULT VALUE OF 300.0 VOLTS FALLS INTO THE THERMAL GROUP
Fatal Error -10400. THE ENERGY SPECIFIED IN COLS. 13-25 OF CARD TYPE 14 OR THE DEFAULT VALUE OF 300.0 VOLTS FALLS ABOVE THE HIGHEST ENERGY IN THE PROBLEM

Subroutine CARD15

Fatal Error -10100. CARD PRESUMED TO BE TYPE 15 NOT FOUND
Fatal Error -10200. FOIL LABELS MUST BE NON-BLANK
Fatal Error -10300. THE FIRST MATERIAL LABEL ON A TYPE 15 CARD WAS BLANK
Fatal Error -10400. MATERIALS IN FOILS MUST CORRESPOND TO LIBRARY MATERIAL
Fatal Error -10500. MATERIALS MAKING UP A GIVEN FOIL MUST BE DISTINCT
Fatal Error -10600. CARD PRESUMED TO BE TYPE 15 NOT FOUND
TABLE V. Contd.

CSIO10 (AREA 4) Contd.

Subroutine CARD15 (contd.)

Fatal Error -10700. FOIL LABELS MUST BE NON-BLANK
Fatal Error -10800. THE FIRST MATERIAL LABEL ON A TYPE 15 CARD WAS BLANK
Fatal Error -10900. POSITIVE FOIL THICKNESSES MUST BE SPECIFIED
Fatal Error -11000. POSITIVE FOIL THICKNESSES MUST BE SPECIFIED

Subroutine CARD16

Fatal Error -10100. CARD PRESUMED TO BE TYPE 16 NOT FOUND
Fatal Error -10200. FISSION SPECTRUM NUCLIDE IDENTIFICATION LABELS ON TYPE 16 CARDS MUST CORRESPOND TO LIBRARY FISSION SPECTRA LABELS
Fatal Error -10300. ONLY ONE TYPE 16 CARD MAY BE SPECIFIED WITH COLS. 13-18 BLANK
Fatal Error -10400. FISSIONABLE NUCLIDE IDENTIFICATION LABELS ON TYPE 16 CARDS MUST CORRESPOND TO PROBLEM NUCLIDE IDENTIFICATION LABELS

Subroutine CARD17

Fatal Error -10100. CARD PRESUMED TO BE TYPE 17 NOT FOUND
Fatal Error -10200. LETHARGY WIDTHS SPECIFIED ON TYPE 17 CARDS MUST BE GREATER THAN ZERO
Fatal Error -10300. FINAL FIXED MESH POINT NUMBERS IN COLS. 31-36 ON TYPE 17 CARDS MUST BE .GE. INITIAL FIXED MESH POINT NUMBERS GIVEN IN COLS. 25-30
Fatal Error -10400. FIXED MESH POINT NUMBERS IN COLS. 55-60 ON TYPE 17 CARDS MUST BE .GE. INITIAL MESH POINT NUMBERS GIVEN IN COLS. 49-54
Fatal Error -10500. THE FIRST FIXED MESH POINT NUMBER MUST BE 1
Fatal Error -10600. THE FIXED MESH POINT NUMBERS MUST ALL BE SPECIFIED
Fatal Error -10700. A MAXIMUM OF 500 FIXED ENERGY MESH POINTS ARE PERMITTED
Fatal Error -10800. THE UNRESOLVED ENERGY REGION FALLS BELOW THE FIXED ENERGY GRID
TABLE V. Contd.

CSI010 (AREA 4) Contd.

Subroutine CARD18

Fatal Error -10100. CARD PRESUMED TO BE TYPE 18 NOT FOUND
Error 10200. ALL MATERIALS NAMED ON TYPE 18 CARDS MUST CORRESPOND TO SOME PROBLEM MATERIAL

Subroutine CARD21

Fatal Error -10100. CARD PRESUMED TO BE TYPE 21 NOT FOUND
Fatal Error -10200. CARD PRESUMED TO BE TYPE 21 NOT FOUND
Fatal Error -10300. EACH COMPOSITION LABEL ON TYPE 21 CARDS MUST CORRESPOND TO SOME COMPOSITION LABEL ON DATA SET A.NIP TYPE 14 CARDS
Fatal Error -10400. THE FIRST COMPOSITION LABEL ON THE TYPE 21 CARDS MUST BE NON-BLANK

Subroutine CARD22

Fatal Error -10100. CARD PRESUMED TO BE TYPE 22 NOT FOUND
Fatal Error -10200. MATERIAL LABELS ON TYPE 22 CARDS MUST CORRESPOND TO LIBRARY MATERIALS

Subroutine CARD23

Fatal Error -10100. CARD PRESUMED TO BE TYPE 23 NOT FOUND
Fatal Error -10200. MORE THAN NPRMAT+MSORS FISSION SPECTRA TEMPERATURES WERE SPECIFIED ON THE TYPE 23 CARDS
Fatal Error -10300. THE MATERIALS NAMED ON THE TYPE 23 CARDS MUST CORRESPOND TO MATERIALS SPECIFIED ON THE TYPE 06 CARDS AND/OR THE MATERIALS SPECIFIED ON THE DATA SET A.NIP TYPE 14 CARDS, OR THE LABELS FOR THE LIBRARY FISSION SPECTRA DATA

Subroutine CSI010 (MAIN)

Fatal Error -10100. INPUT DATA SET A.MCC2 NOT FOUND
Fatal Error -10200. CARD PRESUMED TO BE TYPE 02 NOT FOUND
Fatal Error -10300. CARD PRESUMED TO BE TYPE 04 NOT FOUND
Fatal Error -10400. CARD PRESUMED TO BE TYPE 03 NOT FOUND
Fatal Error -10500. INPUT DATA SET A.NIP NOT FOUND
TABLE V. Contd.

CSI010 (AREA 4) Contd.

<table>
<thead>
<tr>
<th>Fatal Error</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>-10600</td>
<td>CARD PRESUMED TO BE TYPE 01 NOT FOUND</td>
</tr>
<tr>
<td>-10700</td>
<td>TYPE 06 CARDS MUST BE SUPPLIED FOR HOMOGENEOUS PROBLEMS</td>
</tr>
<tr>
<td>-10800</td>
<td>CARD PRESUMED TO BE TYPE 19 NOT FOUND</td>
</tr>
<tr>
<td>-10900</td>
<td>EXTENDED TRANSPORT APPROXIMATION ORDER MUST BE 1 FOR INCONSISTENT FUNDAMENTAL MODE OPTION</td>
</tr>
<tr>
<td>-11000</td>
<td>LEGENDRE ELASTIC SCATTERING TRANSPORT APPROXIMATION PERMITTED ONLY FOR NON-CONSISTENT FUNDAMENTAL MODE OPTIONS</td>
</tr>
<tr>
<td>-11100</td>
<td>CARD PRESUMED TO BE TYPE 20 NOT FOUND</td>
</tr>
<tr>
<td>-11200</td>
<td>THE BROAD GROUP STRUCTURE SPECIFIED ON THE TYPE 03 CARD DOES NOT CORRESPOND TO ONE OF THE PRESTORED GROUP STRUCTURES</td>
</tr>
</tbody>
</table>

Subroutine RDANIP

<table>
<thead>
<tr>
<th>Fatal Error</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>-10100</td>
<td>CARD PRESUMED TO BE TYPE 04 OF DATA SET A.NIP NOT FOUND</td>
</tr>
<tr>
<td>10200</td>
<td>ONLY REFLECTIVE OR PERIODIC BOUNDARY CONDITIONS ARE ALLOWED AND THE SAME CONDITION APPLIES TO BOTH SIDES OF THE CELL. THE PERIODIC CONDITION IS BEING USED</td>
</tr>
<tr>
<td>-10300</td>
<td>DATA SET A.NIP TYPE 06 CARDS MUST BE SUPPLIED IF COLS. 37-42 ON CARD TYPE 03 OF DATA SET A.MCC2 ARE NON-ZERO</td>
</tr>
<tr>
<td>-10400</td>
<td>DATA SET A.NIP TYPE 14 CARDS MUST BE SUPPLIED IF COLS. 37-42 ON CARD TYPE 03 OF DATA SET A.MCC2 ARE NON-ZERO</td>
</tr>
<tr>
<td>-10500</td>
<td>DATA SET A.NIP TYPE 15 CARDS MUST BE SUPPLIED IF COLS. 37-42 ON TYPE 03 CARD OF DATA SET A.MCC2 ARE NON-ZERO</td>
</tr>
<tr>
<td>10600</td>
<td>ONLY THE REFLECTIVE BOUNDARY CONDITION IS ALLOWED AT THE LEFT BOUNDARY OF A CYLINDRICAL CELL</td>
</tr>
<tr>
<td>10700</td>
<td>ONLY WHITE BOUNDARY CONDITIONS ARE ALLOWED FOR THE RIGHT BOUNDARY OF A CYLINDRICAL CELL.</td>
</tr>
</tbody>
</table>
Subroutine STRTCH

Fatal Error -10100.  IF THE ATOMIC DENSITY OF SOME MATERIAL IS NOT
SUPPLIED ON THE TYPE 06 CARDS, THE MATERIAL MUST
APPEAR IN SOME HETEROGENEOUS REGION

Fatal Error -10200.  EACH MATERIAL MUST CORRESPOND TO SOME LIBRARY MATERIAL

Subroutine TESTBG

Fatal Error -10100.  THE HIGHEST BROAD GROUP AS READ FROM DATA SET
XS.ISO MAY NOT LIE ABOVE THE HIGHEST ENERGY IN
THE LIBRARY

Fatal Error -10300.  THE HIGHEST BROAD GROUP ENERGY AS READ FROM
DATASET XS.ISO DOES NOT FALL ON AN ULTRA-FINE-
GROUP BOUNDARY

Fatal Error -10500.  THE SPECIFIED BROAD GROUP STRUCTURE AS READ FROM
DATASET XS.ISO DOES NOT FALL ON ULTRA-FINE-GROUP
BOUNDARIES

Subroutine TYPE06

Fatal Error -10100.  CARD PRESUMED TO BE TYPE 06 OF DATA SET A.NIP
NOT FOUND

Fatal Error -10200.  REGION LABELS MUST BE NON-BLANK

Fatal Error -10300.  INVALID REGION BOUNDARY COORDINATES GIVEN ON DATA
SET A.NIP TYPE 06 CARDS. EACH REGION LOWER BOUNDARY
COORDINATE MUST BE .GE.0. AND .LT. THE CORRESPONDING
UPPER BOUNDARY COORDINATE FOR THAT REGION

Fatal Error -10400.  THE LOWEST MESH POINT FOR CYLINDERS MUST FALL AT 0.

Fatal Error -10500.  REGION BOUNDARIES FOR SEQUENTIAL REGIONS MUST AGREE
TO AT LEAST 1.E-4

Subroutine TYPE14

Fatal Error -10100.  CARD PRESUMED TO BE TYPE 14 OF DATA SET A.NIP NOT
FOUND

Fatal Error -10200.  COMPOSITION LABELS MUST BE NON-BLANK

Fatal Error -10300.  THE FIRST MATERIAL LABEL ON A TYPE 14 CARD OF DATA
SET A.NIP WAS BLANK

Fatal Error -10400.  MATERIALS IN HETEROGENEOUS REGIONS MUST CORRESPOND
TO LIBRARY MATERIALS
TABLE V. Contd.

CSI010 (AREA 4) Contd.

Subroutine TYPE14 (contd.)

Fatal Error -10500. MATERIALS MAKING UP A GIVEN COMPOSITION MUST BE DISTINCT

Fatal Error -10600. CARD PRESUMED TO BE TYPE 14 OF DATA SET A.NIP NOT FOUND

Fatal Error -10700. COMPOSITION LABELS MUST BE NON-BLANK

Fatal Error -10800. THE FIRST MATERIAL LABEL ON A TYPE 14 CARD OF DATA SET A.NIP WAS BLANK

Subroutine TYPE15

Fatal Error -10100. CARD PRESUMED TO BE TYPE 15 OF DATA SET A.NIP NOT FOUND

Fatal Error -10200. COMPOSITION LABELS MUST BE NON-BLANK

Fatal Error -10300. THE FIRST REGION LABEL ON A TYPE 15 CARD OF DATA SET A.NIP MUST BE NON-BLANK

Fatal Error -10400. A COMPOSITION REFERRED TO ON A DATA SET A.NIP TYPE 15 CARD MUST CORRESPOND TO SOME COMPOSITION DEFINED ON A TYPE 14 CARD

Fatal Error -10500. A REGION REFERRED TO ON A DATA SET A.NIP TYPE 15 CARD MUST CORRESPOND TO SOME REGION DEFINED ON THE TYPE 06 CARDS

Fatal Error -10600. ONLY ONE COMPOSITION MAY BE ASSIGNED TO A GIVEN REGION

Fatal Error -10700. CARD PRESUMED TO BE TYPE 15 OF DATA SET A.NIP NOT FOUND

Fatal Error -10800. COMPOSITION LABELS MUST BE NON-BLANK

Fatal Error -10900. A COMPOSITION REFERRED TO ON A DATA SET A.NIP TYPE 15 CARD MUST CORRESPOND TO SOME COMPOSITION DEFINED ON A TYPE 14 CARD

Fatal Error -11000. THE FIRST REGION LABEL ON A TYPE 15 CARD OF DATA SET A.NIP MUST BE NON-BLANK

Fatal Error -11100. A REGION REFERRED TO ON A DATA SET A.NIP TYPE 15 CARD MUST CORRESPOND TO SOME REGION DEFINED ON THE TYPE 06 CARDS

Fatal Error -11200. EVERY REGION ON AN A.NIP TYPE 06 CARD MUST ALSO BE PRESENT ON A TYPE 15 CARD
TABLE V. Contd.

CSC004 (AREA 5)

Subroutine CSC004 (MAIN)
Fatal Error -10100.  PROBLEM MATERIAL NOT IN THE LIBRARY
Fatal Error -10200.  PROBLEM MATERIAL IS NOT IN THE LIBRARY

Subroutine MATRIX
Fatal Error -10100.  DETERMINANT IS SINGULAR

CSC005 (AREA 6)

Subroutine ADMSTR
Fatal Error -10100.  PROBLEM MATERIAL IS NOT IN THE LIBRARY

Subroutine CSC005 (MAIN)
Fatal Error -10100.  PROBLEM MATERIAL NOT IN THE LIBRARY

CSC006 (AREA 6.5)

Subroutine CSC006 (MAIN)
Fatal Error -10100.  PROBLEM MATERIAL IS NOT IN THE LIBRARY

CSC008 (AREA 7)

Subroutine CSC008 (MAIN)
Fatal Error -999.  ERROR IN BPOINTER ALLOCATION

Subroutine SETCHI
Fatal Error -1  THE FISSION DISTRIBUTION SPECIFIED FOR THE PROBLEM IS NOT ON THE LIBRARY
Fatal Error -2  ALL FISSION DISTRIBUTIONS WERE NOT FOUND
Fatal Error -3  ALL FISSION DISTRIBUTIONS WERE NOT FOUND

Subroutine SETSCT
Fatal Error -1  ALL PROBLEM MATERIALS COULD NOT BE FOUND
Subroutine SETSCT (contd.)

Error 2  NONE OF THE MATERIALS ON THE OLD DATASET OLDSGS ARE USED IN THIS PROBLEM. ALL MICROSCOPIC CROSS SECTIONS MUST BE CALCULATED

Error 3  THE OLD DATASET OLDSGS HAS A DIFFERENT ENERGY STRUCTURE THAN THE PRESENT PROBLEM (DIFFERENT NUMBER OF GROUPS OR DIFFERENT STARTING ENERGY). MICROSCOPIC CROSS SECTIONS WILL BE RECALCULATED

Error 4  FIRST ORDER SCATTERING MATRICES ARE REQUIRED BY PROBLEM BUT ARE NOT AVAILABLE ON OLD DATASET OLDSGS. ALL MICROSCOPIC CROSS SECTIONS MUST BE RECALCULATED

Fatal Error -999  ERROR IN BPOINTER ALLOCATION

Subroutine SIGMAC

Fatal Error -1  ALL PROBLEM MATERIALS COULD NOT BE FOUND ON LIBRARY FILE

CSC009 (AREA 8)

Subroutine BGFL1

Fatal Error -170  ALL PROBLEM MATERIALS COULD NOT BE FOUND

Subroutine BGFL2

Fatal Error -200  ALL PROBLEM MATERIALS COULD NOT BE FOUND ON FILE MCC2P5

Fatal Error -320  NO CORRESPONDENCE CAN BE FOUND BETWEEN PROBLEM MATERIAL AND INELASTIC MATERIAL

Fatal Error -500  ALL PROBLEM MATERIALS TO BE EDITED COULD NOT BE FOUND

Subroutine BSQITR

Error 1001  BUCKLING ITERATION NOT FEASIBLE-ZERO BUCKLING IS ASSUMED

Subroutine DRIVER

Error 515  INHOMOGENEOUS SOURCE CALCULATION IS MEANINGFUL ONLY FOR SUBCRITICAL CONFIGURATION
TABLE V. Contd.

CSC009 (AREA 8) Contd.

Subroutine FILE1
Fatal Error -1000
ALL PROBLEM MATERIALS COULD NOT BE FOUND

Subroutine FILE6
Fatal Error -9000
ALL PROBLEM MATERIALS COULD NOT BE FOUND
Fatal Error -9010
ALL PROBLEM MATERIALS WITH INELASTIC AND/OR \((N,2N)\) DATA COULD NOT BE FOUND
Fatal Error -9020
ALL PROBLEM MATERIALS WITH INELASTIC AND/OR \((N,2N)\) DATA COULD NOT BE FOUND

Subroutine INIT
Fatal Error -1000
ALL FISSION SPECTRA MUST BE VECTORS
Error 1001
PROBLEM CHI VECTORS ARE NOT PROPERLY NORMALIZED

Subroutine ISOCHI
Fatal Error -500
FISSION SPECTRUM FOR PROBLEM MATERIAL M COULD NOT BE FOUND

Subroutine CSC009 (MAIN)
Fatal Error -999
AN ERROR HAS OCCURRED IN ALLOCATING VARIABLY DIMENSIONED ARRAYS

Subroutine REORDR
Fatal Error -1000
ALL UNRESOLVED RESONANCES WERE NOT PROCESSED

Subroutine RESCAT
Fatal Error -300
ALL RESOLVED RESONANCE MATERIALS COULD NOT BE FOUND

Subroutine RESCS
Error 1001
THERE ARE UNRESOLVED MATERIALS IN PROBLEM BUT UNRESOLVED ULTRA-FINE-GROUP CROSS SECTIONS ARE NOT AVAILABLE FROM FILE UNREG

Subroutine SETBG
Error 200
FIXED SOURCE CANNOT BE WRITTEN TO FILE SRATES
Fatal Error -999
ERROR IN BPOINTER ALLOCATIONS
TABLE V. Contd.

CSCO10 (AREA 9)

Subroutine SETIN

Fatal Error -999 AN ERROR HAS OCCURRED IN ALLOCATING VARIABLY DIMENSIONED ARRAYS

Subroutine BGPN

Error 280 INHOMOGENEOUS PROBLEM IS POSSIBLE ONLY IF EIGENVALUE IS LESS THAN UNITY

Subroutine BSQTR

Error 1001 BUCKLING ITERATION NOT FEASIBLE-ZERO BUCKLING IS ASSUMED

Subroutine HOMOG

Error 1 AT LEAST TWO ISOTOPES ON FILE ISOTXS HAVE THE SAME NAME. ONLY THE CROSS SECTIONS OF THE FIRST ARE PROCESSED

Fatal Error -2 SCATTERING TYPE IS NOT DEFINED

Error 3 NO UPSCATTER IS PERMITTED. UPSCATTER MATRIX ELEMENTS WILL NOT BE PROCESSED

Fatal Error -4 ALL PROBLEM ISOTOPES COULD NOT BE FOUND ON FILE ISOTXS

Subroutine CSCO10 (MAIN)

Fatal Error -1 SET FISSION VECTOR MUST BE PRESENT ON FILE ISOTXS IF NO EXTERNAL SOURCE IS PROVIDED

Fatal Error -999 ERROR IN BPOINTER ALLOCATION

CSCO11 (RABANL)

Subroutine CSCO11 (MAIN)

Fatal Error -10100. PROBLEM MATERIAL NOT IN THE LIBRARY

Fatal Error -10200. FOIL MATERIAL NOT IN THE LIBRARY

Subroutine MANAGR

Fatal Error -10100. INSUFFICIENT STORAGE PROVIDED FOR AREA 10 EXECUTION

Subroutine MATRIX

Fatal Error -10100. DETERMINANT IS SINGULAR
TABLE V. Contd.

CSC011 (RABANL) Contd.

Subroutine MERGER

Fatal Error -10100. THE PROBLEM CONTAINS NO RESOLVED RESONANCES

Fatal Error -10200. THE DATA SET Sbrates IS NOT CONSISTENT WITH THE AREA 10 UPPER ENERGY OF THE CURRENT PROBLEM

Fatal Error -10300. THE DATA SET Sbrates IS NOT CONSISTENT WITH THE NUMBER OF ULTRA FINE GROUPS IN THE CURRENT PROBLEM

Subroutine RATES

Fatal Error -10100. A NEGATIVE COLLISION RATE HAS BEEN ENCOUNTERED

Subroutine SOARCE

Fatal Error -10100. A NEGATIVE SOURCE HAS BEEN COMPUTED

CSE009 (ISOTXS Editor)

Subroutine CSE009 (MAIN)

Error 10000 CARD IS OF WRONG TYPE. SHOULD BE CARD OF TYPE 01

Subroutine XSEDIT

Fatal Error -10000 CARD IS OF WRONG TYPE. SHOULD BE CARD OF TYPE 02

Fatal Error -20000 REQUESTED ISOTOPE NOT FOUND IN LIBRARY

CSE007 (Generate XS.ISO from ISOTXS)

Subroutine CTD

Fatal Error -998 SET YOU HAVE ASKED TO ADD TO IS INCOMPATIBLE IN ENERGY STRUCTURE OR GROUPS

Fatal Error -999 ERROR IN BPOINTER ALLOCATION

Subroutine CTS

Fatal Error -998 SET YOU HAVE ASKED TO ADD TO IS INCOMPATIBLE IN ENERGY STRUCTURE OR GROUPS

Fatal Error -999 ERROR IN BPOINTER ALLOCATION

Subroutine PRINXD

Error 500 FILE ISOTXS CONTAINS UNDEFINED SCATTERING TYPE
TABLE V. Contd.

CSE007 (Generate XS.ISO from ISOTXS) Contd.

Subroutine PRINXS

Error 500  FILE ISOTXS CONTAINS UNDEFINED SCATTERING TYPE

Subroutine CSE012

CSE012 (XS.ISO Editor)

Fatal Error -10000.  DATA SET XS.ISO NOT PROVIDED
Fatal Error -10100.  TYPE 01 CARD NOT FOUND
Fatal Error -10200.  TYPE 02 CARD NOT FOUND

Subroutine SORTNM

Fatal Error -10000.  CARD TYPE 01 NOT FOUND
Fatal Error -10100.  CARD TYPE 01 NOT FOUND
Fatal Error -10200.  ISOTOPE LABELS MUST BE NON-BLANK
Fatal Error -10300.  EACH ISOTOPE SPECIFIED ON AN ACSE12 CARD MUST CORRESPOND TO SOME ISOTOPE IN THE XS.ISO DATA SET

reed/rite

Fatal Error -900  LOGICAL UNIT NUMBER IS OUT OF RANGE
Fatal Error -910  MODE INDEX OUT OF RANGE
Fatal Error -920  RECORD NUMBER OUT OF RANGE
Fatal Error -930  NUMBER OF WORDS IS NEGATIVE
Fatal Error -940  MISSING DD CARD FOR FILE LUN
Fatal Error -950  SIO ACCESS ERROR
Error 960  WRITING A RECORD WITH NWDS=0
Fatal Error -999  ATTEMPTING TO READ PAST END OF FILE
VII. PROGRAMMING INFORMATION

The MC²-2 code system was developed within the ARC System modular environment on IBM hardware with an OS operating system. Great care was taken in the programming to limit the degree of system dependence. A number of local conventions were adopted to permit ease of code conversion. These local conventions supplemented the procedures adopted by the CCCC(1). Two standalone versions of MC²-2 were created based on the ARC System modular program: (i) an IBM version for use on any IBM 360 or 370 operating system with at least 600K bytes of storage and (ii) a CDC version for use on CDC 7600 hardware with 50K words of SCM, 60K words of directly addressable LCM, and SEGMENTATION LOADER capability as offered with SCOPE 3.4. In this chapter some of the details of the MC²-2 code are given along with a description of the differences between the IBM and CDC versions of the code. A guide for the implementation of both standalone versions of the code is provided.

A. Program Structure

The standalone versions of the MC²-2 code were adapted from the ARC System modular programs by creating a primary overlay for each of the MC²-2 modules (c.f. Chapter VI). Figure 16 shows the overlay control cards for the IBM version and Figure 17 shows the directives required for a segmented load of the CDC version of the code. The segmentation loader available with the SCOPE 3.4 operating system was used by MC²-2 to avoid the need to insert special OVERLAY and PROGRAM statements and to permit the passing of arguments across overlays.

The programming language used in MC²-2 is almost entirely FORTRAN. The few machine language subprograms used are discussed in Section D below. There is a one-to-one correspondence between the FORTRAN source code of the IBM and CDC versions. Changes required to account for word length differences, large core memory use, or ENTRY point differences, for example, are flagged by CDC* and/or CIBM comment cards. Testing of the FORTRAN code was performed using the IBM FORTRAN H, OPT=2, compiler whereas the CDC code was compiled using the FTN 4.5, OPT=1 compiler. Extensive use is made of comment cards throughout the FORTRAN source code in an attempt to make the code as self-documenting as possible.

B. ARC System Routines

The user specified BCD (card) input to MC²-2 follows the ARC System conventions (1) as discussed in Chapter VI. The FORTRAN routines SCAN and STUFF read and process the input as discussed in Reference 1.
ENTRY MAIN
INSERT MAIN
INSERT SNIFF, SEEK, REED, TIMER, ERROR
INSERT PONTR, PUTPNT, BULK, FREE, WIPOUT, GETPNT, IGET, IPT2, PUTM
INSERT IPTERR, ILAST, REDEF, REDEFM, PURGE, STATUS, PRT11, PRT11E
INSERT PRT12, PRT12E, PRTR1, PRTR1E, PRTR2, PRTR2E
INSERT ALLOC$, LOC, TIME, CLOCK#, DATE, ABEND, TRACER, SECOND, JOBID
INSERT PRT1E, PRT1A, PRT1I
INSERT MIXER, SIGMAX, QUICK1, CSLAB1, SIGESC
INSERT QL, PIXP1, GRAPH
INSERT MATRIX
INSERT LENGTH, OUTPUT, NUMBER, ARRAY, SPECS, EDITS, REALMW, INTEGL
INSERT TIMING, OPTUNR, IOPUT, STFARC, LOCATE, TABLES, PTERL, LCMSIZ, BFLAGS
OVERLAY ALPHA
OVERLAY CODE
OVERLAY SCAN
OVERLAY STUFF, STUFF1
OVERLAY ALPHA
OVERLAY CSI010, SPACER, PRNT1D, PRNTAE, DISPOS, GOWEST
OVERLAY UNITS, CRDCNT, LBSPEC
OVERLAY BETA
OVERLAY TESTBG, CARD05, CARD06, CARD07, CARD09
OVERLAY BETA
OVERLAY RDANIP, TYPE06, TYPE14, TYPE15, EDGE1, GEOM
OVERLAY BETA
OVERLAY STRTCH, HETERO, CARD10, CARD11, CARD12, SXLXSR, CSDMGI, CARD14
OVERLAY CARD15, CARD16, CARD17, CARD18, FOILS, CARD21, CARD22, CARD08, CARD23
OVERLAY BETA
OVERLAY WRITER, ENTPR
OVERLAY REC1
OVERLAY ALPHA
OVERLAY CSC004, SETUPU, UNRINT, DRCTOR, EDITUN
OVERLAY ESMEH, PACKER
OVERLAY WZERO, QUICKJ, INTERP
OVERLAY RATION, MULTIP, FILE3, BOUNDY, DRCUNR
OVERLAY ALPHA
OVERLAY CSC005, ADMSTR, SETUPR, SIFTER, RATNL
OVERLAY REORDR, STUFIT, NSIG0
OVERLAY JINT, OVLAP, WINNER, JINTGL, TRIPLE, LORENT, EDITLZ
OVERLAY BOUND, PHILE1, FILE4
OVERLAY TRIPIN
OVERLAY ALPHA
OVERLAY CSC006, EDITSP, EDITAT, EDITRS, PONTRL, WRISIT, INTRAC
OVERLAY MAININ
OVERLAY ALPHA
OVERLAY CSC008
OVERLAY NSCR7
OVERLAY BETA
OVERLAY SIGAVG, SIGMAC, SETCHI

Fig. 16. IBM Overlay Control
Fig. 16. IBM Overlay Control (Contd.)
Fig. 17. CDS Segmentation Loader Directives
The code \( \text{MC}^{2}-2 \) uses the dynamic storage capability, B POINTER, described in Reference 1, to manage all variable dimension array allocations. A one-to-one correspondence between the IBM and CDC versions of this subprogram package has been retained except for the machine dependent routines ALLOC and LOCF which are discussed in Section D below. The bulk storage capability of the IBM version of B POINTER has been modified to manage arrays in large core memory of the CDC 7600. Appendix E describes some of the characteristics of the B POINTER subprogram package.

The ARC System routine SNIFF is used throughout the code to assign logical unit numbers to named data files. Both the IBM and CDC standalone versions of the code use a modification of the routine SNIFF which calls the CCCC subroutine SEEK described in Section C below.

C. CCCC Standard Subroutines

The Committee on Computer Code Coordination has specified a number of standard routines (2) to be used in RRD funded code development. In principle the routines may be installation dependent. The \( \text{MC}^{2}-2 \) code uses the standard routines REED, RITE, TIMEK and SEEK as specified in Reference 2. While it is possible to substitute installation dependent code, simple versions of these routines are provided with both the IBM and CDC standalone versions of \( \text{MC}^{2}-2 \).

1. SEEK

The subroutine SEEK is used by \( \text{MC}^{2}-2 \) to return the logical unit number associated with a named data file. With only two exceptions, all files referenced by \( \text{MC}^{2}-2 \) are assigned unit numbers through calls to subroutine SEEK. The two exceptions are the BCD files input (5) and printed output (6). While it should be possible to use installation dependent versions of SEEK, it is obvious that any changes in unit allocation must also be reflected in the Job Control Language required for the IBM version of \( \text{MC}^{2}-2 \) (Fig. 11) or the program card of the CDC version. A single initialization call to SEEK is made from the main program driver of \( \text{MC}^{2}-2 \). In Table VI information is provided about the various files referenced by \( \text{MC}^{2}-2 \). Detailed formats for the interface files MCC2F1 - MCC2F8, ISOTXS and XSISO, card input files A.MCC2, A.NIP, A.STP015, ACS009 and ACSE12, and some of the other important files are given in the Appendices B, C and D. It should be noted from Table VI that each named file in the IBM version of the program is assigned a unique logical unit number. Restrictions on the number of unit definitions permitted by CDC 7600 software made it necessary to use the same unit number for more than one file. This equivalencing of files was specified to retain full program generality. The file assignment is specified in the initialization call to SEEK from the main program driver. In spite of the large number of files required, even the largest problem requires that a maximum of seven files be open at any particular time in the calculation.

In Table VI there is a column indicating the modules ( overlays) which reference a particular file for reading and/or writing. Many of these references are conditional and depend upon the particular problem specifications. Extensive use is made of the various SEEK options to determine whether a particular file is available for reading and/or writing.
<table>
<thead>
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<th>IBM (CDC)</th>
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<th>Modules Referencing File*</th>
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| PRBCHI | 34 (34)             | Problem Dependent Fission Spectrum Data | CSC008 (W)  
|        |                     |                                     | CSC009 (R,W) |
| PRBSPC | 35 (35)             | Problem Specifications              | CSC010 (R,W)  
|        |                     |                                     | CSC004 (R)  
|        |                     |                                     | CSC005 (R)  
|        |                     |                                     | CSC006 (R)  
|        |                     |                                     | CSC008 (R)  
|        |                     |                                     | CSC009 (R)  
|        |                     |                                     | CSC010 (R)  
|        |                     |                                     | CSC011 (R)  
|        |                     |                                     | CSE009 (R)  
|        |                     |                                     | CSE007 (R)  |
| RESINT | 36 (38)             | Resolved Resonance Integrals        | CSC005 (W)  
|        |                     |                                     | CSC006 (R,W)  
|        |                     |                                     | CSC009 (R)  |
| SCR001 | 37 (39)             | Scratch                             | CSC005 (R,W)  
|        |                     |                                     | CSC008 (R,W)  
|        |                     |                                     | CSC009 (R,W)  
|        |                     |                                     | CSC011 (R,W)  |
| SCR002 | 38 (40)             | Scratch                             | CSC005 (R,W)  
|        |                     |                                     | CSC008 (R,W)  
|        |                     |                                     | CSC009 (R,W)  
|        |                     |                                     | CSC011 (R,W)  |
| SCR003 | 39 (41)             | Scratch                             | CSC004 (R,W)  
|        |                     |                                     | CSC005 (R)  
|        |                     |                                     | CSC006 (R,W)  
|        |                     |                                     | CSC009 (R,W)  
|        |                     |                                     | CSC011 (R,W)  |
| SCR004 | 40 (42)             | Scratch                             | CSC009 (R,W)  
<p>|        |                     |                                     | CSC011 (R,W)  |</p>
<table>
<thead>
<tr>
<th>Name</th>
<th>Logical Unit Number</th>
<th>IBM (CDC)</th>
<th>Contents</th>
<th>Modules Referencing File*</th>
</tr>
</thead>
<tbody>
<tr>
<td>SCRO05</td>
<td>41 (43)</td>
<td>IBM (CDC)</td>
<td>Scratch</td>
<td>CSC009 (R,W)</td>
</tr>
<tr>
<td>SIGMAP</td>
<td>42 (44)</td>
<td>IBM (CDC)</td>
<td>Ultra-Fine-Group Background Cross Section</td>
<td>CSC006 (R,W)</td>
</tr>
<tr>
<td>SMSIGS</td>
<td>43 (45)</td>
<td>IBM (CDC)</td>
<td>Ultra-Fine-Group Elastic Transfer Matrices</td>
<td>CSC008 (R,W)</td>
</tr>
<tr>
<td>SPECTR</td>
<td>44 (46)</td>
<td>IBM (CDC)</td>
<td>Ultra-Fine-Group Spectrum</td>
<td>CSC009 (R)</td>
</tr>
<tr>
<td>SPECXS</td>
<td>45 (47)</td>
<td>IBM (CDC)</td>
<td>Ultra-Fine-Group Cross Sections and Moderating Parameters</td>
<td>CSC008 (R,W)</td>
</tr>
<tr>
<td>SRAATES</td>
<td>46 (48)</td>
<td>IBM (CDC)</td>
<td>Ultra-Fine-Group Microscopic Scattering Collision Density and Sources</td>
<td>CSC009 (W)</td>
</tr>
<tr>
<td>UNREG</td>
<td>47 (49)</td>
<td>IBM (CDC)</td>
<td>Unresolved Resonance Ultra-Fine-Group Cross Sections</td>
<td>CSC008 (W)</td>
</tr>
<tr>
<td>UNRES</td>
<td>48 (50)</td>
<td>IBM (CDC)</td>
<td>Unresolved Cross Sections at E* Points</td>
<td>CSC004 (R,W)</td>
</tr>
<tr>
<td>XSISO</td>
<td>49 (51)</td>
<td>IBM (CDC)</td>
<td>File 1 of ARC System Broad Group File</td>
<td>CSI010 (R)</td>
</tr>
<tr>
<td>XSISO5</td>
<td>50 (52)</td>
<td>IBM (CDC)</td>
<td>File 2 of ARC System Broad Group File</td>
<td>CSE007 (R,W)</td>
</tr>
<tr>
<td>IRESCS</td>
<td>51 (53)</td>
<td>IBM (CDC)</td>
<td>Integral Transport Derived Broad Group Cross Sections</td>
<td>CSC011 (R,W)</td>
</tr>
<tr>
<td>Name</td>
<td>Logical Unit Number</td>
<td>IBM (CDC)</td>
<td>Contents</td>
<td>Modules Referencing File*</td>
</tr>
<tr>
<td>------------</td>
<td>---------------------</td>
<td>-----------</td>
<td>--------------------------------------------------------------------------</td>
<td>---------------------------</td>
</tr>
<tr>
<td>BIGXS1</td>
<td>52 (54)</td>
<td>IBM (CDC)</td>
<td>Ultra-Fine-Group Macroscopic Scattering Data, Foil Data in Integral Transport Module, For IBM 25 Files are defined BIGXS1 - BIGXSP with unit Numbers 52-76.</td>
<td>CSC008 (R,W) CSC009 (R) CSC011 (R,W)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>For CDC 14 Files are defined BIGXS1 - BIGXSE with unit Numbers 54, 55, 11, 12, 13, 20, 21, 30, 32, 33, 44, 51, 52, 53</td>
<td></td>
</tr>
<tr>
<td>RANDOM**</td>
<td>77 (-)</td>
<td>IBM (CDC)</td>
<td>Random Access Data File Not Used In Standalone Code Releases</td>
<td>CSC009 (R,W)</td>
</tr>
<tr>
<td>RESDAT</td>
<td>78 (37)</td>
<td>IBM (CDC)</td>
<td>Selected Resonance Parameters</td>
<td>CSC005 (W) CSC009 (R)</td>
</tr>
<tr>
<td>ACS009</td>
<td>79 (36)</td>
<td>IBM (CDC)</td>
<td>BCD Input for ISOTXS Editor</td>
<td>STUFF (W) CSE009 (R)</td>
</tr>
<tr>
<td>ACSE12**</td>
<td>80 (-)</td>
<td>IBM (CDC)</td>
<td>BCD Input for XS.ISO Editor</td>
<td>STUFF (W) CSE012 (R)</td>
</tr>
</tbody>
</table>

*R Read

W Write

** Not Referenced in Standalone Version of MC²-2
2. **REED/RITE**

The standard routines REED and RITE are used to perform the non-formatted (binary) I/O operations for $MC^2$-2. The ARC System modular version of REED/RITE makes use of three access methods, standard FORTRAN, asynchronous FORTRAN and a special random access I/O package SIO\(^{(40)}\). The IBM and CDC standalone versions of $MC^2$-2 contain a far simpler version of REED/RITE which uses standard FORTRAN I/O. The CCCC specifications of REED and RITE did not account for the possibility of multilevel data transfers as required by the CDC version of $MC^2$-2 to permit the transfer of data between large core memory and disk files without use of a buffer array in small core memory. In order to permit such transfers the routines DRED and DRIT were used in the CDC version of the code. The argument lists to DRED/DRIT are precisely the same as the calls to REED/RITE but the array address into (from) which data are transferred is assumed to be in large core memory. This convention differs from a recent proposal to the CCCC where a pointer rather than an address was recommended. Changes to conform with the recommended versions of DRED/DRIT would be quite simple because of the limited number of calls to these routines.

3. **TIMER**

The standard subroutine TIMER is used by $MC^2$-2 to provide timing and problem identification information. These data are not essential to the execution of the $MC^2$-2 program. As a consequence, the CDC version of TIMER is in large part a dummy program. It calls only the standard CDC system code SECOND to provide CPU timing data. The IBM version of TIMER makes use of a number of assembler language routines to provide time and edit information. These assembler routines are described in Section D below.

D. **Machine Language Routines**

Machine language routines are used in $MC^2$-2 to provide capability which does not exist in the FORTRAN language. A brief description of these sub-programs is provided in this section.

1. **ALLOC**

The subroutine PoINTr of the dynamic allocation subprogram package BPOINTER assigns storage dynamically at run time based on user input specifications. The routine ALLOC is called to assign and free this storage. The IBM version of the code ALLOC makes use of the OS macros GETMAIN and FREEMAIN to perform this function. The CDC version of ALLOC is a FORTRAN function which calls the COMPASS routine MEMGET to perform the allocation.

2. **LOCF**

The function subprogram LOCF is used by subroutine PoINTr to obtain the address of the dynamic storage container and the common block /ARRAY/. This function is a standard routine of CDC FORTRAN. The IBM version of the function is coded in assembler language. Since the CDC version of LOCF does not obtain the address of LCM variables, the CDC version of PoINTr assumes that the LCM common block /ARRAY2/ is located at the start of LCM (address 1).
3. **GOWEST**

   The subroutine GOWEST is used to left-justify Hollerith variables. The IBM version of the routine is written in assembler language. The CDC version of the routine is written in FORTRAN and uses the standard CDC FORTRAN version of the function SHIFT.

4. **FILEID**

   The subroutine FILEID is used in subroutine BGFLE1 of module CSC009 to obtain the dataset name associated with the file ISOTXS. It is an assembler language routine in the IBM version of the code and a dummy FORTRAN routine in the CDC code.

5. **CVD**

   The subroutine CVD is used in subroutine BGFLE2 of module CSC009 to convert a variable from integer to Hollerith format. The IBM version of CVD is written in assembler language and the CDC version of the routine uses the FORTRAN ENCODE capability.

6. **TIME**

   TIME is used by the IBM version of subroutine TIMER to return the wall clock time in the form HH.MM.SS. TIME is not referenced in the CDC version of the code.

7. **CLOCK**

   CLOCK is used by the IBM version of subroutine TIMER to return the wall clock time in units of .01 seconds. CLOCK is not referenced in the CDC version of the code.

8. **DATE**

   The function subprogram DATE is called by the IBM version of subroutine TIMER to return the current date in the form MM/DD/YY. DATE is not referenced by the CDC version of the code.

9. **SECOND**

   The subroutine SECOND is called by TIMER to return the elapsed CPU time in seconds. An IBM assembler language version of SECOND which uses the STIMER and TTIMER macro-instructions is provided. The CDC version of the code requires the standard system version of the subroutine SECOND.

10. **ABEND**

    The subroutine ABEND is called by subroutine ERROR to force an abnormal termination of the job with a DUMP. The IBM version of ABEND is an assembler language routine which invokes the macro-instruction ABEND. An abnormal termination code USER 16 is given and a dump is written to the file SYSUDUMP or SYSABEND. The CDC version of ABEND is a FORTRAN routine which calls the FORTRAN routine EXIT.
11. **JOBID**

   JOBID is used by the IBM version of subroutine TIMER to return the job name supplied on the user's job card. JOBID is not referenced by the CDC version of the code.

12. **FXP**

   FXP is a fast exponential function. The algorithm is described in Appendix A. The IBM version of FXP is programmed in assembler language. An equivalent FORTRAN routine is provided with the CDC version of the code.

13. **DISPOS**

   The subroutine DISPOS is used by the module CSIO10 to determine whether the file SRATES is given a permanent or temporary disposition. The IBM version of DISPOS is programmed in assembler language. The CDC version of DISPOS is a dummy FORTRAN routine which returns a flag to the calling routine indicating a temporary disposition for the file.

14. **TRACER**

   TRACER is used by the IBM version of REED/RITE to provide traceback information in case of an error in REED/RITE. The IBM version of TRACER is programmed in assembler language. TRACER is not referenced in the CDC version of the code.

---

### E. Program Implementation

Both the IBM and CDC versions of the program MC²-2 are available from the Argonne Code Center. Each version of the code requires a program tape and a library tape. A description of the tapes along with a step-by-step implementation strategy for each version of the program is described below.

---

1. **IBM Code Implementation**

   The IBM program tape is written as described in Table VII. The source code for MC²-2 is contained on Files 1 and 2 of the program tape. A brief description of each of the subprograms of File 1 is given in Table VIII. The assembler language subprograms on File 2 of the tape were discussed in Section D above. Creation of object code for input to the linkage editor is the first step required for implementation of the MC²-2 program. It is recommended that this step be performed in the following manner: (i) preallocate an object module dataset; (ii) compile File 1 Fortran code; (iii) assemble File 2 assembler code. The preallocation may be performed by submitting the job shown in Fig. 18. The user may clearly specify any DSN, VOL or UNIT information consistent with local naming conventions. In all of the examples which follow, ANL conventions will be used but the essential nature of each step is intended to be system independent. The compilation of the File 1 subprograms should be performed using the highest level of optimization available. Routinely this means use of the FORTRAN H compiler with OPT=2 specified. It should be noted that FORTRAN compilers are often system dependent in the sense of release identification and system generation (SYSGEN) options. The Level 21.7
compiler is currently in use at ANL but other releases of IBM compilers have been used without problem. The SIZE parameter on the standard ANL Fortran H compiler was set at 215K at SYSGEN time. Several of the MC²-2 subroutines are too large to compile with this specification. A second Fortran H compiler is available at ANL which was specified with SIZE=450K at SYSGEN time. This compiler is used at ANL to compile the subroutines CSI010, DRCTOR, ELSCAT, CSC009, SETBG, CSC011, RATES and SIFTIT since these routines will not compile (ADCON TABLE EXCEEDED) with the smaller compiler. The compilation of File 1 code may be performed in one job step as shown in Fig. 19 or by breaking up the code into a number of smaller blocks. The latter procedure is recommended as it permits one to work with smaller blocks of source code. In order to break up the file into such manageable blocks, one can use the IBM utility IEBGENER to create a partitioned data set (PDS) and then compile each member of the PDS separately into the PDS created by the preallocation step of Fig. 18. If this mode of operation is used, a recommended breakup of the source language is by module as indicated in Table VIII. Whether one uses a PDS or the tape as input, it is recommended that the code be compiled and link edited (with NCAL specified) as shown in Fig. 19. The final step in the processing of the source language tape is the assembly of the assembler language routines on File 2 of the tape. This is done in a straightforward manner as illustrated in Fig. 20. The File 2 routines should not be broken into blocks although all of File 2 (944 source cards) may be copied as a single member of the source language PDS if desired.

If the user does not wish to work directly with source code as recommended above, an object library PDS is available on File 3 of the program tape. One may bypass the steps above and use the IBM utility IEHMOVE to load the object library to a disk pack as shown in Fig. 21. The blocksize of the object module was set to 6K so that it may be moved to either a 2314 or 3330 disk pack. This is not the recommended procedure unless there are particular problems involved in operating with the two files of source code.

A sample problem input deck is provided on File 4 of the program tape. Prior to executing this sample problem three further steps are required: (i) preparation of MC²-2 binary libraries; (ii) modification of sample problem linkage editor instructions to conform with the object library preparation completed above; (iii) modification of the JCL procedure provided with sample problem.

A library tape is provided along with the MC²-2 program tape. This second tape contains eight binary sequential files in the format of files MCC2F1 - MCC2F8 described in Appendix C. These files must be copied to a direct access device (e.g. disk pack) as the next step in program implementation. A sample of the job control required to copy these files is given in Fig. 22. The space requirements for these files (on a 3330 disk pack) are given in Table VII. The data available on these library files were processed from the ENDF/B-IV data files by the code ETOE-II. A summary of the library specifications is given in Table IX. The Argonne Code Center also has available four BCD tapes which contain this same eight file library in BCD format along with a Fortran program, MC²-2 LIBGEN, which reads the BCD files and writes the eight binary files. This library generation program is described in Appendix F.
Having copied the eight library files to a direct access device, the only remaining steps in implementation involve modification of the sample problem linkage edit and JCL procedure to conform with local conventions. The linkage edit step of the sample problem deck builds an executable load module from the object library segments created by compilation and assembly of Files 1 and 2 of the library tape respectively (or alternatively copy of File 3). The user must modify the sample problem deck to reference this object library on the JCL card with the DDNAME MYLIB. Following the linkage edit SYSIN card the user must INCLUDE all members of the object library. The INCLUDE cards provided with the sample problem deck reference the members available on the PDS of File 3 of the library tape. It is obvious that the user must also modify the procedure name FTHEP and step names to conform with local conventions. If desired the load module created in this step may be given a permanent disposition so that the edit step may be bypassed on future problem executions thus saving a considerable amount (∼2 minutes) of I/O time.

The JCL procedure (c.f. Fig. 11) ARCSP015, which follows the linkage edit step of the sample problem input must be modified to conform with local conventions. Symbolic parameters have been provided to ease the burden of this modification. For example the parameter UNITSCR should be changed in the PROC statement to reference the standard system direct access scratch unit, FULLBLK should be set to 6136 if 3330 disk packs are not available, etc. In addition the parameters MCC2F1 through MCC2F8 should be modified to conform with the data set names assigned to the eight MC^2 library files copied from the library tape. The parameter PRELIB should be set to the data set name (permanent or temporary) assigned to the MC^2 load module.
Table VII
IBM Code Center Tape Description

1) Program Tape (Non-Labelled, 9 trk, 800 bpi)

<table>
<thead>
<tr>
<th>File</th>
<th>Description</th>
<th>RECFM</th>
<th>LRECL</th>
<th>BLKSIZE</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Fortran Source (EBCDIC)</td>
<td>FB</td>
<td>80</td>
<td>3200</td>
</tr>
<tr>
<td>2</td>
<td>Assembler Source (EBCDIC)</td>
<td>FB</td>
<td>80</td>
<td>3200</td>
</tr>
<tr>
<td>3</td>
<td>Load Module (Binary)</td>
<td>FB</td>
<td>80</td>
<td>800</td>
</tr>
<tr>
<td>4</td>
<td>Sample Problem (EBCDIC)</td>
<td>FB</td>
<td>80</td>
<td>3200</td>
</tr>
</tbody>
</table>

2) Library Tape (Non-Labelled, 9 trk, 1600 bpi)

<table>
<thead>
<tr>
<th>File</th>
<th>Space (units of 3330 Tracks)</th>
<th>RECFM</th>
<th>LRECL</th>
<th>BLKSIZE</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>VBS</td>
<td>X</td>
<td>6447</td>
</tr>
<tr>
<td>2</td>
<td>9</td>
<td>VBS</td>
<td>X</td>
<td>6447</td>
</tr>
<tr>
<td>3</td>
<td>6</td>
<td>VBS</td>
<td>X</td>
<td>6447</td>
</tr>
<tr>
<td>4</td>
<td>11</td>
<td>VBS</td>
<td>X</td>
<td>6447</td>
</tr>
<tr>
<td>5</td>
<td>223</td>
<td>VBS</td>
<td>X</td>
<td>6447</td>
</tr>
<tr>
<td>6</td>
<td>289</td>
<td>VBS</td>
<td>X</td>
<td>6447</td>
</tr>
<tr>
<td>7</td>
<td>1</td>
<td>VBS</td>
<td>X</td>
<td>6447</td>
</tr>
<tr>
<td>8</td>
<td>334</td>
<td>VBS</td>
<td>X</td>
<td>6447</td>
</tr>
</tbody>
</table>
Figure 18
Preallocation of Object Library

// EXEC PGM=IEFBR14
//OBJECT DD DSN=MCC2.OBJLIB,DISP=(NEW,CATLG),UNIT=SHRT3330,
// SPACE=(CYL,(5,3,1)),VOL=SER=,DCB=BLKSIZE=6144
/

Figure 19
Compilation of Fortran Subprograms

// EXEC FTHCEP,OPTIONS='OPT=2',COMPILE=FORTH450,
// EDTOPTS='LET,LIST,MAP,DCBS,NCAL'
//FTH.SYSIN DD UNIT=TAPE9TRK,DISP=OLD,LABEL=(1,NL),
// VOL=(,RETAIIN,SER=nmmmmn),
// DCB=(RECFM=FB,LRECL=80,BLKSIZE=3200,DEN=2)
//EDT.SYSLMOD DD DISP=OLD,DCB=BLKSIZE=6144,
// DSN=MCC2.OBJLIB(anyname_1)
/

Figure 20
Assembly of File 2 CSECTS

// EXEC ASMCEP,EDTOPTS='LIST,MAP,DCBS'
//ASM.SYSIN DD UNIT=TAPE9TRK,DISP=OLD,LABEL=(2,NL),
// VOL=(,RETAIIN,SER=nmmmmn),
// DCB=(RECFM=FB,LRECL=80,BLKSIZE=3200,DEN=2)
//EDT.SYSLMOD DD DISP=OLD,DCB=BLKSIZE=6144,
// DSN=MCC2.OBJLIB(anyname_2)
/

Figure 21
Copy Object Module from File 3 of Program Tape to Disk

// EXEC PGM=IEHMOVE
//SYSPRINT DD SYSOUT=A
//SYSSUT1 DD DISP=SHR,UNIT=3330,VOL=SER=SCR001
//OBJECT DD DISP=OLD,UNIT=3330,VOL=SER=PACKxx
//TAPE DD DISP=(OLD,PASS),UNIT=TAPE9TRK,VOL=(,RETAIIN,SER=nmmmmn),
// DCB=(RECFM=FB,LRECL=80,BLKSIZE=800,DEN=2),
// LABEL=(3,NL),DSN=FILE3
//SYSSIN DD *
COPY FROM=2400=(nmmmmn,3),TO=3330=PACKxx,FROMDD=TAPE,
 DSNAME=MCC2.OBJLIB
/
/*
Fig. 22. Copy of MC²-2 IBM Binary Library Files
TABLE VIII. Function of MC²-2 Subprograms

Driver and System Subprograms

MAIN (000010 - 002110)*

Main program driver for MC²-2. Initializes SEEK, calls system routines to read and spool BCD input and calls all modules.

SEEK (002120 - 004290)

CCCC routine returns logical unit numbers associated with named data file.

REED/RITE (004300 - 006500)

CCCC routine performs all binary I/O data transfer operations.

TIMER (006510 - 007830)

CCCC routine performs all timing and system dependent editing (date, ID, etc.) operations.

ERROR (007840 - 008450)

Prints error numbers and calls ABEND for job termination in case of FATAL error.

SNIFF (008460 - 008700)

Dummy ARC System interface routine calls SEEK to obtain unit information.

BPOINTER (008710 - 021230)

Dynamic allocation subprogram package - c.f. Appendix

CODE (021240 - 022650)

Reads a BCD card image and inspects it; called by SCAN and STUFF modules.

SCAN (022660 - 024880)

Reads entire BCD input stream from logical unit number 5 and spools the data to file ARC. Calls SEEK to initialize files in BLOCK=OLD.

*Numbers in brackets are sequence numbers of routine on MC²-2 program tape.
<table>
<thead>
<tr>
<th>Subprogram</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>STUFF (024890 - 026270)</td>
<td>Locates next block of data from file ARC for processing.</td>
</tr>
<tr>
<td>STUFF1 (026280 - 029800)</td>
<td>Reads and process next block of BCD data from file ARC.</td>
</tr>
<tr>
<td>PRNT1A (029810 - 031020)</td>
<td>Edits one-dimensional Hollerith arrays.</td>
</tr>
<tr>
<td>PRNT1E (031030 - 032250)</td>
<td>Edits one-dimensional floating point single precision arrays.</td>
</tr>
<tr>
<td>PRNT1I (032260 - 033470)</td>
<td>Edits one-dimensional integer arrays.</td>
</tr>
<tr>
<td>MIXER (033480 - 034950)</td>
<td>Homogenizes smooth u.f.g. total cross sections for homogeneous mixture and each heterogeneous region.</td>
</tr>
<tr>
<td>SIGMAX (034960 - 036560)</td>
<td>Calculates optical thickness to left and right of each slab region.</td>
</tr>
<tr>
<td>QUICK1/QUICKW (036570 - 038070)</td>
<td>Calculates the real and imaginary parts of the complex W function.</td>
</tr>
<tr>
<td>MATRIX (038080 - 039830)</td>
<td>Matrix inversion routine.</td>
</tr>
<tr>
<td>CSLAB1/CSLAB (039840 - 040460)</td>
<td>Calculates Dancoff factor for slab region.</td>
</tr>
<tr>
<td>SIGESC (040470 - 040800)</td>
<td>Calculates escape cross section for cylindrical two-region pin cells.</td>
</tr>
</tbody>
</table>
TABLE VIII. Function of MC²-2 Subprograms (Contd.)

QL (040810 - 043580)

Calculates ratio of Legendre functions of the second kind,
\[ \frac{Q_{N+1}}{Q_N} \] - c.f. Appendix A.

GRAPH (043590 - 043650)

Dummy routine to substitute for Simplotter driver.

CSIOLO (043660 - 060380)

Main program driver for MC²-2 input processor.

CARD06 (060390 - 062630)

Reads type 06 cards of file A.MCC2 and orders materials
consistent with library.

CARD15 (062640 - 066460)

Reads and processes type 15 cards of file A.MCC2.

CARD22 (066470 - 068170)

Reads type 22 cards of file A.MCC2 and loads arrays.

CARD09 (068180 - 071100)

Reads and processes type 09 cards of file A.MCC2.

CARD14 (071110 - 072970)

Reads and processes type 14 cards of file A.MCC2.

CARD18 (072980 - 074070)

Reads and processes type 18 cards of file A.MCC2.

CARD10 (074080 - 075330)

Reads and processes type 10 cards of file A.MCC2.

TYPE06 (075340 - 078580)

Reads and processes type 06 cards of file A.NIP.

TYPE14 (078590 - 081610)

Reads and processes type 14 cards of file A.NIP.
TABLE VIII. Function of MC\textsuperscript{2}-2 Subprograms (Contd.)

**TYPE15 (081620 - 086030)**
Reads and processes type 15 cards of file A.NIP.

**CARD16 (086040 - 087860)**
Reads and processes type 16 cards of file A.MCC2.

**CARD21 (087870 - 089690)**
Reads and processes type 21 cards of file A.MCC2.

**SPACER (089700 - 090260)**
Reads past cards in a BCD file.

**CARD23 (090270 - 091960)**
Reads and processes type 23 cards of file A.MCC2.

**CARD11 (091970 - 093130)**
Reads and processes type 11 cards of file A.MCC2.

**CARD08 (093140 - 097070)**
Reads and processes type 08 cards of file A.MCC2.

**HETERO (097080 - 098250)**
Generates homogeneous atom densities from A.NIP data.

**CARD17 (098260 - 102370)**
Reads and processes type 17 cards of file A.MCC2.

**CSDMGI (102380 - 103130)**
Determines interface energy between multigroup and continuous slowing down solution algorithms.

**PRNTAE (103140 - 103860)**
Edits Hollerith and single precision floating point arrays.

**TESTBG (103870 - 105610)**
Tests broad group energy structure for compatibility with ultra-fine-group energies.
TABLE VIII. Function of MC²-2 Subprograms (Contd.)

CARD12 (105620 - 112160)
Reads and processes type 12 cards of file A.MCC2.

CARD07/SETGRP (112170 - 117750)
Reads and processes type 07 cards of file A.MCC2; processes prestored broad-group structures.

CARD05 (117760 - 122280)
Reads and processes type 05 cards of file A.MCC2.

RDANIP (122290 - 127690)
Controls the reading of type 06, 14, 15 cards of file A.NIP.

EDGEOM (127700 - 129190)
Edits binary file GEOM1

FOILS (129200-129640)
Loads foil atom density array FOILDN

STRTCH (129650 - 131600)
Ensures that all materials in heterogeneous problem appear in homogeneous mixture.

PRNTID (131610 - 132830)
Edits one-dimensional double precision floating point array.

WRITER (132840 - 135310)
Writes the binary file PRBSPC.

SXLSXR (135320 - 137340)
Calculates arrays SXL, SXR used to obtain slab optical thickness.

EDTPRB (137350 - 145270)
Edits file PRBSPC.

Main driver for MC²-2 unresolved resonance calculation.
<table>
<thead>
<tr>
<th>Subprogram</th>
<th>Function</th>
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</thead>
<tbody>
<tr>
<td>UNRINT/UNRUNT</td>
<td>Calculates the single level unresolved resonance integral including interference scattering and self overlap.</td>
</tr>
<tr>
<td>PACKER</td>
<td>Reads unresolved resonance data from library file MCC2F3 and processes data.</td>
</tr>
<tr>
<td>INTERP</td>
<td>Linearly interpolates input array onto a second array on a different energy grid.</td>
</tr>
<tr>
<td>SETUPU</td>
<td>Identifies mixture materials with unresolved data.</td>
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<tr>
<td>QUICKJ</td>
<td>Calculates the isolated J integral with or without interference scattering using a single level representation.</td>
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<tr>
<td>DRCTOR</td>
<td>Allocates, loads arrays and directs calculation of unresolved resonance cross sections.</td>
</tr>
<tr>
<td>EDITUN</td>
<td>Edits file UNRES.</td>
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<tr>
<td>ESMESH</td>
<td>Sets up correspondence between input and collapsed energy mesh.</td>
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<tr>
<td>WZERO</td>
<td>Calculates real part of the function $W(o,x)$ using a rational approximation.</td>
</tr>
<tr>
<td>CSC005</td>
<td>Main driver for $MC^2$-2 resolved resonance calculation.</td>
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</tbody>
</table>
TABLE VIII: Function of MC²-2 Subprograms (Contd.)

ADMSTR (187710 - 191750)

Reads MC²-2 library data and controls calculation of resolved resonance integrals.

STUFIT (191760 - 193860)

Reads resolved data from file MCC2F4 and loads arrays in compressed form.

JINT (193870 - 204290)

Calculates isolated resonance integrals including interference scattering using either single level or multi-level formalisms.

EDITLZ (204300 - 205880)

Edits file LOPENZ.

NSICO (205890 - 206950)

Calculates $N_0$ for homogeneous and heterogeneous mixtures.

LORENT/LORANT (206960 - 209070)

Calculates ultra-fine-group integrals of Lorentzian shape resonance integrals.

WINNER (209080 - 210390)

Determines which neighboring resolved resonances contribute to overlap integral.

OVRLAP/OVRLOP (210400 - 216960)

Calculates overlap integrals for each resolved resonance.

RATNL (216970 - 217510)

Calculates real part of $W(0,x)$ using a rational approximation.

SETUPR (217520 - 217990)

Identifies mixtures with resolved resonance data.

TRIPLE (218000 - 219450)

Calculates infinite integrals of products of $\psi$ and $\chi$. 
### TABLE VIII. Function of MC$^2$-2 Subprograms (Contd.)

<table>
<thead>
<tr>
<th>Subprogram</th>
<th>Function</th>
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<tr>
<td>JINTGL (219460 - 222330)</td>
<td>Calculates isolated $J$ integral including interference scattering for the single level representation.</td>
</tr>
<tr>
<td>SIFTER (222340 - 228020)</td>
<td>Selects materials from resolved data file MCC2F4, controls reordering of resonances and selects overlap candidates.</td>
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<tr>
<td>REORDR (228030 - 231250)</td>
<td>Arranges resolved resonances in order of decreasing energy and deletes those that fall outside range of problem.</td>
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<tr>
<td>CSC006 (231260 - 239090)</td>
<td>Main driver for resolved-unresolved resonance interaction module.</td>
</tr>
<tr>
<td>INTRAC (239100 - 242260)</td>
<td>Reads files ATNUAT and RESINT and calculates interaction factors.</td>
</tr>
<tr>
<td>POTNTL (242270 - 245890)</td>
<td>Calculates resonance background cross sections and writes file SIGMAP.</td>
</tr>
<tr>
<td>EDITAT (245900 - 248660)</td>
<td>Edits file ATNUAT.</td>
</tr>
<tr>
<td>EDITRS (248670 - 250540)</td>
<td>Edits file RESINT.</td>
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<tr>
<td>WRISIT (250550 - 251560)</td>
<td>Calculates resolved overlap factors to be associated with each grid point.</td>
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<td>EDITSP (251570 - 252880)</td>
<td>Edits file SIGMAP.</td>
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<tr>
<td>CSC008 (252890 - 259500)</td>
<td>Main driver for macroscopic data calculations.</td>
</tr>
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</table>
TABLE VIII. Function of MC²-2 Subprograms (Contd.)

SIGMAC (259510 - 265370)
Calculates macroscopic total, elastic and \( \nu E_f \) ultra-fine-group cross sections.

SETCHI (265380 - 269330)
Calculates fission spectra distributions and writes file PRBCHI.

SETSCT (269340 - 278160)
Controls calculation of elastic matrices, transport cross sections and moderating parameters.

ELSCAT/ELSCT1 (278170 - 290780)
Calculates \( P_0 \) and \( P_1 \) ultra-fine-group elastic transfer matrices.

CALCFN (290790 - 292630)
Calculates \( (2n+1)F_n(u) \) at all hyper-fine-group boundaries.

FNAVG (292640 - 294260)
Calculates group averaged values of elastic expansion coefficients.

SIGAVG (294270 - 296400)
Calculates group averaged cross sections from data pairs using interpolation laws.

SETCSD (296410 - 298790)
Prepares coefficients for calculation of moderating parameters.

MODPAR (298800 - 305270)
Calculates continuous slowing down moderating parameters.

XTRN (305280 - 308120)
Calculates ultra-fine-group extended transport cross sections.

EDIT1 (308130 - 309270)
Edits elastic transfer matrices.

EDIT2 (309280 - 311930)
Edits macroscopic ultra-fine-group vectors.
TABLE VIII. Function of MC²-2 Subprograms (Contd.)

CSC009 (311940 - 322980)

Main program driver for ultra-fine-group spectrum and broad-group cross section calculation.

FILE1 (322990 - 324560)

Loads data from record 5 of file MCC2F1 to determine storage requirements for inelastic data.

FILE6 (324570 - 331140)

Reads the file MCC2F6 inelastic and (n,2n) data and writes the file GRPORD.

ATNSRC (331150 - 332070)

Reads file ATNUAT to determine number of spin states and resonances.

EGRID (332080 - 333080)

Sets up energies at which unresolved attenuation factors act.

REORDR (333090 - 336350)

Reads unresolved resonance integrals from file ATNUAT and orders them by energy.

MATCH (336360 - 339070)

Reads resolved resonance integrals from file RESINT and sets up problem material - resonance material correspondence.

INIT (339080 - 340870)

Sets initial fission source distribution.

SETIN (340880 - 347570)

Sets up storage for inelastic and (n,2n) data.

DRIVER (347580 - 354540)

Controls ultra-fine-group spectrum calculation.

MGSPEC/MGSPC1 (354550 - 358240)

Solves multigroup spectrum equations.

CSDSPC/CSDSP1 (358250 - 363430)

Solves continuous slowing down spectrum equations.
TABLE VIII. Function of $MC^2$-2 Subprograms (Contd.)

FISSOR/FISOR1 (363440 - 366990)

Calculates ultra-fine-group fission source and eigenvalue.

BSQITR (367000 - 368940)

Tests on convergence of buckling search and sets next buckling guess.

PARAB (368950 - 369350)

Computes coefficients for parabolic fit to three points.

INSCAT/INSC1 (369360 - 376090)

Calculates inelastic and $(n,2n)$ ultra-fine-group scattering source.

PROBIN (376100 - 378370)

Calculates discrete inelastic scattering source taking account of energy-angle correlation.

TABINT (378380 - 381170)

Calculates inelastic $(n,2n)$ scattering probability from tabulated function.

EDTUFG (381180 - 381600)

Edits ultra-fine values of array input.

SETBG (381610 - 391130)

Controls calculation of broad-group cross sections.

BGSPEC (391140 - 394860)

Calculates broad-group fluxes and currents; sets correspondence between broad- and ultra-fine-groups.

INSG (394870 - 402660)

Calculates inelastic and $(n,2n)$ broad group scattering source.

RESCS (402670 - 408030)

Calculates homogeneous broad group resonance capture, fission and total cross sections.
TABLE VIII. Function of MC²-2 Subprograms (Contd.)

RESCAT (408040 - 412060)
Calculates resolved resonance broad group elastic transfer matrices.

BGFLE1 (412070 - 415090)
Sets data and writes first three records of file ISOTXS.

BGFLE? (415100 - 421560)
Writes isotope dependent data to file ISOTXS.

ISOCHI (421570 - 422650)
Calculates broad-group chi vectors by isotope.

PRINXS/PRNXS1 (422660 - 429660)
Calculates broad-group non-resonance cross section vectors.

BGSCAT (429670 - 434230)
Calculates non-resolved resonance broad-group elastic scattering transfer matrices.

SRATE (434240 - 435890)
Writes the file SRATES for use by RABANL.

DOI0/DOI01/DOI02/DOI03 (435900 - 438780)
Prepares data for file SRATES.

ORIGIN (438790 - 438840)
Dummy routine to replace SIMPLOTTER subroutine.

CSCOIO (438850 - 444400)
Main driver for broad-group fundamental mode spectrum calculation.

HOMOG (444410 - 448100)
Prepares macroscopic broad group data.
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<tr>
<th>Function</th>
<th>Description</th>
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<tr>
<td>BGN (448110 - 451640)</td>
<td>Solves broad-group $P_N$ equations.</td>
</tr>
<tr>
<td>BSQTR (451650 - 453570)</td>
<td>Controls buckling search calculation.</td>
</tr>
<tr>
<td>CRAMER (453580 - 453980)</td>
<td>Calculates coefficients for parabolic fit to three sets data points.</td>
</tr>
<tr>
<td>BGSORS (453990 - 454540)</td>
<td>Calculates inhomogeneous broad-group source by summing ultra-fine-group sources.</td>
</tr>
<tr>
<td>CSE009 (454550 - 458210)</td>
<td>Main driver for editor of broad-group cross section file ISOTXS.</td>
</tr>
<tr>
<td>XEDIT (458220 - 463840)</td>
<td>Edits isotope cross section data from file ISOTXS.</td>
</tr>
<tr>
<td>CSCO11 (463850 - 481310)</td>
<td>Main driver for integral transport theory resolved resonance calculation.</td>
</tr>
<tr>
<td>E2E3E4/E2/E3/E4 (481320 - 483230)</td>
<td>This function obtains the exponential integrals $E_2(x)$, $E_3(x)$, and $E_4(x)$ by interpolation on tabular values or asymptotic expansions as appropriate.</td>
</tr>
<tr>
<td>FREEUP (483240 - 483760)</td>
<td>Closes data sets MCC2F1, MCC2F4, and SRATES.</td>
</tr>
<tr>
<td>MERGER (483770 - 489790)</td>
<td>Forms the union of all unique problem and foil materials and computes arrays.</td>
</tr>
</tbody>
</table>
TABLE VIII. Function of MC²-2 Subprograms (Contd.)

SPOOL (489800 - 495000)

Reads in the elastic, fission, capture, and total ultra fine group cross sections from scratch data sets.

FLIPIT (495010 - 495630)

Converts a slab cell with reflective boundary conditions to the equivalent cell with periodic boundaries.

SYM (495640  496320)

Determines symmetrical mesh interval pairs for slab geometry.

SIFTIT (496330 - 507750)

Selects materials from data set MCC2F4, calls STUFER to load arrays, and calls MANAGR to proceed with the integral theory resolved resonance calculation.

STUFER (507760 - 510000)

Reads data set MCC2F4, loads arrays, multiplies SIGO by the isotope abundances, and obtains the square roots of the resolved resonance energies.

REARNG (510010 - 511040)

Arranges resonances in order of decreasing energy.

EZ3/EZ4 (511050 - 511840)

This function obtains S3(Z,H) defined as the sum of E3(Z+KH) for K between zero and infinity. EZ3 is used for optically thin unit cells.

YZ3 (511850 - 512940)

Obtains the difference in the sums of E3(Y+KH) and E3(Y+DEL+KH) for K equal zero to infinity, S3(Y,H) - S3(Y+DEL,H).

YZ4 (512950 - 513790)

Obtains the difference in the sums of E4(Y+KH) and E4(Y+DEL+KH) for K equal zero to infinity, S4(Y,H) - S4(Y+DEL,H).

XTRAP/XTRAP4 (513800 - 514510)

Obtains S3(Z3,H) defined as the sum of E3(Z3+KH) for K between zero and infinity using gaussian quadrature.
TABLE VIII. Function of MC²-2 Subprograms (Contd.)

PFUNC (514520 - 515070)

'Obtains the slab collision escape probability.

SOARCE/SORCEL/SORCEF (515080 - 523730)

Computes the scattering source into the current hyper-fine-group.

MANAGR (523740 - 539000)

Acts as the driver to complete the integral transport theory calculation.

RESXSC/RESTES/XSECT (539010 - 544420)

Determines the resolved resonances to be included for the calculation of the hyper-fine-groups within each intermediate group, and computes the resolved resonance related cross sections for each hyper-fine-group.

RATES/RATESF (544430 - 559260)

Obtains the collision rates for the current hyper-fine-group and for each mesh interval of each region in the cell.

PREEDT (559270 - 561730)

Reads the data set IRESCS and writes out the rearranged data onto scratch data sets, one for each region, in preparation for editing the integral transport resonance cross sections.

EDTICS (561740 - 567650)

Reads scratch data sets, loads arrays, and edits the resolved resonance cross sections.

PREFOL (567660 - 569850)

Reads data set SCR005 and writes out the rearranged data onto scratch data sets, one for each foil, in preparation for editing the resonance foil cross section.

EDTFOL (569860 - 572050)

Reads scratch data sets, load arrays, and edits the resolved resonance cross sections for foil materials.


### TABLE VIII. Function of MC²-2 Subprograms (Contd.)

**DRIVED (572060 - 576610)**

Acts as the driver for the editing functions of the integral transport theory calculation.

**PREEDI (576620 - 577880)**

Reads the data set IRESCS and loads arrays for the case when arrays can be core contained in preparation for editing the integral transport theory resonance cross sections.

**EDTICI (577890 - 583220)**

Edits the resolved resonance transport theory resonance cross sections when arrays can be core contained.

**PREFOI (583230 - 584500)**

Reads scratch data set and loads arrays for the case when arrays can be core contained in preparation for editing foil cross sections.

**EDTFOI (584510 - 585960)**

Edits resolved resonance cross sections for foil material when arrays can be core contained.

**DRIVEI (585970 - 589070)**

Acts as the driver for the editing functions of the integral transport theory calculation when arrays can be core contained.
TABLE IX. MC²-2 ENDF/B-IV Library Files

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Maximum Energy: $1.419 \times 10^7 \text{ eV}$

Lethargy Width: 1/120

Number of groups: 2082

Number of Materials: 104
TABLE IX. MC²-2 ENDF/B-IV Library Files (Cont'd.)

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TABLE IX. MC²-2 ENDF/B-IV Library Files (Cont'd.)

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<td></td>
<td></td>
<td>Fission Spectrum</td>
</tr>
<tr>
<td>HYDRGN</td>
<td>1769</td>
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</table>

U This material has unresolved resonance data
R This material has resolved resonance data
F This material has fission spectrum data
2. **CDC Code Implementation**

The implementation of the MC\(^2\)-2 code has been performed at two CDC computer laboratories - Lawrence Berkeley Laboratory and Brookhaven National Laboratory. Each laboratory has one CDC 7600 computer with 65,536 (60-bit) words of small core memory and 512,000 (60-bit) words of large core memory. Also each laboratory has two CDC 6600 computers with 65,536 (60-bit) words of central memory. MC\(^2\)-2 was implemented only on the CDC 7600 computers. The examples in this section display the control cards suitable for each installation. The essential nature of each step is intended to be system independent. Each CDC installation has local conventions but Brookhaven National Laboratory adheres almost entirely to standard CDC conventions. The user will find all the necessary CDC control card information and FORTRAN usage in the following four manuals.

1. FORTRAN Extended 4 Reference Manual (Publication No. 60305600, Rev. G)
2. SCOPE 2.1 Reference Manual (Publication No. 60342600, Rev. H)

The CDC program tape is written as described in Table X. The source code for M\(\text{C}^2\)-2 is contained on Files 1 and 2 of the program tape. A brief description of each of the FORTRAN subprograms of File 1 is given in Table VIII, and the subprograms and sequence numbers in this table are the same for both IBM and CDC codes. The source code differs in that all cards between two cards with CDC* in columns 1-4 have a C in column 1 on the IBM tape and a blank in column 1 on the CDC tape. The opposite change is true of cards between two cards with CIBM in columns 1-4. The 14 subprograms on File 2 of the tape are discussed in Table XI. The first 13 subprograms are written in FORTRAN, and the last subprogram, MEMGET, is a COMPASS routine. Creation of object code for input to the segmentation loader is the first step required for implementation of the MC\(^2\)-2 program. The compilation of File 1 subprograms and the first 13 subprograms of File 2 should be performed using the highest level of optimization available that will give the correct object code. Currently, this means use of the FORTRAN extended compiler with OPT=1 specified. The FORTRAN extended compiler is necessary because of the presence of LEVEL 2 statements. At the present time there are errors in code generated with the OPT=2 FORTRAN extended compiler. Also the CDC FORTRAN compiler release of 4.4 or later was used. Earlier releases generated incorrect object code for all available optimizations. Figure 23 displays the control cards necessary for reading the two files of the source program tape, compilation of the FORTRAN code, assembly of the one COMPASS routine and writing of the object code onto a magnetic tape. Depending on the installation, it may be necessary to isolate the one COMPASS routine in File 2 before assembly.
This is currently a requirement at the Berkeley site because of interface problems with their FORTRAN extended compiler. Therefore the CDC UPDATE routine was used to separate the FORTRAN and COMPASS source code. Generally for CDC computers, source code can be mixed FORTRAN and COMPASS subprograms. The FORTRAN compiler will recognize COMPASS routines and invoke the COMPASS assembler and then control will be returned to the FORTRAN compiler.

Figure 24 displays the control cards which read the generated object code from the magnetic tape. The segmented loader is then invoked and it builds the segments from the object code in accordance with the directives issued to the segmented loader. These directives are provided on File 3 of the program tape. The INCLUDE directives must be specified in a manner which is dependent on the CDC 7600 computer operating system. For an operating system less (greater) than SCOPE 2.0, a subroutine specified in the verb field must (must not) be specified in the specification field. For example, if subroutines A, B, and C are to appear in the same segment, then the directive statement under a SCOPE operating system equal or greater than 2.0 will be expressed as

A INCLUDE B,C

For a 7600 computer operating system less than 2.0 or the Berkeley 'BKY' operating system, the equivalent directive statement must be stated as

A INCLUDE B,C,A

The segmented loader resolves I/O routines and mathematical subroutines with the system library called FTN4LIB (Berkeley) or FORTRAN (Brookhaven). The executable code now resides on the file designated as MCCA. This file is written onto a magnetic tape.

Two library tapes are provided along with the MC^2-2 program tape. These library tapes contain eight binary sequential files with a total of 4559 records and 2,767,155 words in the format of the files MCC2F1-MCC2F8 described in Appendix C. These library tapes were written at the Berkeley Laboratory on 7 track unlabeled tapes at a density of 800 BPI and x-mode binary. Appendix F describes the process used for generating the MC^2-2 library files on a single 1600 BPI tape from these two 7 track tapes. These files must be copied to a direct access device (e.g. disk pack) as the next step in program implementation. Since no private disk space was available, the library was copied from tape to disk for each problem execution as illustrated in Fig. 25. The data set names assigned to the eight binary MC^2-2 library files are TAPE22-TAPE29 as displayed in Fig. 25. The data available on these library files were processed from the ENDF/B-IV data files by the code ETOE-2. A summary of the library specifications is given in Table IX. The Argonne Code Center also has available four BCD tapes which contain this same eight file library in BCD format along with a FORTRAN program, MC^2-2 LIBGEN, which reads the BCD files and writes the eight binary files. Appendix F illustrates this process. The binary library tapes generated at Berkeley Laboratory were made from the FORTRAN program MC^2-2 LIBGEN.

The control cards used to execute an MC^2-2 problem are given in Fig. 25. The executable code generated by the segmented loader and the eight binary library files are copied from tape to a disk pack. Note that the eight
binary library files are copied from tape to disk for every problem execution. For the Berkeley example the TAPE control card and its appropriate directives require 34 charge units (one charge unit costs the user about 7 cents) to transfer the binary library files from tape to disk pack and assign a data set name to each file. Brookhaven does not have a comparable control card. The control cards used to transfer the library files from tape to disk pack in the Brookhaven example are very inefficient. Staging the data and using the COPYBF control cards to assign a data set name to each of the eight files requires twice the disk space since two copies of the library exist on disk packs.

When this method was used at Berkeley for comparison purposes the STAGE command required 8 charge units to transfer all the binary data from tape to disk and the COPYBF control cards which assign data set names to each file require an additional 267 charge units. The user should be aware of the BPOINTER container array size allocated in SCM and LCM and the appropriate field length specified on the CDC control card preceding MC²-2 problem execution. The size of the dynamic storage capability, BPOINTER, described in Reference 1 and briefly in Appendix E, used to manage all variable dimension array allocations, is provided for on card type 02 of data set A.MCC2. For the CDC version of the code, a container array is allocated in SCM (up to 22,000 decimal words available in small core plus another 10,000 decimal words if no small core buffers exist) as well as a container array in LCM (up to 131,072 decimal words in directly addressable large core memory). Almost all of the large BPOINTER arrays in the CDC version of the MC²-2 code are placed in the container array in LCM. At this time, no known limitations due to core size are placed upon executions of the CDC version of this code.

Two BCD sample problem input decks are provided on File 4 of the program tape. The first problem displays the execution of a homogeneous consistent P₁ problem. The type 01 card of data set A.STP015 is set to execute Areas 4, 5, 6, 6.5, 7, 8, and 9 and to edit the broad group cross sections. The second sample problem shows the execution of a homogeneous resolved resonance integral transport calculation. The type 01 card of data set A.STP015 is set to execute Areas 4 and 10. Data set UNREG, the unresolved resonance ultra-fine-group cross sections, (called TAPE 49) was saved from the first problem. This data set is input to the second problem by specifying DATASET=UNREG under the data set initialization BLOCK=OLD.
TABLE X. CDC Code Center Tape Description

<table>
<thead>
<tr>
<th>File Number</th>
<th>Contents</th>
<th>Number of Card Images</th>
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<tbody>
<tr>
<td>1</td>
<td>MC²-2 Subprograms See Table VIII</td>
<td>58907</td>
</tr>
<tr>
<td>2</td>
<td>MC²-2 Subprograms for CDC Code See Table XI</td>
<td>654</td>
</tr>
<tr>
<td>3</td>
<td>Directives Required for Segmented Loader See Fig. 17</td>
<td>48</td>
</tr>
<tr>
<td>4</td>
<td>Two Sample MC²-2 Problem Input Decks</td>
<td>150</td>
</tr>
</tbody>
</table>
TABLE XI. Function of \textit{MC}^2-2\textit{ Subprograms for CDC Code

\textbf{ALLOC1/ALLOC2} (000010 - 000760)*

Assign storage for the dynamic allocation subprogram package BPOINTER.

\textbf{FREE1/FREE2} (000770 - 001010)

Dummy FORTRAN routine that releases the storage of the dynamic storage container array that was allocated by the subroutine ALLOC1/ALLOC2.

\textbf{ABEND/ABSTOP} (001020 - 001080)

Called by subroutine \textit{ERROR} to force an abnormal termination of the job with a DUMP.

\textbf{FXPI/FXPT} (001090 - 001580)

Fast exponential function.

\textbf{COWEST} (001590 - 001840)

Left-justify Hollerith variables.

\textbf{DISPOS} (001850 - 001950)

Used by module CSI010 to determine whether the file \textit{SRATES} is given a permanent or temporary disposition. CDC code always sets a temporary disposition to the file.

\textbf{FILEID} (001960 - 002110)

A dummy routine that is used in subroutine \textit{BGFLE1} of module CSC009 to obtain the dataset name associated with the file \textit{ISOTXS}.

\textbf{CVD} (002120 - 002240)

Used in subroutine \textit{BGFLE2} of module CSC009 to convert a variable from integer to Hollerith format.

\textbf{DRED/DRIT} (002250 - 004040)

FORTRAN routine that performs the non-formatted (binary) I/O operations between LCM and disk files without use of a buffer array in small core memory.

\textbf{ZERO10} (004050 - 004150)

FORTRAN routine that initializes the common block \textit{/INITIO/} which is common to subroutines \textit{REED} and \textit{DRED}.\n
TABLE XI. Function of MG^2-2 Subprograms for CDC Code (Contd.)

BUOPEN/BCLOSE (004160 - 004200)

A dummy FORTRAN routine that is intended to open/close dataset buffers.

ERF (004210 - 005130)

A FORTRAN written function that evaluates the error function.

PRTECS (005140 - 006320)

A FORTRAN subroutine that edits a one-dimensional floating point single precision array located in LCM.

MEMGET/MEMGET1 (006330 - 006540)

A COMPASS routine that performs the allocation for ALLOC1/ALLOC2.

* Numbers in brackets are sequence numbers of routine on File 2 of CDC program tape.

† This is a FORTRAN routine for the CDC code. See Section D above for a further description of this routine.
Fig. 23. Compilation and Assembly of CDC Source Code to Generate Object Code
Fig. 24. Build the Segments from Object Code Using the Segmentation Loader
Fig. 25. Execution of MC$^2$-2 Problem
APPENDIX A

SPECIAL FUNCTION EVALUATIONS
I. Legendre Functions of the Second Kind

In the $B_N$ approximation the extended transport cross section depends on a ratio of Legendre functions of the second kind,

$$R = \frac{Q_{N+1}(z)}{Q_N(z)}$$

where

$$1 \leq N \leq 9$$

$$z = \frac{i\Sigma}{B}$$

and the buckling $B$ can be either real or imaginary. The calculation of the ratio $R$ depends upon both $N$ and $z$. In Table XII the computational option is identified with the values of $N$ and $z$. In the expressions below defining the options $B$ is used to represent the real or imaginary part of $\sqrt{B^2}$.

1) **Option 1 (Analytic)**

$$R_1 = \frac{1}{2} \left[ \left( 1 + \frac{3\Sigma^2}{B^2} \right) \tan^{-1} \frac{B}{\Sigma_t} - \frac{3\Sigma}{B} \right]$$

2) **Option 2 (Analytic)**

$$R_2 = \left[ \frac{3\Sigma^2}{B^2} - 1 \right] \frac{\Sigma_t}{2B} \ln \left| \frac{1 + B/\Sigma_t}{1 - B/\Sigma_t} \right| - \frac{3\Sigma}{B}$$

3) **Option 3 (Hypergeometric Series)**

$Q_N$ and $Q_{N+1}$ are calculated using an eleven term hypergeometric series expansion,

$$(30)$$

$$Q_N(x) = B(N, 0; x) F\left(\frac{1}{2}, \frac{1}{2}; N + \frac{3}{2}; -t\right)$$

$$x = \frac{\Sigma_t}{B}, \quad t = \frac{x - (x^2 - 1)^{1/2}}{2(x^2 - 1)^{1/2}}$$
with the coefficients of the eleven term summation precalculated. The ratio, $R_3$, is then calculated from $Q_{N+1}(x)/Q_N(x)$.

4) **Option 4 (Backward Recursion)**

The ratio $R_4$ is calculated using Gautschi's backward recursion relation (31). Setting

$$
\nu = N + 9
$$

$$
S = - \frac{B^2}{|B^2|}
$$

$$
r_0 = 0
$$

the recursive relationship

$$
r_n = \frac{\nu - n + 1}{\nu - n + 2} \frac{B}{\sum t} \left[ 1 + \frac{\nu - n + 1}{\nu - n + 2} \right] + S r_{n-1}
$$

is used to define $r_9$. The ratio $R$ is then given by

$$
R_4 = \begin{cases} 
-ir_9 & B^2 > 0 \\
9 & B^2 < 0 
\end{cases}
$$

5) **Option 5 (Forward Recursion)**

The ratio $R_5$ is calculated using the standard forward recursion relation. Setting

$$
r_o = \begin{cases} 
-\frac{\tan^{-1}B}{\sum t} & B^2 > 0 \\
\frac{1}{2} \ln \left| \frac{1 + \sum t/B}{1 - \sum t/B} \right| & B^2 < 0 
\end{cases}
$$

$$
r_1 = \frac{\sum t}{B} S r_o - 1
$$

$$
S = - \frac{B^2}{|B^2|}
$$
the recursive relationship
\[ r_{n+1} = \frac{\Sigma t}{B} s^{n+1} r_n - r_{n-1} + \frac{\Sigma t}{B} s^{n+1} r_n \]
\[- \left( \frac{\Sigma t}{B} s^{n+1} r_n - r_{n-1} \right) / (n + 1) \quad n = 1, 2, \ldots, N \]
is used and \( R \) is defined
\[
R_5 = \begin{cases} 
\frac{r_{N+1}}{r_N} & B^2 < 0 \\
i \frac{r_{N+1}}{r_N} & B^2 < 0
\end{cases}
\]

6) **Option 6 (Relationship with \( P_N \))**

Use is made of the relationship between Legendre functions of the first kind \( P_n(z) \) and the second kind \( Q_N(z) \) to calculate the ratio \( R_6 \). Since the forward recursion relation is stable for all \( P_n \), the Legendre functions of the first kind are calculated directly from it,

\[ P_0(z) = 1 \]
\[ |P_1(z)| = \frac{\Sigma t}{B} \]
\[ |P_n(z)| = (-)^{n+1} \frac{\Sigma t}{B} |P_{n-1}(z)| - |P_{n-2}(z)| + (-)^{n+1} \frac{\Sigma t}{B} |P_{n-1}(z)| \]
\[ - \left[ (\Sigma t) |P_{n-1}(z)| - |P_{n-2}(z)| \right] / (n - 1) \]
\[ n = 2, 3, \ldots, N + 1 \]

From the \( P_n(z) \), the non-singular part of \( Q_N(z) \) and \( Q_{N+1}(z) \) is calculated,

\[ (-) \left[ \begin{array}{c} N \\ 2 \end{array} \right] + 1 \]
\[ W_N = \frac{2N + 1}{N + 1} P_N - \frac{2N - 3}{3N} P_{N-2} + \frac{2N - 7}{5(N - 1)} P_{N-4} + \ldots \]
\[ (-) \left[ \begin{array}{c} N+1 \\ 2 \end{array} \right] + 2 \]
\[ W_{N-1} = \frac{2N - 1}{N} P_{N-1} + \frac{2N - 5}{3(N - 1)} P_{N-3} + \ldots \]

The functions \( Q_N \) and \( Q_{N+1} \) are then calculated as,
\[ Q_{N+1} = (-)^{\left[ \frac{N+1}{2} + 1 \right]} \left( \frac{\pi}{2} - \tan^{-1} \frac{\Sigma t}{B} \right) \left| P_{N+1} \left\{ \frac{i \Sigma t}{B} \right\} \right| + \mathcal{W}_N \]

\[ Q_N = (-)^{\left[ \frac{N}{2} + 2 \right]} \left( \frac{\pi}{2} - \tan^{-1} \frac{\Sigma t}{B} \right) \left| P_N \left\{ \frac{i \Sigma t}{B} \right\} \right| + \mathcal{W}_{N-1} \]

and

\[ R_6 = \frac{Q_{N+1}}{Q_N} \]
### TABLE XII  Legendre Function Evaluation

| N | $R^2$ | $|\Sigma_{\xi}/\xi|$ | Option                  |
|---|-------|----------------|------------------------|
| 1 | $> 0$ | all           | 1 Analytic             |
| 1 | $< 0$ | all           | 2 Analytic             |
| $> 1$ | $< 0$ | (1.0, 1.15] | 3 Hypergeometric series|
| $> 1$ | $< 0$ | 1.15         | 4 Backward recursion   |
| $> 1$ | $> 0$ | $> 1.0$     | 4 Backward recursion   |
| $> 1$ | $< 0$ | $\leq 1.0$  | 5 Forward recursion    |
| $< 4$ | $> 0$ | $\leq 1.0$  | 5 Forward recursion    |
| $> 1$ | $> 0$ | (0.0, 0.45] | 5 Forward recursion    |
| $\geq 4$ | $> 0$ | (0.45, 1.0] | 6 Relationship with $P_N$ |
II. A Fast Exponential Subroutine - FXP

Approximately half of the central processor time in a heterogeneous slab calculation in the RABANL module of MC2-2 is devoted to the calculation of exponentials, $e^{-|x|}$. In the ultra-fine-group calculation, about 25% of the CPU time for a problem with many isotopes is spent in the calculation of exponentials to treat the inelastic and $(n,2n)$ evaporation laws. The standard IBM Fortran exponential function is quite general with regard to permissible arguments and quite accurate. On the other hand it is relatively slow ($\approx 9 \times 10^{-6}$ sec. on a 360/195). Large gains in speed at the expense of accuracy and core storage are obtained by use of an assembler language routine FXP. For arguments in the range $0 \leq x \leq 18$, the program FXP uses a linear interpolation scheme

$$ e^{-x} \approx y_i - m_i x \quad 0 \leq i < 1022 $$

where

$$ y_i = y^*_i + i\Delta m_i \quad 0 \leq i \leq 1022 $$
$$ m_i = \frac{y^*_i - y^*_{i+1}}{\Delta} \quad 0 \leq i \leq 1022 $$
$$ y^*_i = e^{-\Delta} y^*_{i-1} \quad 0 < i \leq 1022 $$
$$ y^*_0 = \frac{2}{\Delta} \frac{(1 - e^{-\Delta})}{(1 + e^{-\Delta})} $$

$$ \Delta' = 18.0/1022 $$

This approximation was shown by Olson to be sufficiently accurate for calculations of collision probabilities in the RABID code. The programming of the assembler language routine FXP was optimized to a 195 by A. Hinds of ANL. Computation times less than half that of the Fortran exponential functions are typical of FXP on an IBM 370/195. A Fortran equivalent of FXP is available with the CDC code. The Fortran routine is approximately 20% faster than the CDC library exponential routine.
III. Calculation of Doppler-Broadened Line Shape Functions

In the computation of Doppler-broadened resonance cross sections, use is made of the symmetric and anti-symmetric line shape functions. These functions, usually denoted as $\psi$ and $\chi$, are defined in terms of the real and imaginary parts of the error function for complex arguments as

$$\psi(a,b) = \frac{a\sqrt{\pi}}{2} \text{Re} \ W\left(\frac{ab}{2}, \frac{a}{2}\right)$$  \hspace{1cm} (A.1)

$$\chi(a,b) = a\sqrt{\pi} \text{Im} \ W\left(\frac{ab}{2}, \frac{a}{2}\right)$$  \hspace{1cm} (A.2)

where

$$W(z) = W(x,y) = \exp(-z^2) \text{erfc}(-iz)$$  \hspace{1cm} (A.3)

and $z = x + iy$.

Re$W(x,y)$ and Im$W(x,y)$ were precalculated using the methods described in Ref. 32 and stored in coarse and fine mesh tables as indicated below. In the fine mesh tables, $y$ ranges between -0.02 and 0.5 with the mesh -0.02(0.02)0.5 while in the coarse mesh tables $y$ ranges between 0.4 and 3.0 with the mesh 0.4(0.1)3.0. In both tables, $x$ ranges between -0.1 and 3.9 with the mesh -0.1(0.1)3.9.

If $|x| \leq 3.9$ and $y \leq 3.0$, the Re$W$ and Im$W$ are obtained using the six-point bivariate interpolation formula (25.2.67) of Ref. 33 in either the fine or coarse mesh tables as appropriate to the value of $y$.

If $|x| > 3.9$ or $y > 3.0$ but $|x| \leq 6.0$ and $y \leq 6.0$, $W(z)$ is approximated by

$$W(z) = iz \sum_{i=1}^{3} \frac{a_i}{z^2 - b_i}$$  \hspace{1cm} (A.4)

where

$$a_1 = 0.4613135$$
$$b_1 = 0.1901635$$
$$a_2 = 0.09999216$$
$$b_2 = 1.7844927$$
$$a_3 = 0.002883894$$
$$b_3 = 5.5253437$$

Setting $z = x + iy$, Eq. A.4 yields
\[
\text{KeW} = \sum_{i=1}^{3} \frac{a_i \left[ -y (x^2 - y^2 - b_i) + 2x^2y \right]}{(x^2 - y^2 - b_i)^2 + 4x^2y^2}
\]
(A.5)

\[
\text{ImW} = \sum_{i=1}^{3} \frac{a_i \left[ x (x^2 - y^2 - b_i) + 2xy^2 \right]}{(x^2 - y^2 - b_i)^2 + 4x^2y^2}
\]
(A.6)

If \(|x| > 6.0\) or \(y > 6.0\) but \(|x| \leq 100.0\) and \(y \leq 100.0\), \(W(z)\) is approximated by

\[
W(z) = \frac{2}{\pi} \sum_{i=1}^{2} \frac{c_i}{z^2 - d_i}
\]
(A.7)

where

\[
\begin{align*}
c_1 &= 0.5124242 \\
d_1 &= 0.2752551 \\
c_2 &= 0.0517636 \\
d_2 &= 2.724745
\end{align*}
\]

Thus

\[
\text{ReW} = \sum_{i=1}^{2} \frac{c_i \left[ -y (x^2 - y^2 - d_i) + 2x^2y \right]}{(x^2 - y^2 - d_i)^2 + 4x^2y^2}
\]
(A.8)

\[
\text{ImW} = \sum_{i=1}^{2} \frac{c_i \left[ x (x^2 - y^2 - d_i) + 2xy^2 \right]}{(x^2 - y^2 - d_i)^2 + 4x^2y^2}
\]
(A.9)

If \(|x| > 100.0\) or \(y > 100.0\), the code uses an asymptotic approximation. The integral representation of \(W(z)\) is given by formula 7.1.4 of Ref. 33 as

\[
W(z) = \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t^2}}{z - t} \, dt
\]
(A.10)

\[
\sum_{j=1}^{N} w_j \frac{1}{z - t_j}
\]
(A.11)

where the \(w_j\) and \(t_j\) are the weights and abscissae for the Hermite quadrature. In particular, for very large \(x\) or \(y\), we set \(N = 2\) and ignore \(t_i\) relative to \(z\) so that

\[
W(z) \approx \frac{2i}{\pi} \frac{w}{z}
\]
(A.12)

where \(w = \sqrt{\pi}/2\). Setting \(z = x + iy\), we have finally

\[
\text{ReW} = \frac{y}{\sqrt{\pi} \left( x^2 + y^2 \right)}
\]
(A.13)
For the special case of $x = 0$, Eq. A.3 becomes

$$W(0, y) = e^{y^2} \text{erfc}(y).$$  \hspace{1cm} (A.15)

If $y < 2.0$, Eq. A.15 is evaluated using the rational approximation (7.1.26) of Ref. 33. If $2.0 \leq y \leq 6.0$, Eq. A.15 is evaluated using Eq. A.5 with $x$ set equal to zero. If $6.0 < y \leq 100.0$, Eq. A.15 is evaluated using Eq. A.8 with $x$ set equal to zero. Finally, for $y > 100.0$, Eq. A.15 is evaluated using Eq. A.13 with $x$ set equal to zero.
IV. Numerical Methods Used in Calculating the Isolated Resonance Integral

The three terms of the factored isolated resonance integral $J(\beta, \theta, 0, 0)$, $I(\beta, \theta, a)$, and $M(\beta, \theta, a)$ given respectively in Eqs. III.46–III.48 are evaluated using fixed point Gauss-Jacobi quadrature or asymptotic algorithms depending upon the value of $\beta$. The code calculates the quantity

$$T1 = \frac{\beta + \psi(\theta, 0)}{\psi(\theta, 0)}.$$  \hspace{1cm} (A.16)

If $T1 > 4.5$, asymptotic expressions are evaluated as described later. Otherwise, the code evaluates the integrals as follows. \hspace{1cm} (25)

The variable of integration is changed from $x$ to $u$ using the transformation

$$x = K \frac{u}{\sqrt{1 - u^2}},$$ \hspace{1cm} (A.17)

so that in general

$$\int_0^{\infty} f(x) dx = \frac{1}{K} \int_0^{1} \frac{du}{\sqrt{1 - u^2}} \cdot f(x(u))\int_0^{1} \frac{du}{\sqrt{1 - u^2}}$$

$$= \frac{\pi}{N} \frac{1}{K} \left\{ \frac{1}{2} f(0) + \sum_{i=2}^{(N-1)/2} \frac{f(x(u_i))}{1 - u_i^2} \right\} + R_N.$$ \hspace{1cm} (A.18)

The Gauss-Jacobi quadrature points $u_1$ are given by

$$u_1 = \cos \left( \frac{(2i - 1) \pi}{2N} \right),$$ \hspace{1cm} (A.19)

the quadrature weights are constant and equal to $\pi/N$, and the remainder is given

$$R_N = \frac{\pi}{(2N)!} \frac{f(2N)(\xi)}{2^{2N-1}}, \hspace{1cm} 0 < \xi < 1.$$ \hspace{1cm} (A.20)

The value selected for $N$ (either 9 or 13) and the value for $K$ is determined as shown in Fig. 26 based upon the values of $\theta$ and $\beta$.

Now when $T1 \geq 4.5$, Hwang has shown that one may write

$$J(\beta, \theta, 0, 0) = T \int_0^{\infty} dx \frac{\psi(\theta, x)}{\beta + S \psi(\theta, x)}$$

$$\approx T \left\{ \frac{\pi}{\beta + \rho} + S^2 \frac{\int_0^{\infty} \psi^3(\theta, x) dx}{(\beta + \rho)^3} - \frac{\pi \rho^2}{(\beta + \rho)^3} \right\}.$$ \hspace{1cm} (A.21)
Fig. 26. Gauss-Jacobi Quadrature Selection
\[ I(\beta, \theta, a) = Ta^2 \int_0^\infty dx \frac{\psi}{\beta + S\psi} \cdot \frac{\chi^2}{(\beta + S\psi)^2 - a^2\chi^2} \]
\[ + \frac{4a^2}{3} T \frac{\int_0^\infty \psi^3 dx}{(\beta + \rho)^3} \tag{A.22} \]

\[ M(\beta, \theta, a) = a \int_0^\infty dx \frac{\chi^2}{(\beta + S\psi)^2 - a^2\chi^2} \]
\[ + \frac{2\pi a(\beta + 3\rho)\rho}{S(\beta + \rho)^3} - \frac{8aS}{3(\beta + \rho)^3} \int_0^\infty \psi^3 dx \tag{A.23} \]

In Eqs. A.21-A.23,
\[ \rho = \frac{S}{2} \psi(\sqrt{2} \theta, 0) \tag{A.24} \]
and \( \psi(\sqrt{2} \theta, 0) \) is evaluated using Eq. A.15.

The third order integral which appears in Eqs. A.21-A.23 is evaluated using a power series expansion, or if \( \theta > 2.5 \), an asymptotic expansion.

For \( \theta \leq 2.5 \)
\[ \int_0^\infty \psi^3(\theta, x) dx \approx \frac{\pi}{2} \left\{ \frac{\rho}{S} \left[ 3 \psi(\sqrt{2/3} \theta, 0) - \sqrt{3\pi/2} \theta e^{\frac{\theta^2}{2}} \right] + \frac{3}{2} \beta^2 S_1 \right\} \tag{A.25} \]

where
\[ S_1 = \frac{1}{4} + 6 \sum_{n=1} \frac{A_n}{n} \sum_{m=1}^n B_m \theta^{2m} \tag{A.26} \]

and
\[ A_n = \frac{n!}{1 \cdot 3 \cdot 5 \cdots (2n + 1)} \frac{1}{2^n} \]
\[ B_m = \frac{1}{(3/2)^m} \cdot 4 \cdot m! \tag{A.27} \]

For \( \theta > 2.5 \)
\[ \int_0^\infty \psi^3(\theta, x) dx \approx \frac{\pi}{8} \left\{ \frac{3}{2} \left[ \frac{2}{3} \theta^2 e^{\frac{2\theta^2}{3}} E_1(\frac{2}{3} \theta^2) - h_1 + h_2 - h_3 + h_4 \right] \right\} \tag{A.28} \]
where

\[ E_1 \text{ is the exponential integral defined in Eq. A.37 and} \]

\[ h_1 = 1 - \frac{2}{3} \theta^2 e^{\frac{2}{3} \theta^2} E_1(\frac{2}{3} \theta^2) \]

\[ h_2 = \frac{1}{3} \theta^2 - h_1 \]

\[ h_3 = \frac{5}{6} \theta^4 - \frac{10}{9} h_2 \]

\[ h_4 = \frac{105}{4\theta^6} - \frac{7}{6} h_3 \]  \hspace{1cm} (A.29)

For \( x < 10 \), \( E_1(x) \) is evaluated using the rational expression 5.1.54 of Ref. 33 and for \( x \geq 10 \), the rational expression 5.1.55 of Ref. 33.

For the case of \( \beta > 10^{10} \), the code uses the first term in Eq. A.21 for \( J \) and sets \( I \) and \( M \) equal to 0.
V. Quadratures for Statistical Integration

In the calculation of unresolved resonance cross sections, integrals of the form

\[ \langle f(x,y) \rangle = \int_0^\infty P_\mu(x)dx \int_0^\infty P_\nu(y)f(x,y)dy \]  

(A.30)

are required where \( P_\mu \) is the Chi-squared distribution of order \( \mu \) given by

\[ P_\mu(x)dx = \frac{\mu}{\Gamma(\mu/2)} \frac{1}{\Gamma(\mu/2)^{1/2}} \exp \left( -\frac{\mu x}{2} \right) \]  

(A.31)

Eq. A.30 is evaluated using the method described by Hwang as

\[ \langle f(x,y) \rangle = \sum_{j=1}^{10} \sum_{k=1}^{10} A_j A_k f(x_j, y_k) \]  

(A.32)

where the \( A_j \) and \( x_j \) have been calculated for \( \mu = 1, 2, 3, \) and 4. The ten point quadrature is used for both neutron and fission width distributions.

For odd \( \mu \)

\[ x_j = 2z_j^2/\mu \]  

(A.33)

\[ A_j = 2w_j^S z_j^{\mu-1}/\Gamma(\mu/2) \]  

(A.34)

while for even \( \mu \)

\[ x_j = (1-s_j)/(1+s_j) \]  

(A.35)

\[ A_j = \mu w_j^L \left( \frac{\mu}{2} x_j \right)^{\mu/2-1} \exp \left( -\frac{\mu x_j}{2} \right) /[\Gamma(\mu/2)(1+s_j)^2] \]  

(A.36)

In Eqs. A.33 and A.34, \( z_j \) and \( w_j^S \) are respectively the ordinates and weights of the half-range Gauss-Hermite quadrature derived by Steen, et al. (36) while in Eqs. A.35 and A.36, \( s_j \) and \( w_j^L \) are respectively the usual Gauss-Legendre ordinates and weights.

Table XIII lists \( A_j \) and \( x_j \) for \( \nu = 1, 2, 3, \) and 4 and \( j = 1, 2, \ldots, 10. \)
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VI. Numerical Methods Used in Calculating Slab Collision Rates

a. Exponential Integrals

The exponential integral $E_n(x)$ is defined as

$$E_n(x) = \int_1^\infty \frac{e^{-xt}}{t^n} \, dt$$  \hspace{1cm} (A.37)

The integrals $E_2(x)$, $E_3(x)$, and $E_4(x)$ are obtained using the following algorithms.

$E_2(x)$ is evaluated using the series expansion (5.1.11) of the Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables (33) for $E_1(s)$ along with the recursion relationship

$$E_{n+1}(x) = \frac{1}{n} \left[ e^{-x} - x E_n(x) \right]$$  \hspace{1cm} (A.38)

to yield

$$E_2(x) \approx 1 - x (1 - \gamma - \ln x) - \frac{x^2}{1 \cdot 2!} + \frac{x^3}{2 \cdot 3!} - \frac{x^4}{3 \cdot 4!}$$  \hspace{1cm} (A.39)

where Euler's constant $\gamma$ has the value $\gamma = 0.5772156649 \ldots$

For $x < 0.6$, $E_3(x)$ as in the case of $E_2(x)$ uses (5.1.11) of Ref. 33 with successive application of Eq. A.38 to yield

$$E_3(x) \approx 0.5 - x + \frac{x^2}{2} (1.5 - \gamma - \ln x) + \frac{x^3}{3!} - \frac{x^4}{2 \cdot 4!} + \frac{x^5}{3 \cdot 5!} - \frac{x^6}{4 \cdot 6!} \ldots$$  \hspace{1cm} (A.40)

For $0.6 \leq x \leq 6.4$, $E_3(x)$ is obtained by linear interpolation in a table of $E_3$ with tabular entries $0(0.01)2(0.02)4(0.08)6.4$. The table values are calculated using the polynomial approximation (5.1.53) of Ref. 33 if $0 \leq x \leq 1$ and the rational approximation (5.1.56) of Ref. 33 if $x > 1$ to obtain $E_1(x)$, and successive application of Eq. A.38.

For $6.4 < x \leq 80$, $E_3(x)$ is evaluated using the first three terms of the series representation of $E_n(x)$ for large $n$ (5.1.52) of Ref. 33 so that

$$E_3(x) \approx \frac{e^{-x}}{x + 3} \left[ 1 + \frac{3}{(x + 3)^2} + \frac{3(3 - 2x)}{(x + 3)^4} \right]$$  \hspace{1cm} (A.41)

Beyond $x = 80$, $E_3$ is assumed to be zero.
For $0 \leq x \leq 6.4$, $E_4(x)$ is obtained by linear interpolation in a Table of $E_4$ with table entries the same as for the $E_3$ table mentioned above. The table values were obtained as in the case of $E_3$ with one more application of the recursion relation Eq.A.38.

For $6.4 < x < 80$, $E_4$ is evaluated as in the case of $E_3$ using (5.1.52) of Ref. 33 so that

$$E_4(x) \approx \frac{e^{-x}}{x + 4} \left[ 1 + \frac{4}{(x + 4)^2} + \frac{4(4 - 2x)}{(x + 4)^4} \right]$$  \hspace{1cm} (A.42)

Beyond $x = 80$, $E_4$ is assumed to be zero.

b. Slab Collision Escape Probability

The probability of escape without a collision from a slab with optical thickness $x$ is given by

$$P = \frac{0.5 - E_3(x)}{x}$$  \hspace{1cm} (A.43)

If $x \geq 0.6$, $P$ is evaluated with $E_3(x)$ being obtained as described earlier using table interpolation or using Eq.A.41 as appropriate to the range of $x$.

For $x < 0.6$, use of Eq.A.40 in Eq.A.43 yields

$$P \approx 1 - \frac{x}{2} (1.5 - \gamma - \ln x) - \frac{x^2}{3!} + \frac{x^3}{2\cdot4!} - \frac{x^4}{3\cdot5!} + \frac{x^5}{4\cdot6!} - \frac{x^6}{5\cdot7!}$$  \hspace{1cm} (A.44)

c. Infinite Sums of Exponential Integrals

In the case of a unit cell of optical thickness $h$, the collision rate calculation involves evaluation of infinite sums of exponential integrals. Numerical procedures have been developed (6) for evaluating the functions

$$S_n(z,h) = \sum_{k=0}^{\infty} E_n(z + kh) = \int_{1}^{\infty} \frac{e^{-zt}}{(1 - e^{-ht})t^n} dt$$  \hspace{1cm} (A.45)

which make use of fast and accurate Gaussian quadrature formulas.

The code evaluates $S_3(z,h)$ using

$$S_3(z,h) \approx \sum_{i=1}^{M} \left[ \frac{w_{i,3} \exp(t_{i,3})}{1 - \exp(-ht_{i,3})} \right] \exp(-zt_{i,3}) + C(z,h)$$  \hspace{1cm} (A.46)

where

$$C(z,h) = \begin{cases} 0.004126 + 0.00628 \exp(-19.8h) & \text{if } z < 0.3 \\ 0, & \text{if } z \geq 0.3 \end{cases}$$  \hspace{1cm} (A.47)
and the abscissae $t_{1,3}$ and weights $w_{1,3}$ are precalculated as described in Ref. 37 data and stored as data in the code.

The number of terms $M$ used in the sum in Eq. A.46 lay between 1 and 4 depending upon the value of $z$. If

$$z \leq 3.16,$$  \hspace{1cm} M \text{ is determined by truncating to an integer} \hspace{1cm} M = 0.633 \left(7.89 - z\right). \hspace{1cm} \text{(A.48)}$$

For $3.16 < z \leq 13.7$, $M$ is determined from

$$M = 1.0 + 6.2/z. \hspace{1cm} \text{(A.49)}$$

For $z > 13.7$, $S_3(z,h)$ is assumed to be zero.

$S_4(z,h)$ is evaluated as

$$S_4(z,h) \approx \sum_{i=1}^{N} \left[ \frac{w_{1,4} \exp(t_{1,4})}{1 - \exp(-ht_{1,4})} \right] \exp(-zt_{1,4}) \hspace{1cm} \text{(A.50)}$$

with the abscissae and weights again precalculated and stored.

$N$ lay between 1 and 4 depending upon $z$. If $z \leq 3.64$, $M$ is determined by truncating to an integer

$$N = 0.549 \left(9.10 - z\right). \hspace{1cm} \text{(A.51)}$$

For $3.64 < N \leq 15.6$, $M$ is determined from

$$N = 1.0 + 6.81/z. \hspace{1cm} \text{(A.52)}$$

For $z > 15.6$, $S_4(z,h)$ is assumed to be zero.

In addition to the infinite sums $S_n(z,h)$, the code requires differences of these sums

$$D_n(y,\Delta,h) = S_n(y, h) - S_n(y + \Delta, h). \hspace{1cm} \text{(A.53)}$$

The $D_n(y,\Delta,h)$ are evaluated using various algorithms depending upon the cell optical thickness and the incremental length $\Delta$. In particular, the method of Gaussian quadrature for the evaluation of the $S_n$ described above is least accurate for either $z$ or $h$ small.

For $\Delta > 0.02$ and $h \leq 0.2$, if $z > 1.147h^{1.4}$, the $S_3(z,h)$ of Eq. A.53 are evaluated using the Euler-Maclaurin series

$$S_3(z,h) \approx \frac{1}{12} \left\{ e^{-z} \left[ \frac{4 - 2z}{h} + 3 - \frac{h^3}{60z} \left( 1 - \frac{h^2}{21z^2} \left( 1 + z + \frac{z^2}{2} \right) \right) \right] \right.$$  

$$\left. + E_2(z) \left[ h - 3z + \frac{2z^2}{h} \right] \right\} \hspace{1cm} \text{(A.54)}$$
If \( z < 1.147h^{1.4} \) but \( z + h > 1.147h^{1.4} \),
\[
S_3(z, h) = E_3(z) + S_3(z + h, h)
\]
where \( S_3(z + h, h) \) is evaluated using Eq.A.54.

If \( z + h < 1.147h^{1.4} \) but \( z + 2h > 1.147h^{1.4} \),
\[
S_3(z, h) = E_3(z) + E_3(z + h) + S_3(z + 2h, h)
\]
where again \( S_3(z + 2h, h) \) uses Eq.A.54. In Eqs.A.54-A.56, the \( E_2(z) \) and \( E_3(z) \) are obtained using the methods described above for obtaining the exponential integrals.

If \( \Delta > 0.02 \) and \( h > 0.2 \), the \( S_3(z, h) \) of Eqs.A.53 are evaluated using Gaussian quadrature as described earlier in the discussion relating to Eq.A.46 with the number of terms used in the quadrature determined using Eqs.A.48 and A.49.

If \( \Delta \leq 0.02 \), a Taylor series expansion is used to obtain
\[
D_3(y, \Delta, h) = S_3(y, h) - S_3(y + \Delta, h) = S_3(z - \frac{\Delta}{2}, h) - S_3(z + \frac{\Delta}{2}, h)
\]
\[
\approx \Delta \cdot \left[ S_2(y + \Delta/2, h) + \frac{\Delta^2}{24} S_0(y + \Delta/2, h) + \frac{\Delta^4}{1920} S_{-2}(y + \Delta/2, h) \right].
\]

(A.57)

For \( y + \Delta/2 < 0.6 \), only the \( S_2 \) and the \( S_0 \) are retained and the first few terms of the series in Eq.A.57 are evaluated by directly summing the \( E_2 \) and \( E_0 \) functions as
\[
S_1 = \Delta \cdot \left\{ E_2(y + \Delta/2) + E_2(y + \Delta/2 + h) + E_2(y + \Delta/2 + 2h) + \ldots \right. \\
+ \frac{\Delta^2}{24} \left[ E_0(y + \Delta/2) + E_0(y + \Delta/2 + h) + E_2(y + \Delta/2 + 2h) + \ldots \right] \right\}
\]
\[
(A.58)
\]
where the direct summation in Eq.A.58 is continued as long as \( y + \Delta/2 + kh < 0.6 \), and \( E_0(z) = \exp(-z)/z \).

When \( y + \Delta/2 + kh \geq 0.6 \), the remainder of the series of Eq.A.57 is obtained as follows. \( S_2 \) is obtained using the Gaussian quadrature algorithm
\[
S_2(y + \Delta/2 + kh, h) = \sum_{i=1}^{4} \left[ \frac{w_{i,2} \exp(t_{i,2})}{1 - \exp(-ht_{i,2})} \right] \exp \left\{ -(y + \Delta/2 + kh)t_{i,2} \right\}
\]
\[
(A.59)
\]
using precalculated and stored weights and abscissae. Then, using the fact that

$$\frac{3 E_n(z)}{3z} = - E_{n-1}(z)$$

(A.60)

we may rewrite Eq. A.57 as

$$S_2 = \Delta \cdot S_2(y + \Delta/2 + kh, h) \left\{ 1 + \frac{\Delta^2}{24} t_{1,2}^2 + \frac{\Delta^4}{1920} t_{1,2}^4 \right\}$$

(A.61)

with Eq. 23 used to obtain $S_2$. Thus finally

$$D_3(y, \Delta, h) = S_1 + S_2.$$  (A.62)

The $D(y, \Delta, h)$ are similarly evaluated using various algorithms depending upon the cell optical thickness $h$ and the incremental length $\Delta$.

For $\Delta > 0.02$ and $h \leq 0.2$, if $z > 1.818h^{2.5}$, the $S_4(z, h)$ of Eq.A.53 are evaluated using the Euler-Maclaurin series

$$S_4(z, h) \approx \frac{1}{12} \left\{ e^{-z} \left[ \frac{3 - z}{h} + 2 + \frac{h^3}{60z^2} (1 - z) \right] 
+ E_3(z) \left[ \frac{z^2}{h} - h - 2z - \frac{h^3}{30z^2} \right] \right\}.$$  (A.63)

If $z \leq 1.818h^{2.5}$ but $z + h > 1.818h^{2.5}$,

$$S_4(z, h) = E_4(z) + S_4(z + h, h)$$  (A.64)

where $S_4(z + h, h)$ is evaluated using Eq.A.63. In Eqs.A.63 and A.64, the $E_3(z)$ and $E_4(z)$ are obtained using the methods described earlier for obtaining the exponential integrals.

If $\Delta > 0.02$ and $h > 0.2$, the $S_4(z, h)$ of Eq.A.53 are evaluated using Gaussian quadrature as described earlier in the discussion relating to Eq.A.50 with the number of terms used in the quadrature determined using Eqs.A.51 and A.52.

If $\Delta$ is $\leq 0.02$, a Taylor series expansion is used as in the case of $D_3(y, \Delta, h)$ to obtain

$$D_4(y, \Delta, h) = S_4(y, h) - S_4(y + \Delta, h) \approx \Delta \cdot S_3(y + \Delta/2, h) \left\{ 1 + \frac{\Delta^2}{24} t_{1,3}^2 \right\}$$  (A.65)

with $S_3$ being obtained using the Gaussian quadrature of Eq.A.46.
VII. Cylindrical Transmission Probabilities

As given in Ref. 5, for a cylindrical region \( i \) having outer radius \( r_i \)
inner radius \( r_{i-1} \), and macroscopic cross section \( \Sigma_i \), the transmission
probabilities from inner surface to outer surface \( T_{i1}^{OI} \) and from outer surface
to outer surface \( T_{i1}^{OO} \) are given by

\[
T_{i1}^{OI} = \frac{4}{\pi} \int_0^{\pi/2} d\phi \cos \phi K_{13} \{ \Sigma_i f_i(\phi) \} \quad (A.66)
\]

\[
T_{i1}^{OO} = \frac{4}{\pi} \int_0^{\pi/2} d\phi \cos \phi \left[ K_{13} \{ \Sigma_i g_i(\phi) \} - \frac{r_{i-1}}{r_i} K_{13} \{ \Sigma_i h_i(\phi) \} \right] \quad (A.67)
\]

where

\[
K_{13}(\xi) = \int_0^{\pi/2} e^{-\xi \csc \theta} \sin^2 \theta \, d\theta \quad (A.68)
\]

\[
f_i(\phi) = -r_{i-1} \cos \phi + \left\{ r_i^2 - r_{i-1}^2 \sin^2 \phi \right\}^{1/2} \quad (A.69)
\]

\[
g_i(\phi) = 2r_i \cos \phi \quad (A.70)
\]

\[
h_i(\phi) = 2 \left\{ r_i^2 - r_{i-1}^2 \sin^2 \phi \right\}^{1/2} \quad (A.71)
\]

The \( T_{i1}^{OI} \) and \( T_{i1}^{OO} \) are tabulated as a function of \( x \) and \( z \) where

\[
x_i = \frac{r_{i-1}}{r_i} \quad (A.72)
\]

\[
z_i = \Sigma_i (r_i - r_{i-1}) \quad (A.73)
\]

with \( x \) ranging between 0.0 and 1.0 and \( z \) between 0.0 and 8.0. For both
\( T_{i1}^{OI} \) and \( T_{i1}^{OO} \), the mesh for \( z \) is 0(0.01)0.4(0.02)1.0(0.04)2.6(0.06)5.0(0.10)8.0.
For \( T_{i1}^{OI} \), the \( x \) mesh increment is 0.04, and for \( T_{i1}^{OO} \), the \( x \) mesh increment is
0.02.

The \( K_{13} \) used in Eqs. A.66 and A.67 were obtained from an extended precision
(real*16) function KIN which computes \( K_{13}(x) \) for \( 1 \leq N \leq 10 \) and \( x \geq 0 \)
using the following algorithms.

For \( x > 39.0 \), KIN returns the value 0.0 for all \( N \). For \( 0.0 < x < 39.0 \),
\( K_{12} \) and \( K_{13} \) are evaluated using the rational expressions given by
I. Gargantine and T. Pomentale(38).
For $0.0 < x \leq 2.0$, $K_{10}(x) = K_0(x)$ is obtained from the polynomial approximations (9.8.5) and (9.8.1) of the Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables (33) and for $x > 2.0$, $K_{11}$ is obtained from the polynomial approximation (9.8.6) of Ref. 33.

$K_{11}$ is obtained for $0.0 < x \leq 7.0$ in terms of $K_{10}$ and $K_{12}$ as

$$K_{11}(x) = K_{10}(x) - \frac{1}{x} K_{12}(x)$$

where $K_{10}$ is obtained as indicated above and $K_{12}(x) = K_2(x)$ is obtained using the polynomial approximations (9.8.7) and (9.8.3) of Ref. 33 when $0.0 < x \leq 2.0$, and using the polynomial approximation (9.8.8) of Ref. 33 when $x > 2.0$. For $x > 7.0$, $K_{11}$ is obtained from the polynomial approximation (11.1.18) of Ref. 33.

For $n > 3$, the recursion relationship

$$n K_{1n+1}(x) = (n - 1) K_{1n}(x) + x \left[ K_{1n-2}(x) - K_{1n}(x) \right]$$

(A.75)

is used.

For $x = 0.0$, KIN uses stored precalculated data to return

$$K_{1n}(0) = \frac{(\pi)^{1/2}}{2} \left[ \frac{n!}{\Gamma(n + \frac{1}{2})} \right]$$

(A.76)

where

$$\Gamma(n + \frac{1}{2}) = (\pi)^{1/2} \left( \frac{\pi}{2} \right)^{1/2} \frac{n!}{(2n - 1)!}$$

The extended precision (real*16) numerical integration of Eqs. A.66 and A.67 was accomplished using an adaptive Simpson's rule quadrature with convergence criteria adjusted for different ranges of $x$ and $z$ to achieve at least six significant figure agreement with very small convergence criterion results.

For a given $x$ and $z$, $T_0^I$ and $T_0^O$ are obtained using the six point bivariate interpolation formula (25.2.67) of Ref. 33 within the body of the table and the four point formula (25.2.66) of Ref. 33 in the first $x$ or $z$ intervals.

Outside the range of the table $T_0^I$ is set to zero and an approximate polynomial fit similar to that used in the RABBLE code (5) is used for $T_0^O$. 
APPENDIX B

MC$^2$-2 BCD INPUT FILES
APPENDIX B. MC²-2 BCD Input Files. A.MCC2

C*******************************************************************************
C
C PREPARED 3/8/76 AT ANL

C
C A.MCC2

C GENERAL BCD INPUT FOR MC²-2-II AND SDX CALCULATIONS

C
C THIS IS A USER SUPPLIED BCD DATA SET.

C THE LIST FOR EACH RECORD IS GIVEN IN TERMS

C OF THE BCD FORMAT OF THAT DATA CARD.

C COLUMNS 1-2 CONTAIN THE CARD TYPE NUMBER.

C BLANK FIELDS PRODUCE THE DEFAULT OPTIONS.

C*******************************************************************************

CR

PROBLEM TITLE (TYPE 01)

CL FORMAT-----(I2,4X,11A6)

CD COLUMNS CONTENTS..IMPLICATIONS, IF ANY

CD ======== ================================================

CD 1-2 01

CD 7-72 ANY ALPHANUMERIC CHARACTERS.

CN ANY NUMBER OF TYPE 01 CARDS MAY BE USED.

C

C*******************************************************************************

CR

CONTAINER ARRAY SPECIFICATIONS (TYPE 02)

CL FORMAT-----(I2,4X,3I6)

CD COLUMNS CONTENTS..IMPLICATIONS, IF ANY

CD ======== ================================================

CD 1-2 02

CD 7-12 SIZE OF MAIN CORE CONTAINER ARRAY IN 8 BYTE WORDS,

CD TYPICALLY 30000 (DEFAULT=30000).

CD FOR CDC USERS TYPICALLY 20000 (DEFAULT=20000).

CD 13-19 SIZE OF BULK CORE CONTAINER ARRAY IN 8 BYTE WORDS,

CD TYPICALLY 0, (DEFAULT=0).

CD FOR CDC USERS TYPICALLY 100000 (DEFAULT=100000).

CD MAXIMUM ALLOWABLE=131072.
APPENDIX B. MC$^2$-2 BCD Input Files. A.MCC2 (Contd.)

<table>
<thead>
<tr>
<th>CD</th>
<th>19-24</th>
<th>POINTR DEBUGGING EDIT, TYPICALLY 0.</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD</td>
<td>0</td>
<td>NO DEBUGGING PRINTOUT (DEFAULT).</td>
</tr>
<tr>
<td>CD</td>
<td>1</td>
<td>DEBUGGING DUMP PRINTOUT.</td>
</tr>
<tr>
<td>CD</td>
<td>2</td>
<td>DEBUGGING TRACE PRINTOUT.</td>
</tr>
<tr>
<td>CD</td>
<td>3</td>
<td>FULL DEBUGGING PRINTOUT.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>CN</th>
<th>NO TYPE 02 CARD WILL GIVE THE FOLLOWING DEFAULT</th>
</tr>
</thead>
<tbody>
<tr>
<td>CN</td>
<td>VALUES FOR IBM USERS.</td>
</tr>
<tr>
<td>CN</td>
<td>MAIN CORE CONTAINER=30000</td>
</tr>
<tr>
<td>CN</td>
<td>BULK CORE CONTAINER=0</td>
</tr>
<tr>
<td>CN</td>
<td>PRINT OPTION FLAG=0</td>
</tr>
<tr>
<td>CN</td>
<td>FOR THE DEFAULT VALUES ON THE TYPE 02 CARD, THE</td>
</tr>
<tr>
<td>CN</td>
<td>REGION PARAMETER OF THE JOB CARD SHOULD BE</td>
</tr>
<tr>
<td>CN</td>
<td>REGION=700K</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>CN</th>
<th>NO TYPE 02 CARD WILL GIVE THE FOLLOWING DEFAULT</th>
</tr>
</thead>
<tbody>
<tr>
<td>CN</td>
<td>VALUES FOR CDC USERS.</td>
</tr>
<tr>
<td>CN</td>
<td>MAIN CORE CONTAINER=20000</td>
</tr>
<tr>
<td>CN</td>
<td>BULK CORE CONTAINER=100000</td>
</tr>
<tr>
<td>CN</td>
<td>PRINT OPTION FLAG=0</td>
</tr>
<tr>
<td>CN</td>
<td>FOR THE DEFAULT VALUES ON THE TYPE 02 CARD, THE</td>
</tr>
<tr>
<td>CN</td>
<td>REDEFINE FIELD LENGTH CONTROL CARD SHOULD SPECIFY</td>
</tr>
<tr>
<td>CN</td>
<td>RPL(160000,L=400)</td>
</tr>
</tbody>
</table>

---

CR  | GENERAL PROBLEM SPECIFICATIONS (TYPE 03)

<table>
<thead>
<tr>
<th>CI</th>
<th>FORMAT-----(T2,4X,4I6,A6,6T6)</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>CD</th>
<th>COLUMNS</th>
<th>CONTENTS...IMPLICATIONS, IF ANY</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD</td>
<td>1-2</td>
<td>03</td>
</tr>
<tr>
<td>CD</td>
<td>7-12</td>
<td>FUNDAMENTAL MODE TYPE.</td>
</tr>
<tr>
<td>CD</td>
<td>1...P1 (DEFAULT).</td>
<td></td>
</tr>
<tr>
<td>CD</td>
<td>2...B1.</td>
<td></td>
</tr>
<tr>
<td>CD</td>
<td>3...CONSISTENT P1.</td>
<td></td>
</tr>
<tr>
<td>CD</td>
<td>4...CONSISTENT B1.</td>
<td></td>
</tr>
<tr>
<td>CD</td>
<td>13-18</td>
<td>ORDER OF EXTENDED TRANSPORT APPROXIMATION (DEFAULT=1).</td>
</tr>
<tr>
<td>CD</td>
<td>19-24</td>
<td>CONTINUOUS SLOWING DOWN MODERATING PARAMETER OPTION.</td>
</tr>
<tr>
<td>CD</td>
<td>0...IMPROVED GREULING GOERTZEL (DEFAULT).</td>
<td></td>
</tr>
<tr>
<td>CD</td>
<td>1...GREULING GOERTZEL.</td>
<td></td>
</tr>
<tr>
<td>CD</td>
<td>25-30</td>
<td>MAXIMUM NUMBER OF HYPERFINE GROUPS PER ULTRAFINE GROUP</td>
</tr>
<tr>
<td>CD</td>
<td>USED IN EVALUATION OF ELASTIC SCATTERING MATRICES</td>
<td></td>
</tr>
</tbody>
</table>

---
APPENDIX B. MC$^2$-2 BCD Input Files. A.MCC2 (Contd.)

CD 31-36 BROAD GROUP STRUCTURE TYPE.
   ANL9...ANL 9 GROUP STRUCTURE.
   ANL11...ANL 11 GROUP STRUCTURE.
   ANL27...ANL 27 GROUP STRUCTURE.
   ANL28...ANL 28 GROUP STRUCTURE.
   BOND26...BONDARENKO 26 GROUP STRUCTURE.
   FFTF30...FFTF 30 GROUP STRUCTURE.
   HANS16...HANSEN-ROACH 16 GROUP STRUCTURE.
   SDX156...SDX 156 GROUP STRUCTURE.
   USS212...UNIVERSAL SUPERGROUP 712 GROUP STRUCTURE.
   USS226...UNIVERSAL SUPERGROUP 226 GROUP STRUCTURE.
   WARD9...WARD 9 GROUP STRUCTURE.

CD 37-42 FUEL GEOMETRY.
   0...HOMOGENEOUS.
   1...SLAB.
   2...CYLINDER.

CD 43-48 RESOLVED RESONANCE OVERLAP OPTION.
   0...INCLUDE OVERLAP CALCULATION FOR THE NUMBER OF NEIGHBORING RESONANCES DESIGNATED IN COLS. 55-60 (DEFAULT).
   1...OMIT OVERLAP CALCULATION.

CD 49-54 UNRESOLVED RESONANCE SELF-OVERLAP OPTION.
   0...INCLUDE SELF-OVERLAP CALCULATION (DEFAULT).
   1...OMIT SELF-OVERLAP CALCULATION.

CD 55-60 NUMBER OF RESOLVED RESONANCES TO BE TESTED FOR OVERLAP ON EACH SIDE OF EACH RESOLVED RESONANCE (DEFAULT=4).
   THIS FIELD IS IGNORED IF COLS. 43-48 ARE 1.

CD 61-66 RESERVED FOR FUTURE USE.

CD 67-72 INELASTIC AND (N,2N) ULTRA-FINE-GROUP TREATMENT.
   0...APPROXIMATE TREATMENT (DEFAULT).
   1...RIGOROUS ENERGY-ANGLE CORRELATION ACCOUNTED FOR.

C IF CARD TYPE 03 IS NOT SUPPLIED, ALL DEFAULT OPTIONS WILL BE UTILIZED.
C IF COLS. 37-42 ARE NON-ZERO, CARD TYPES 04, 06, 14, AND 15 OF DATA SET A.NIP MUST BE SUPPLIED TO SPECIFY THE HETEROGENEOUS PROBLEM GEOMETRY AND COMPOSITIONS.
C IF COLS. 7-12 ARE 1 OR 2, COLS. 13-18 MUST BE 1.
C COLS. 31-36 ARE IGNORED IF ANY TYPE 05 OR 07 CARDS ARE SUPPLIED OR IF THE DATA SET XS.ISO IS DECLARED TO BE OLD IN THE EXECUTION DECK.
APPENDIX B. MC²-2 BCD Input Files. A.MCC2 (Contd.)

C-----------------------------------------------

C GENERAL PROBLEM CONSTANTS (TYPE 04)

C-----------------------------------------------

C FORMAT----(12,10X,5E12.5)

C-----------------------------------------------

COLUMNS CONTENTS...IMPLICATIONS, IF ANY
-----------------------------------------------

1-2 04

CD 13-24 CONTINUOUS SLOWING DOWN INTEGRATION FACTOR THETA
(DEFAULT=0.5).

CD 25-36 MASS OF MATERIAL USED IN DETERMINATION OF THE DATA
MANAGEMENT STRATEGY FOR THE SPECTRUM CALCULATION.

CD COLS 25-36 SHOULD BE LESS THAN OR EQUAL TO THE MASS OF
THE LIGHTEST MATERIAL IN THE PROBLEM (EXCLUDING H).

CD IF COLS. 25-36 ARE BLANK, THE MANAGEMENT STRATEGY IS
SELECTED BY THE BUILT IN ALGORITHM. IF COLS. 25-36
CONTAIN A VALUE LARGER THAN THE LIGHTEST MASS MATERIAL
IN THE PROBLEM, THE LATTER WILL BE USED INSTEAD.

CD 37-48 BOUNDARY ENERGY IN EV. BETWEEN THE MULTIGROUP FLUX
SOLUTION AND THE CONTINUOUS SLOWING DOWN FLUX
SOLUTION. THE BOUNDARY ENERGY MUST BE GREATER THAN
THE ENERGY OF THE HIGHEST RESOLVED RESONANCE IN THE
PROBLEM. THE DEFAULT VALUES WILL SATISFY THIS
REQUIREMENT.

CD 49-60 CONSTANT A1 USED IN THE EQUIVALENCE PRINCIPLE.

CD 61-72 CONSTANT A2 USED IN THE EQUIVALENCE PRINCIPLE.

C

IF COLS. 49-60 ARE BLANK, COLS. 49-60 AND

COLS. 61-72 ARE SET EQUAL TO 1.35 IF COLS 37-42 ON.

CARD TYPE 03 CONTAIN A 2 AND THEY ARE SET EQUAL TO

1.09 IF COLS. 37-42 ON CARD TYPE 03 CONTAIN A 1.

IF COLS. 49-60 ARE NON-BLANK AND COLS. 61-72 ARE
BLANK, COLS. 61-72 ARE SET EQUAL TO COLS. 49-60.

IF NO CARD TYPE 04 IS SUPPLIED, ALL DEFAULT OPTIONS
WILL BE UTILIZED.

C-----------------------------------------------

C BROAD GROUP ENERGIES (TYPE 05)

C-----------------------------------------------
APPENDIX B. MC$^2$-2 BCD Input Files. A.MCC2 (Contd.)

```
FORMAT----(I2,10X,3(I6,E12.5))

COLUMNS CONTENTS...IMPLICATIONS, IF ANY
------ =--------------------------------------------
1-2   05

13-18 BROAD GROUP NUMBER.

19-30 UPPER ENERGY OF GROUP (EV).

31-36 BROAD GROUP NUMBER.

37-48 UPPER ENERGY OF GROUP (EV).

49-54 BROAD GROUP NUMBER.

55-66 UPPER ENERGY OF GROUP (EV).

THE BROAD GROUP STRUCTURE MAY BE SPECIFIED USING TYPE
05 CARDS OR TYPE 07 CARDS OR A COMBINATION OF EACH.
ALTERNATIVELY, ONE OF THE PRESERVED GROUP STRUCTURES
SPECIFIED IN COLS. 31-36 ON THE TYPE 03 CARD OR THE
BUILT IN DEFAULT DESCRIBED BELOW MAY BE USED.
GROUP 1 IS THE GROUP OF HIGHEST ENERGY. THE THERMAL
GROUP HAVING THE LARGEST GROUP NUMBER HAS AS UPPER
ENERGY THE INTERFACE BETWEEN THE THERMAL GROUP AND
EPI-THERMAL GROUPS. AS MANY TYPE 05 CARDS ARE USED AS
ARE NECESSARY TO SPECIFY THE ENERGIES. IF COLS. 31-36
OR 49-54 ARE BLANK, THE REST OF THE DATA ON THE TYPE 05-
CARDS ARE IGNORED.

IF ONLY THE BROAD GROUP NUMBER ONE UPPER ENERGY IS
SPECIFIED AND IF NO TYPE 07 CARDS ARE SUPPLIED, A FIXED-
0.5 LETHARGY WIDTH BROAD GROUP STRUCTURE IS CONSTRUCTED-
EXTENDING DOWN FROM THE SPECIFIED ENERGY TO THE LOWEST
ENERGY IN THE LIBRARY. IF TYPE 07 CARDS ARE SUPPLIED,
THE TYPE 07 DATA ARE USED WITH THE SPECIFIED UPPER
ENERGY TO CONSTRUCT THE BROAD GROUP STRUCTURE.
IF MORE THAN ONE BROAD GROUP ENERGY BOUNDARY IS
SPECIFIED ON THE TYPE 05 CARDS, ANY TYPE 07 CARDS
SUPPLIED WILL BE ignored.

IF COLS. 31-36 ON CARD TYPE 03 ARE BLANK AND
IF NO TYPE 05 CARDS ARE SUPPLIED AND NO TYPE 07 CARDS
ARE SUPPLIED, A FIXED 0.5 LETHARGY WIDTH BROAD GROUP
STRUCTURE IS CONSTRUCTED COVERING THE ENERGY RANGE
OF THE LIBRARY.
```
APPENDIX B. MC²-2 BCD Input Files. A.MCC2 (Contd.)

HOMOGENEOUS COMPOSITION SPECIFICATIONS (TYPE 06)

FORMAT----(T2,10X,2A6,3E12.5,I6)

COLUMNS CONTENTS...IMPLICATIONS, IF ANY

1-2 06

13-18 NUCLIDE IDENTIFICATION LABEL ON LIBRARY.

19-24 PROBLEM MATERIAL LABEL. THIS LABEL CAN BE ANY ALIAS NAME. IF COLS. 19-24 ARE BLANK, THE MATERIAL NAMED IN COLS. 13-18 WILL BE USED.

25-36 MATERIAL ATOMIC CONCENTRATION USED TO COMPUTE HOMOGENEOUS CROSS SECTIONS FOR USE IN THE SPECTRUM CALCULATION (ATOMS/CC*1.E-24).

37-48 MATERIAL TEMPERATURE IN DEGREES K (DEFAULT=300.).

49-50 EPSHET, USED TO DETERMINE NEAREST NEIGHBORING PLATE CONTAINING MATERIAL NAMED IN COLUMNS 13-18. IF A PLATE K CONTAINS MATERIAL I, THEN NEIGHBORING PLATES ARE SEARCHED TO FIND THE NEAREST PLATE M WHICH SATISFIES THE CONDITION N(I,M)*DX(M).CP.EPSHET*N(I,K)*DX(K), WHERE N(I,M) IS THE ATOM DENSITY OF MATERIAL I IN PLATE M AND DX(M) IS THE THICKNESS OF PLATE M. (DEFAULT VALUE=0.1).


ONE TYPE 06 CARD MUST BE GIVEN FOR EACH MATERIAL PRESENT IN THE MACROSCOPIC MIXTURE OF THE SPECTRUM. COMPOSITION IF COLS. 37-42 ON CARD TYPE 03 ARE ZERO OR IF CARD TYPE 03 IS NOT SUPPLIED. IF NO TYPE 06 CARD IS GIVEN, THE MACROSCOPIC MIXTURE IS DERIVED FROM THE DATA ON THE A.MIP CARD TYPES 06, 14, AND 15. IN THIS CASE, ALL MATERIALS WILL BE ASSUMED TO HAVE A TEMPERATURE OF 300 DEGREES K AND LIBRARY NUCLIDE IDENTIFICATION LABELS WILL BE USED FOR THE PROBLEM MATERIAL LABELS. IF COLS. 25-36 ARE BLANK OR ZERO FOR ANY MATERIAL THE ATOMIC DENSITY FOR THAT MATERIAL IS DERIVED FROM THE A.MIP DATA FOR THE REGIONS. ALTHOUGH MATERIAL LABELS AND TEMPERATURES WILL BE SET BY THE TYPE 06 DATA, ANY ATOMIC DENSITY WHICH IS
APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)


---

EPI-THERMAL BROAD GROUP LETHARGY WIDTHS (TYPE 07)

FORMAT----(I2,10X,2(E12.5,16,16))

<table>
<thead>
<tr>
<th>COLS</th>
<th>CONTENTS...IMPLICATIONS, IF ANY</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-2</td>
<td>07</td>
</tr>
<tr>
<td>13-24</td>
<td>LETHARGY WIDTH.</td>
</tr>
<tr>
<td>25-30</td>
<td>INITIAL BROAD GROUP NUMBER.</td>
</tr>
<tr>
<td>31-36</td>
<td>FINAL BROAD GROUP NUMBER.</td>
</tr>
<tr>
<td>37-48</td>
<td>LETHARGY WIDTH.</td>
</tr>
<tr>
<td>49-54</td>
<td>INITIAL BROAD GROUP NUMBER.</td>
</tr>
<tr>
<td>55-60</td>
<td>FINAL BROAD GROUP NUMBER.</td>
</tr>
</tbody>
</table>

SEE NOTES FOR THE TYPE 05 CARDS.
DATA SHOULD BE SUPPLIED FOR ONLY THE EPI-THERMAL GROUPS. THUS, NO LETHARGY WIDTH SHOULD BE GIVEN FOR THE THERMAL GROUP.
AS MANY TYPE 07 CARDS AS NECESSARY MAY BE USED.
AS A MAXIMUM, THERE MAY BE AS MANY BROAD EPI-THERMAL GROUPS AS THERE ARE ULTRA FINE GROUPS IN THE LIBRARY.
APPENDIX B. MC²-2 BCD Input Files. A.MCC2 (Contd.)

MULTIPLE OF THE LIBRARY GROUP LETHARGY WIDTH.

EXTERNAL SOURCE SPECIFICATIONS (TYPE 08)

<table>
<thead>
<tr>
<th>COLS</th>
<th>CONTENTS...IMPLICATIONS, IF ANY</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-2</td>
<td>08</td>
</tr>
<tr>
<td>13-24</td>
<td>MAGNITUDE OF EXTERNAL SOURCE.</td>
</tr>
<tr>
<td>25-30</td>
<td>HIGHER ENERGY ULTRAFINE GROUP NUMBER TO WHICH SOURCE IN COLS. 13-24 APPLIES.</td>
</tr>
<tr>
<td>31-36</td>
<td>LOWER ENERGY ULTRAFINE GROUP NUMBER TO WHICH SOURCE IN COLS. 13-24 APPLIES.</td>
</tr>
<tr>
<td>37-48</td>
<td>MAGNITUDE OF EXTERNAL SOURCE.</td>
</tr>
<tr>
<td>49-54</td>
<td>HIGHER ENERGY ULTRAFINE GROUP NUMBER TO WHICH SOURCE IN COLS. 37-48 APPLIES.</td>
</tr>
<tr>
<td>55-60</td>
<td>LOWER ENERGY ULTRAFINE GROUP NUMBER TO WHICH SOURCE IN COLS. 37-48 APPLIES.</td>
</tr>
</tbody>
</table>

IF COLS. 13-24 OF THE FIRST TYPE 08 CARD ARE BLANK OR ZERO THEN COLS. 25-30 OF THIS CARD MUST CONTAIN THE FISSION SPECTRUM NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY (A6 FORMAT) SPECIFYING THE EXTERNAL SOURCE. THIS OPTION SHOULD BE USED WHEN A FISSION SPECTRUM SOURCE IS DESIRED FOR A PROBLEM WHICH CONTAINS NO FISSIONABLE NUCLIDES. ALL OTHER TYPE 08 CARDS ARE NEGLECTED IF COLS. 13-24 OF THE FIRST TYPE 08 CARD ARE BLANK OR ZERO.

IF COLS. 37-48 OR 49-54 ON ANY TYPE 08 CARD ARE BLANK OR ZERO, OR IF COLS. 13-24 OR 25-30 ON ANY TYPE 08 CARD AFTER THE FIRST ARE BLANK OR ZERO, THE REST OF THE TYPE 08 DATA ARE IGNORED.

APPENDIX B. MC²-2 BCD Input Files. A.MCC2 (Contd.)

---

**APPENDIX**

**B.**

**MC~²~ BC~D Input Files. A.MCC2**

**CONTD.**

---

**COVERED BY THIS DATA WILL BE ASSIGNED THE EXTERNAL SOURCE VALUE 0.** **AS MANY TYPE 08 CARDS AS NECESSARY MAY BE USED SPECIFY THE EXTERNAL SOURCE DATA.**

---

**BUCKLING SPECIFICATIONS (TYPE 09)**

**FORMAT**

---

**(I2, 10X, 3E12.5, 2I6, E12.5)**

---

**COLUMNS**

---

**CONTENTs...IMPLICATIONS, IF ANY**

---

**1-2**

---

**09**

---

**13-24**

---

**INITIAL BUCKLING GUESS.**

---

**25-36**

---

**SECOND BUCKLING GUESS.**

---

**37-48**

---

**CONVERGENCE CRITERION, EPS, FOR BUCKLING ITERATION TO KEFF=1. ABSOLUTE VALUE OF (KEFF-1)*EP.s.**

---

**49-54**

---

**HIGHER ENERGY ULTRAFINE GROUP NUMBER TO WHICH VALUES OF BUCKLING APPLY.**

---

**55-60**

---

**LOWER ENERGY ULTRAFINE GROUP NUMBER TO WHICH VALUES OF BUCKLING APPLY.**

---

**61-72**

---

**EXTENDED TRANSPORT APPROXIMATION BUCKLING, KAPPA SQUARED.**

---

**AS MANY TYPE 09 CARDS MAY BE USED AS NECESSARY TO SPECIFY THE BUCKLING DATA. IF COLS. 49-54 ARE BLANK, THE BUCKLING DATA WILL BE ASSUMED TO BE GROUP INDEPENDENT. IF COLS. 55-60 ARE BLANK, THE DATA IN COLS. 13-24 WILL APPLY TO THE ULTRAFINE GROUP GIVEN IN COLS. 49-54. IF COLS. 61-72 ARE BLANK, THE BUCKLING GIVEN IN COLS. 13-24 ON THE FIRST TYPE 09 CARD ENCOUNTERED WILL BE USED FOR KAPPA SQUARED. NOTE THAT THE SECOND BUCKLING GUESS IN COLS. 25-36 AND THE CONVERGENCE CRITERION IN COLS. 37-48 ARE PERTINENT ONLY FOR ENERGY INDEPENDENT BUCKLING PROBLEMS WHICH WILL ITERATE ON BUCKLING TO KEFF=1. IF COLS. 37-48 ARE BLANK OR ZERO, THE SECOND BUCKLING GUESS IS IGNORED AND NO BUCKLING ITERATION IS PERFORMED. COLS. 25-48 WILL BE IGNORED IF COLS. 49-54 ARE NON-BLANK. ANY GROUP NOT COVERED BY THIS DATA WILL BE ASSIGNED THE BUCKLING VALUE 0.**
COLUMNS 61-72 ARE IGNORED AFTER READING THE FIRST TYPE 09 CARD.

---

**Thermal Group Cross Section Data (Type 10)**

**Format:** (I2,4X,A6,5E12.5)

<table>
<thead>
<tr>
<th>Columns</th>
<th>Contents...Implications, if Any</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-2</td>
<td>10</td>
</tr>
<tr>
<td>7-12</td>
<td>Nuclide identification label on the library (Cols. 13-18 on type 06 cards).</td>
</tr>
<tr>
<td>13-24</td>
<td>Microscopic thermal group capture cross section (barns)</td>
</tr>
<tr>
<td>25-36</td>
<td>Microscopic thermal group fission cross section (barns)</td>
</tr>
<tr>
<td>37-49</td>
<td>Number of neutrons emitted per fission in the thermal group.</td>
</tr>
<tr>
<td>49-50</td>
<td>Microscopic thermal group total cross section (barns).</td>
</tr>
<tr>
<td>61-72</td>
<td>Thermal group average reciprocal velocity (sec/cm) (default=1./2.2E+5).</td>
</tr>
</tbody>
</table>

As many type 10 cards are used as necessary to specify the thermal group values. Any material not specified on a type 10 card will be assigned thermal group cross sections equal to the last epi-thermal group values. The first positive value encountered in cols. 61-72 of any type 10 card will be used for the average thermal group reciprocal velocity. The thermal group velocity is not material dependent.

---

**Auxiliary Thermal Group Cross Section Data (Type 11)**

**Format:** (I2,4X,A6,5E12.5)

<table>
<thead>
<tr>
<th>Columns</th>
<th>Contents...Implications, if Any</th>
</tr>
</thead>
<tbody>
<tr>
<td>---------</td>
<td>---------------------------------</td>
</tr>
</tbody>
</table>

---

APPENDIX B. MC²-2 BCD Input Files. A.MCC2 (Contd.)
APPENDIX B. MC²-2 BCD Input Files. A.MCC2 (Contd.)

CD  1-2  11
CD  7-12 NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY
CD               (COLS. 13-18 ON TYPE 06 CARDS).
CD  13-24 MICROSCOPIC THERMAL GROUP N-ALPHA CROSS SECTION (BARNs).-
CD  25-36 MICROSCOPIC THERMAL GROUP N-P CROSS SECTION (BARNs).-
CD  37-48 MICROSCOPIC THERMAL GROUP N-D CROSS SECTION (BARNs).-
CD  49-60 MICROSCOPIC THERMAL GROUP N-H2 CROSS SECTION (BARNs).-
CD  61-72 MICROSCOPIC THERMAL GROUP N-HE3 CROSS SECTION (BARNs).-
C
C AS MANY TYPE 11 CARDS ARE USED AS NECESSARY TO
C SPECIFY THE AUXILIARY THERMAL GROUP DATA. ANY MATERIAL
C NOT SPECIFIED ON A TYPE 11 CARD WILL BE ASSIGNED
C THERMAL GROUP CROSS SECTIONS EQUAL TO THE LAST
C EPT-THERMAL GROUP VALUES.
C
C-------------------------------------------------
CR RESONANCE HETEROGENEITY SPECIFICATIONS (TYPE 12)
C---------------------------------------------------------------------
CL FORMAT------(I2,4X,A6,5(2A6))
C
C     CONTENTS...IMPLICATIONS, IF ANY
C
C     COLUMNS
C CD  ======  ===========================
C CD  1-2   12
C CD  7-12 NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY
C CD               (COLS. 13-18 ON TYPE 06 CARDS OR IF NO TYPE 06 CARDS
C CD ARE SUPPLIED, COLS. 19-24, 37-42, AND 55-60 ON DATA
C CD SET A.WIP TYPE 14 CARDS).
C CD  13-18 REGION LABEL.
C CD  19-24 REGION LABEL.
C CD  25-30 REGION LABEL.
C CD  31-36 REGION LABEL.
C CD  37-42 REGION LABEL.
C CD  43-48 REGION LABEL.
APPENDIX B. MC2-2 BCD Input Files. A.MCC2 (Contd.)

<table>
<thead>
<tr>
<th>CD</th>
<th>REGION LABEL.</th>
</tr>
</thead>
<tbody>
<tr>
<td>49-54</td>
<td>MATERIALS NOT SPECIFIED ON THE TYPE 12 CARDS WILL RECEIVE A HOMOGENEOUS RESONANCE TREATMENT.</td>
</tr>
<tr>
<td>55-69</td>
<td>FOR CYLINDRICAL GEOMETRY (NGEOM=2) ONLY COLS. 1-2 AND 7-12 ARE PERTINENT. MATERIALS NAMED IN COLS. 7-12 WILL RECEIVE A RESONANCE HETEROGENEITY TREATMENT IN THE CENTRAL PIN REGION OF THE CYLINDRICAL CELL IF THEY ARE PRESENT IN THE PIN REGION AND IF THEY ARE RESONANCE MATERIALS.</td>
</tr>
<tr>
<td></td>
<td>AS AN EXAMPLE, LET MATERIAL M1 APPEAR IN REGIONS R1, R2, R3, R4, AND R5. IF M1 IS TO BE TREATED HOMOGENEOUSLY IN REGIONS R2 AND R5 AND IF IT IS TO RECEIVE THE SAME HETEROGENEITY TREATMENT IN REGION R1 AS IN R3, THEN CARD TYPE 12 WOULD CONTAIN THE FOLLOWING:</td>
</tr>
<tr>
<td></td>
<td>COLUMNS     CONTENTS</td>
</tr>
<tr>
<td></td>
<td>------------  --------</td>
</tr>
<tr>
<td>1-2</td>
<td>12</td>
</tr>
<tr>
<td>7-12</td>
<td>M1</td>
</tr>
<tr>
<td>13-18</td>
<td>R2</td>
</tr>
</tbody>
</table>
APPENDIX B. MC²-2 BCD Input Files. A.MCG2 (Contd.)

CN 19-24 (BLANK)
CN 25-30 R5
CN 31-36 (BLANK)
CN 37-42 R1
CN 43-48 R3
CN 49-54 (BLANK)

Since region R4 is not mentioned, material M1 will be treated heterogeneously in region R4. Since cols. 49-54 are blank, the rest of the data, if any, on the card are ignored.

The resonance region modules will not generate resonance cross sections for material M1 in region R1 but will generate resonance cross sections for material M1 in region R3.

Note that any material in a given region which is either to receive a homogeneous treatment or is to receive the same heterogeneous treatment as in some other region will not have any resonance overlap influence on any other resonance materials in the region in question.

---

CR INTEGRAL TRANSPORT SPECIFICATIONS (TYPE 14)

FORMAT----(I2, 10X, 2E12.5, 4I6)

CD COLUMNS CONTENTS...IMPLICATIONS, IF ANY
CD 1-2 14
CD 13-24 Energy at which integral transport theory treatment begins. (DEFAULT=300.0 EV).
CD 25-36 Criterion used for testing for inclusion of resonances for hyper fine groups within an intermediate group (DEFAULT=0.05). A 0.0 must be specified in cols. 25-36 if all resonances are to be included.
CD 37-42 Number of ultra fine groups per intermediate group (DEFAULT=2).
CD 43-48 Number of hyper fine groups per doppler width (DEFAULT=4).
CD 49-54 Transverse leakage option. 0... OMIT TRANSVERSE LEAKAGE CORRECTION (DEFAULT). 1... INCLUDE TRANSVERSE LEAKAGE CORRECTION USING THE
APPENDIX B. MC\textsuperscript{2}-2 BCD Input Files. A.MCC2 (Contd.)

BUCKLING SPECIFIED IN COLS. 61-72 ON THE TYPE 09 CARD.

INGROUP SCATTERING OPTION.

0...INCLUDE INGROUP SCATTERING (DEFAULT).

1...OMIT INGROUP SCATTERING.

IF INVOKED BY THE PATH DRIVER, RESOLVED RESONANCE BROADGROUP CROSS SECTIONS WILL BE RECOMPUTED USING INTEGRAL TRANSPORT THEORY ALGORITHMS FOR ALL BROAD GROUPS WHOSE LOWER ENERGIES ARE .LT. THE VALUE SPECIFIED. THE INTERMEDIATE GROUPS ARE USED TO DETERMINE WHICH RESONANCES ARE TO BE INCLUDED FOR THE HYPER FINE GROUPS CONTAINED IN THAT INTERMEDIATE GROUP USING THE CRITERION SPECIFIED IN COLS. 25-36. THE CODE WILL ADJUST THE HYPER FINE GROUP WIDTH TO BE AN INTEGRAL SUB-MULTIPLE OF THE ULTRA FINE GROUP WIDTH WITH A MAXIMUM HYPER FINE GROUP WIDTH OF 0.001. IF COLS. 43-48 ARE NEGATIVE, A CONSTANT HYPER FINE GROUP WIDTH IS USED FOR ALL BROAD GROUPS BASED ON THE ABSOLUTE VALUE OF THE QUANTITY GIVEN IN COLS. 43-48. IF THE PATH INVOKES AREA 10, THE PROBLEM MIXTURE MUST CONTAIN MATERIALS HAVING RESOLVED RESONANCES.

FOIL SPECIFICATIONS (TYPE 15)

FORMAT----(T2,4X,A6,2(A6,E12.5),2E12.5)

COLUMNS CONTENTS...IMPLICATIONS, IF ANY

1-2 15

7-12 FOIL IDENTIFICATION LABEL.

13-18 NUCLIDE IDENTIFICATION IN THE LIBRARY.


31-36 NUCLIDE IDENTIFICATION IN THE LIBRARY.


49-60 FOIL THICKNESS IN CM.

61-72 FOIL TEMPERATURE IN DEGREES K. (DEFAULT=300.0).
APPENDIX B. MC²-2 BCD Input Files. A.MCC2 (Contd.)

<table>
<thead>
<tr>
<th>COLS. 49-72</th>
<th>ARE PERTINENT ONLY FOR THE FIRST TYPE 15 CARDS SPECIFIED ON TYPE 15 CARDS WILL BE EDITED AT EACH MESH INTERVAL BOUNDARY AS SPECIFIED ON THE DATA SET A.NIP TYPE 06 CARDS FOR HETEROGENEOUS PROBLEMS, OR FOR THE HOMOGENEOUS SPECTRUM FOR HOMOGENEOUS PROBLEMS WHEN RESOLVED RESONANCE CROSS SECTIONS ARE RECOMPUTED USING INTEGRAL TRANSPORT THEORY. IF THE PATH INVOKES AREA 10, THE PROBLEM MIXTURE MUST CONTAIN MATERIALS HAVING RESOLVED RESONANCES.</th>
</tr>
</thead>
</table>

---

FISSION SPECTRUM SPECIFICATIONS (TYPE 16)

<table>
<thead>
<tr>
<th>COLUMNS</th>
<th>CONTENTS...IMPLICATIONS, IF ANY</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-2</td>
<td>16</td>
</tr>
<tr>
<td>7-12</td>
<td>FISSION SPECTRUM NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY.</td>
</tr>
<tr>
<td>13-18</td>
<td>FISSIONABLE NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY.</td>
</tr>
<tr>
<td>19-24</td>
<td>FISSIONABLE NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY.</td>
</tr>
<tr>
<td>25-30</td>
<td>FISSIONABLE NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY.</td>
</tr>
<tr>
<td>31-36</td>
<td>FISSIONABLE NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY.</td>
</tr>
<tr>
<td>37-42</td>
<td>FISSIONABLE NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY.</td>
</tr>
<tr>
<td>43-48</td>
<td>FISSIONABLE NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY.</td>
</tr>
<tr>
<td>49-54</td>
<td>FISSIONABLE NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY.</td>
</tr>
<tr>
<td>55-60</td>
<td>FISSIONABLE NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY.</td>
</tr>
<tr>
<td>61-66</td>
<td>FISSIONABLE NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY.</td>
</tr>
<tr>
<td>67-72</td>
<td>FISSIONABLE NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY.</td>
</tr>
</tbody>
</table>
APPENDIX B. MC\textsuperscript{2}-2 BCD Input Files. A.MCC2 (Contd.)

C
CN
IF NO TYPE 16 CARDS ARE GIVEN, THE FISSION SPECTRUM WILL BE OBTAINED FROM A MIXTURE OF ALL SPECTRA REPRESENTED BY THE MATERIALS PRESENT IN THE SPECTRUM COMPOSITION. THE FISSION SPECTRUM SPECIFIED IN COLS. 7-12 WILL BE USED FOR THE FISSIONABLE NUCLIDES SPECIFIED IN COLS. 13-18, 19-24, ETC. IF COLS. 13-18 OF ANY TYPE 16 CARD ARE BLANK, THE REST OF THAT TYPE 16 CARD IS IGNORED AND THE FISSION SPECTRUM SPECIFIED IN COLS. 7-12 WILL BE USED FOR ANY FISSIONABLE NUCLIDES NOT SPECIFIED ON OTHER TYPE 16 CARDS. ONLY ONE TYPE 16 CARD WITH A BLANK FIELD IN COLS. 13-18 IS PERMITTED. IF NO SUCH CARD IS GIVEN ANY FISSIONABLE NUCLIDE NOT SPECIFIED ON A TYPE 16 CARD WILL BE ASSIGNED ITS OWN FISSION SPECTRUM. AS MANY TYPE 16 CARDS AS NECESSARY MAY BE USED. THE FISSION SPECTRUM IDENTIFICATION LABEL SHOULD BE REPEATED ON ADDITIONAL CARDS. COLS. 13-18, 19-24, ETC. SHOULD CONTAIN LABELS CORRESPONDING TO LABELS IN COLS. 13-18 OF THE TYPE 06 CARDS.

C
C-----------------------------------------------------------------------
CR
UNRESOLVED RESONANCE FIXED ENERGY MESH (TYPE 17)
C
CL
FORMAT-----(I2,10X,2(E12.5,16,16))
C
CD
COLUMNS CONTENTS...IMPlications, IF any
CD
1-2 17
CD
12-24 LETHARGY WIDTH.
CD
25-30 INITIAL FIXED MESH POINT NUMBER.
CD
31-36 FINAL FIXED MESH POINT NUMBER.
CD
37-48 LETHARGY WIDTH.
CD
49-54 INITIAL FIXED MESH POINT NUMBER.
CD
55-60 FINAL FIXED MESH POINT NUMBER.
C
A MAXIMUM OF 500 FIXED ENERGY MESH POINTS MAY BE USED.
AS MANY TYPE 17 CARDS AS NECESSARY MAY BE USED. IF NO TYPE 17 CARD IS SUPPLIED, THE BUILT IN FIXED ENERGY MESH STRUCTURE IS USED. THE LETHARGY WIDTH SPECIFIED IN COLS. 12-24 IS USED FOR POINTS SPECIFIED IN COLS.
APPENDIX B.  $M^2-2$ BCD Input Files.  A.MCC2 (Contd.)

<table>
<thead>
<tr>
<th>Column Numbers</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>25-30</td>
<td>The lethargy width specified in cols. 37-48 is used for points specified in cols. 31-36. The lethargy width specified in cols. 12-24 or 37-48 is used for all remaining points and the rest of the data on the Type 17 cards are ignored. The fixed energy mesh covers the entire energy range as specified on the Type 05 cards.</td>
</tr>
<tr>
<td>49-54</td>
<td>If cols. 25-30 or 49-54 are blank, the value specified in cols. 12-24 and/or cols. 37-40 is used for the mesh point specified in cols. 25-30 and/or cols. 49-54.</td>
</tr>
</tbody>
</table>

---

### Homogeneous Infinitely Dilute Specifications (Type 18)

- **Format:** (I2,4X,11A6)

- **Columns**

  1-2 | COLUMNS | CONTENTS...IMPLICATIONS, IF ANY |
  --- | ======= | ---------------------------------- |
  7-12 | NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY (COLS. 13-18 ON TYPE 06 CARDS). |
  13-18 | NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY (COLS. 13-18 ON TYPE 06 CARDS). |
  19-24 | NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY (COLS. 13-18 ON TYPE 06 CARDS). |
  25-30 | NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY (COLS. 13-18 ON TYPE 06 CARDS). |
  31-36 | NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY (COLS. 13-18 ON TYPE 06 CARDS). |
  37-42 | NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY (COLS. 13-18 ON TYPE 06 CARDS). |
  43-48 | NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY (COLS. 13-18 ON TYPE 06 CARDS). |
  49-54 | NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY (COLS. 13-18 ON TYPE 06 CARDS). |
  55-60 | NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY |
APPENDIX B. MC\(^2\)-2 BCD Input Files. A.MCC2 (Contd.)

**CD**
(COLS. 13-18 ON TYPE 06 CARDS).

**CD**
61-66 NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY
(COLS. 13-18 ON TYPE 06 CARDS).

**CD**
67-72 NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY
(COLS. 13-18 ON TYPE 06 CARDS).

**C**
MATERIALS NAMED ON THE TYPE 18 CARDS WILL BE ASSUMED
TO BE INFINITELY DILUTE FOR THE HOMOGENEOUS RESOLVED
RESONANCE CALCULATION. MATERIALS WHICH ARE ASSUMED TO
BE INFINITELY DILUTE WILL NOT BE INVOLVED IN THE
OVERLAP CALCULATION FOR ANY OTHER MATERIAL.
THEIR RESONANCE INTEGRALS WILL BE SET TO THE
INFINITELY DILUTE LIMIT OF \(\pi/(2 \times \beta)\).
SEE CARD TYPE 12 FOR THE HETEROGENEOUS SPECIFICATIONS.

**C**

**CR**
RESONANCE EDIT OPTIONS (TYPE 19)

**CL**
FORMAT----(T2,4X,6I6)

**CD**
COLUMN CONTENTS...IMPLICATIONS, IF ANY

<table>
<thead>
<tr>
<th>==</th>
<th>==</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-2</td>
<td>19</td>
</tr>
</tbody>
</table>

**CD**
7-12 DATA SET UNRES EDIT FLAG.

**CD**
13-18 DATA SET ATNUAT EDIT FLAG.

**CD**
19-24 DATA SET PESINT EDIT FLAG.

**CD**
25-30 DATA SET SIGMAP EDIT FLAG.

**CD**
31-36 DATA SET LORENZ EDIT FLAG.

**CD**
37-42 BROAD GROUP RESONANCE CROSS SECTION FLAG.

0...INCLUDE RESONANCE CROSS SECTIONS IN THE BROAD GROUP-
CROSS SECTIONS (DEFAULT).

1...OMIT ALL RESONANCE CROSS SECTIONS FROM THE BROAD-
GROUP CROSS SECTIONS.

2...OMIT RESONANCE CAPTURE AND FISSION CROSS SECTIONS-
FROM THE BROAD GROUP CROSS SECTIONS.

**CN**
EACH DATA SET WHOSE EDIT FLAG IS NON-ZERO WILL BE
EDITED. OTHERWISE IT WILL NOT BE EDITED.
### GENERAL PROBLEM EDIT OPTIONS (TYPE 20)

<table>
<thead>
<tr>
<th>Columns</th>
<th>Contents/Implications, if any</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-2</td>
<td>20</td>
</tr>
<tr>
<td>7-12</td>
<td>Ultra-fine-group macroscopic fission, total, transport and scattering cross sections.</td>
</tr>
<tr>
<td></td>
<td>0...Do not edit data (default).</td>
</tr>
<tr>
<td></td>
<td>1...Edit data.</td>
</tr>
<tr>
<td>13-18</td>
<td>Ultra-fine-group macroscopic moderating parameters.</td>
</tr>
<tr>
<td></td>
<td>0...Do not edit data (default).</td>
</tr>
<tr>
<td></td>
<td>1...Edit data.</td>
</tr>
<tr>
<td>19-24</td>
<td>Ultra-fine-group microscopic pl scattering cross sections, p0 and p1 elastic transfer matrices.</td>
</tr>
<tr>
<td></td>
<td>0...Do not edit data (default).</td>
</tr>
<tr>
<td></td>
<td>n...Edit data at ultra-fine-groups 1,n+1,2*n+1,...</td>
</tr>
<tr>
<td>25-30</td>
<td>Ultra-fine-group spectrum.</td>
</tr>
<tr>
<td></td>
<td>0...Edit data (default).</td>
</tr>
<tr>
<td></td>
<td>1...Do not edit data.</td>
</tr>
<tr>
<td>31-36</td>
<td>Broad group resonance cross section edit flag.</td>
</tr>
<tr>
<td></td>
<td>0...Do not edit data (default).</td>
</tr>
<tr>
<td></td>
<td>1...Edit data.</td>
</tr>
<tr>
<td>37-42</td>
<td>Broad group reaction rate edit flag.</td>
</tr>
<tr>
<td></td>
<td>0...Edit data.</td>
</tr>
<tr>
<td></td>
<td>1...Do not edit data.</td>
</tr>
</tbody>
</table>

**Cols. 19-24** should routinely be set at zero (default) as the edit of transfer matrices produces a great deal of paper output.

### COMPOSITION TEMPERATURES (TYPE 21)

| Format: | (I2,10X,3(A6,E12.5)) |
APPENDIX B. MC^2-2 BCD Input Files. A.MCC2 (Contd.)

<table>
<thead>
<tr>
<th>CD</th>
<th>COLUMNS</th>
<th>CONTENTS...IMPLICATIONS, IF ANY</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD</td>
<td>1-2</td>
<td>21</td>
</tr>
<tr>
<td>CD</td>
<td>13-18</td>
<td>COMPOSITION LABEL.</td>
</tr>
<tr>
<td>CD</td>
<td>19-30</td>
<td>TEMPERATURE IN DEGREES K (DEFAULT=300.0).</td>
</tr>
<tr>
<td>CD</td>
<td>31-36</td>
<td>COMPOSITION LABEL.</td>
</tr>
<tr>
<td>CD</td>
<td>37-48</td>
<td>TEMPERATURE IN DEGREES K (DEFAULT=300.0).</td>
</tr>
<tr>
<td>CD</td>
<td>49-54</td>
<td>COMPOSITION LABEL.</td>
</tr>
<tr>
<td>CD</td>
<td>55-66</td>
<td>TEMPERATURE IN DEGREES K (DEFAULT=300.0).</td>
</tr>
</tbody>
</table>

As many type 21 cards as necessary may be used to specify the composition temperatures. Composition labels in cols. 13-18, 31-36, and 49-54 must correspond to labels given in cols. 13-18 on data set A.NIP type 14 cards. The composition temperatures are used only for the integral transport theory calculations.

In the case of homogeneous problems for which cols. 37-42 on the type 03 card are zero, the temperature used for an integral transport theory calculation will be the value specified in cols 19-30 on the first type 21 card provided. If no type 21 cards are given, the temperature for a homogeneous problem will be that specified on the type 06 card for the first material after the input is reordered to correspond to the order of materials in the library.

If the path invokes area 10, the problem mixture must contain materials having resolved resonances.

---

**ISOTOPE IDENTIFICATION (TYPE 22)**

<table>
<thead>
<tr>
<th>CD</th>
<th>COLUMNS</th>
<th>CONTENTS...IMPLICATIONS, IF ANY</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD</td>
<td>1-2</td>
<td>22</td>
</tr>
<tr>
<td>CD</td>
<td>13-18</td>
<td>NUCLIDE IDENTIFICATION LABEL ON LIBRARY.</td>
</tr>
<tr>
<td>CD</td>
<td>19-24</td>
<td>ISOTOPE CLASSIFICATION.</td>
</tr>
</tbody>
</table>
APPENDIX B. MC²-2 BCD Input Files. A.MCC2 (Contd.)

| CD  | 0... UNDEFINED (DEFAULT).   |
| CD  | 1... FISSION.               |
| CD  | 2... FERTILE.               |
| CD  | 3... OTHER ACTINIDE.        |
| CD  | 4... FISSION PRODUCT.       |
| CD  | 5... STRUCTURAL.            |
| CD  | 6... COOLANT.               |
| CD  | 7... CONTROL.               |
| CD  | 25-36 TOTAL THERMAL ENERGY YIELD/FISSION (MEV/FISSION). |
| CD  | 37-48 TOTAL THERMAL ENERGY YIELD/CAPTURE (MEV/CAPTURE). |

---

FISSION SPECTRA TEMPERATURES (TYPE 23)

<table>
<thead>
<tr>
<th>COLUMN</th>
<th>CONTENTS...IMPLICATIONS, IF ANY</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-2</td>
<td>23</td>
</tr>
<tr>
<td>7-12</td>
<td>NUCLIDE IDENTIFICATION LABEL ON LIBRARY.</td>
</tr>
<tr>
<td>13-24</td>
<td>FISSION SPECTRUM TEMPERATURE, E.V.</td>
</tr>
<tr>
<td>25-30</td>
<td>NUCLIDE IDENTIFICATION LABEL ON LIBRARY.</td>
</tr>
<tr>
<td>31-42</td>
<td>FISSION SPECTRUM TEMPERATURE, E.V.</td>
</tr>
<tr>
<td>43-48</td>
<td>NUCLIDE IDENTIFICATION LABEL ON LIBRARY.</td>
</tr>
<tr>
<td>49-60</td>
<td>FISSION SPECTRUM TEMPERATURE, E.V.</td>
</tr>
</tbody>
</table>

NOTE THAT THE TYPE 23 DATA ARE PERTINENT ONLY FOR FISSIONABLE ISOTOPES. THE TEMPERATURES ON THE TYPE 23 CARDS ARE USED TO OVERRIDE THE CORRESPONDING TEMPERATURES OF PROBLEM MATERIALS ON THE LIBRARY FOR USE IN GENERATING FISSION SPECTRA. IF AN EXTERNAL SOURCE IS SPECIFIED SUCH THAT ON THE TYPE 08 CARD COLS. 13-24 ARE BLANK AND COLS. 25-30 CONTAIN THE FISSION SPECTRUM NUCLIDE IDENTIFICATION LABEL ON THE LIBRARY, THEN THAT LABEL AND THE CORRESPONDING LABEL IN COLS. 7-12 ON THE TYPE
APPENDIX B. MC²-2 BCD Input Files. A.MCC2 (Contd.)

CN 23 CARD NEED NOT CORRESPOND TO ONE OF THE PROBLEM MATERIALS. ANY LIBRARY MATERIAL NOT REFERENCED ON THE TYPE 23 CARDS WILL USE THE LIBRARY SPECIFIED.

CN FISSION SPECTRUM TEMPERATURE.

CN IF COLS. 7-12, 25-30, OR 43-48 ARE BLANK ON ANY TYPE 23 CARD, THE REST OF ANY SUPPLIED TYPE 23 DATA WILL BE IGNORED.

CEOFS
APPENDIX B. MC\textsuperscript{2}-2 BCD Input Files. A.NIP

PREPARED 6/13/75 AT ANL

BCD INPUT FOR HETEROGENEOUS MC\textsuperscript{2}-II AND SDX CALCULATIONS

THIS IS A USER-SUPPLIED BCD DATA SET. IT IS AN ABBREVIATED VERSION OF THE DATA SET A.NIP.

THE LIST FOR EACH RECORD IS GIVEN IN TERMS OF THE BCD FORMAT OF THE DATA CARD.

COLUMNS 1 2 CONTAIN THE CARD TYPE NUMBER.

EXTERNAL BOUNDARY CONDITIONS (TYPE 04)

~~~ FORM~~~(I2,10X,216)

~~~ COLUMNS CONTENTS...IMPLICATIONS, IF ANY

~~~ 1-2 04

~~~ 13-18 BOUNDARY CONDITION AT LOWER "X" BOUNDARY OF CELL.

~~~ 19-24 BOUNDARY CONDITION AT UPPER "X" BOUNDARY OF CELL.

~~~ 10...REFLECTIVE.

~~~ 11...PERIODIC.

~~~ 12...WHITE.

THE LEFT BOUNDARY CONDITION MUST BE REFLECTIVE AND THE RIGHT BOUNDARY CONDITION MUST BE WHITE FOR CYLINDRICAL GEOMETRY. THE LEFT AND RIGHT BOUNDARY CONDITIONS MUST BE THE SAME AND MAY BE ONLY REFLECTIVE OR PERIODIC FOR SLAB GEOMETRIES.

REGION BOUNDARY COORDINATES AND MESH STRUCTURE

~~~ FORM~~~(I2,4X,A6,2E12.5,I6)

~~~ COLUMNS CONTENTS...IMPLICATIONS, IF ANY
### APPENDIX B. MC²-2 BCD Input Files. A.NIP (Contd.)

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-2</td>
<td>Region Label (repeated on additional type 06 cards).</td>
</tr>
<tr>
<td>13-24</td>
<td>&quot;X&quot;-direction lower-boundary coordinate.</td>
</tr>
<tr>
<td>25-36</td>
<td>&quot;X&quot;-direction upper-boundary coordinate.</td>
</tr>
<tr>
<td>37-42</td>
<td>Number of intervals in &quot;X&quot; direction.</td>
</tr>
<tr>
<td>43-54</td>
<td>Isotope atom density.</td>
</tr>
<tr>
<td>55-60</td>
<td>Isotope label.</td>
</tr>
<tr>
<td>61-72</td>
<td>Isotope atom density.</td>
</tr>
</tbody>
</table>

- Regions may be defined using the overlay procedure, with the latest region assignment overlaying the previous configuration, or using the usual procedure, with each region's boundaries given explicitly.
- Region labels must be non-blank.
- Only the "X"-direction upper boundaries need to be given for regions after the first.

**Composition Specifications (Type 14)**

<table>
<thead>
<tr>
<th>Column</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-2</td>
<td>14</td>
</tr>
<tr>
<td>13-18</td>
<td>Composition label (repeated on additional type 14 cards).</td>
</tr>
<tr>
<td>19-24</td>
<td>Isotope label.</td>
</tr>
<tr>
<td>25-36</td>
<td>Isotope atom density.</td>
</tr>
<tr>
<td>37-42</td>
<td>Isotope label.</td>
</tr>
<tr>
<td>43-54</td>
<td>Isotope atom density.</td>
</tr>
<tr>
<td>55-60</td>
<td>Isotope label.</td>
</tr>
<tr>
<td>61-72</td>
<td>Isotope atom density.</td>
</tr>
</tbody>
</table>

- Composition labels must be non-blank.
- Isotope labels in cols. 19-24, 37-42, and 55-60 must be non-blank.
APPENDIX B. MC²-2 BCD Input Files. A.NIP (Contd.)

CORRESPOND TO NUCLIDE IDENTIFICATION LABELS ON THE
LIBRARY IF THEY DO NOT CORRESPOND TO ANY OF THE
MATERIALS NAMED ON THE DATA SET A.MCC2 TYPE 06 CARDS.
IN OTHER CASES, THEY MUST CORRESPOND TO SOME PROBLEM
MATERIAL LABEL IN COLS. 19-24 ON THE DATA SET A.MCC2
TYPE 06 CARDS.

---

**COMPOSITION AND REGION ASSIGNMENTS (TYPE 15)**

<table>
<thead>
<tr>
<th>COLUMNS</th>
<th>CONTENTS...IMPLICATIONS, IF ANY</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-2</td>
<td>15</td>
</tr>
<tr>
<td>7-12</td>
<td>COMPOSITION LABEL (REPEATED ON ADDITIONAL TYPE 15 CAPDS).</td>
</tr>
<tr>
<td>13-18</td>
<td>REGION LABEL OF REGION CONTAINING SPECIFIED COMPOSITION.</td>
</tr>
<tr>
<td>19-24</td>
<td>REGION LABEL OF REGION CONTAINING SPECIFIED COMPOSITION.</td>
</tr>
<tr>
<td>25-30</td>
<td>REGION LABEL OF REGION CONTAINING SPECIFIED COMPOSITION.</td>
</tr>
<tr>
<td>31-36</td>
<td>REGION LABEL OF REGION CONTAINING SPECIFIED COMPOSITION.</td>
</tr>
<tr>
<td>37-42</td>
<td>REGION LABEL OF REGION CONTAINING SPECIFIED COMPOSITION.</td>
</tr>
<tr>
<td>43-48</td>
<td>REGION LABEL OF REGION CONTAINING SPECIFIED COMPOSITION.</td>
</tr>
<tr>
<td>49-54</td>
<td>REGION LABEL OF REGION CONTAINING SPECIFIED COMPOSITION.</td>
</tr>
<tr>
<td>55-60</td>
<td>REGION LABEL OF REGION CONTAINING SPECIFIED COMPOSITION.</td>
</tr>
<tr>
<td>61-66</td>
<td>REGION LABEL OF REGION CONTAINING SPECIFIED COMPOSITION.</td>
</tr>
<tr>
<td>67-72</td>
<td>REGION LABEL OF REGION CONTAINING SPECIFIED COMPOSITION.</td>
</tr>
</tbody>
</table>
APPENDIX B. MC\textsuperscript{2}-2 BCD Input Files. A.NIP (Contd.)

CD

CEOF
APPENDIX B. $\text{MC}^2$-2 BCD Input Files. A.STPO15

**C**

PREPARED 2/25/76 AT ANL

**CF**

A.STPO15

**CE**

GENERAL BCD INPUT FOR $\text{MC}^2$-II PATH DRIVER

**CN**

THIS IS A USER SUPPLIED BCD DATA SET.
THE LIST FOR EACH RECORD IS GIVEN IN TERMS
OF THE BCD FORMAT OF THAT DATA CARD.
COLUMNS 1-2 CONTAIN THE CARD TYPE NUMBER.
BLANK FIELDS PRODUCE THE DEFAULT OPTIONS.

**C**

PATH OPTIONS (TYPE 01)

**CL**

FORMAT-----(I2,4X,9I6)

**CD**

COLUMNS CONTENTS...IMPLICATIONS, IF ANY

**CD**

1-2 01

**CD**

7-12 $\text{MC}^2$-II INPUT PROCESSOR CALCULATION
AREA 4 (CSI010).
0... INVOKE INPUT PROCESSOR (DEFAULT).
1...DO NOT Invoke INPUT PROCESSOR.

**CD**

13-18 UNRESOLVED RESONANCE CALCULATION
AREA 5 (CSCO04).
0...DO UNRESOLVED RESONANCE CALCULATION (DEFAULT).
1...DO NOT DO UNRESOLVED RESONANCE CALCULATION.

**CD**

19-24 RESOLVED RESONANCE CALCULATION
AREA 6 (CSCO05).
0...DO RESOLVED RESONANCE CALCULATION (DEFAULT).
1...DO NOT DO RESOLVED RESONANCE CALCULATION.

**CD**

25-30 MACROSCOPIC CROSS SECTION AND MODERATING PARAMETER
CALCULATION
AREA 7 (CSCO08).
0...DO CALCULATION OF MACROSCOPIC CROSS SECTIONS
AND CONTINUOUS SLOWING DOWN MODERATING PARAMETERS
(DEFAULT).
1...DO NOT CALCULATE MODERATING PARAMETERS AND
MACROSCOPIC CROSS SECTIONS.

**CD**

31-36 UFG SPECTRUM AND BROAD GROUP CROSS SECTIONS
CD AREA 8 (CSC009).
  0...DO ULTRA-FINE-GROUP CALCULATION AND BROAD GROUP
      CROSS SECTIONS (DEFAULT).
  1...DO NOT DO ULTRA-FINE-GROUP CALCULATION AND BROAD
      GROUP CROSS SECTIONS.

CD 37-42 BROAD GROUP SPECTRUM CALCULATION
  AREA 9 (CSC010).
  0...DO BROAD GROUP SPECTRUM CALCULATION (DEFAULT).
  1...DO NOT DO BROAD GROUP SPECTRUM CALCULATION.

CD 43-48 BROAD GROUP CROSS SECTION EDITS (CSE009).
  0...EDIT BROAD GROUP CROSS SECTION FILE ISOTXS
      (DEFAULT).
  1...DO NOT EDIT BROAD GROUP CROSS SECTION FILE ISOTXS.

CD 49-54 TSOTXS TO XS.ISO CONVERSION (CSE007).
  0...CREATE EQUIVALENT OF DATA SET ISOTXS IN THE DOUBLE
      PRECISION DATA SET XS.ISO (DEFAULT).
  1...CREATE EQUIVALENT OF DATA SET ISOTXS IN A SINGLE
      PRECISION VERSION OF DATA SET XS.ISO.
  -1...DO NOT CREATE DATA SET XS.ISO.
  (OPTION NOT AVAILABLE IN ARGONNE CODE CENTER VERSION
  OF MC**2-II.)

CD 55-60 HYPER FINE GROUP INTEGRAL TRANSPORT CALCULATION
  AREA 10 (CSC011).
  0...DO NOT DO HYPER FINE GROUP INTEGRAL TRANSPORT
      CALCULATION (DEFAULT).
  1...DO HYPER FINE GROUP INTEGRAL TRANSPORT CALCULATION.

CD 61-66 DATA SET XS.ISO EDIT (CSE012).
  0...DO NOT EXECUTE CSE012 (XS.ISO EDITOR).
  1...EXECUTE CSE012.
  (OPTION NOT AVAILABLE IN ARGONNE CODE CENTER VERSION
  OF MC**2-II.)

CN IF COLS. 13-18 OR COLS. 19-24 ARE 1, AREA 6.5 WILL BE
    EXECUTED TO OBTAIN THE RESOLVED-UNRESOLVED OVERLAP
    CALCULATION.

C

C---------------------------------------------------------------

CR UNRESOLVED RESONANCE OPTION (TYPE 02)

CL FORMAT----(I2,4X,I6)

D COLUMNS CONTENTS...IMPLICATIONS, IF ANY
APPENDIX B. MC\textsuperscript{2}-2 BCD Input Files. A.STP015 (Contd.)

<table>
<thead>
<tr>
<th>CD</th>
<th>1-2</th>
<th>ARPA 10 UNRESOLVED RESONANCE OPTION (CSC011).</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD</td>
<td></td>
<td>0...EXCLUDE UNRESOLVED RESONANCE CROSS SECTIONS FROM THE HYPER FINE GROUP INTEGRAL TRANSPORT CALCULATION (DEFAULT).</td>
</tr>
<tr>
<td>CD</td>
<td>7-12</td>
<td>1...INCLUDE UNRESOLVED RESONANCE CROSS SECTIONS IN THE HYPER FINE GROUP INTEGRAL TRANSPORT CALCULATION.</td>
</tr>
</tbody>
</table>

CEOF
APPENDIX B. MC²-2 BCD Input Files. ACSE12

C***********************************************************************
C- PREPARED 12/09/74 AT ANL
C- CF ACS.Y.l2 BCD INPUT FOR XS.ISO EDITOR CSE012
C- CN THIS IS A USER-SUPPLIED BCD DATA SET.
CN THE LIST FOR EACH RECORD IS GIVEN IN TERMS OF
CN THE BCD FORMAT OF THE DATA CARD.
CN COLUMNS 1-2 CONTAIN THE CARD TYPE NUMBER.
C- C***********************************************************************

C---------------------------------------
CR EDIT SPECIFICATIONS (TYPE 01)
C-
CL FORMAT-----(I2,4X,A6,I6)
C-
CD COLUMNS CONTENTS...IMPLICATIONS, IF ANY
CD ------- -------------------------------
CD 1-2 01
CD 7-12 ISOTOPE LABEL.
CD 13-18 EDIT FLAG.
CD-
CN IF COLS. 7-12 ON THE FIRST TYPE 01 CARD ARE BLANK, THE-
CN ENTIRE XS.ISO DATA SET WILL BE EDITED. IF COLS. 13-18-
CN ARE 0, ALL CROSS SECTION TYPES WILL BE EDITED. IF-
CN COLS. 13-18 ARE 1, ONLY THE PRINCIPAL CROSS SECTIONS-
CN WILL BE EDITED. IF COLS. 13-18 ARE 2, ONLY THE-
CN SCATTERING ARRAYS WILL BE EDITED. IF COLS. 13-18 ARE-
CN 3, ONLY FILE 1 OF DATA SET XS.ISO WILL BE EDITED.
CN IF COLS. 7-12 ARE BLANK ON THE FIRST TYPE 01 CARD BUT-
CN ADDITIONAL TYPE 01 CARDS ARE SUPPLIED, THE ISOTOPE-
CN NAMED IN COLS. 7-12 OF EACH ADDITIONAL CARD WILL BE-
CN EDITED ACCORDING TO THE FLAG SET IN COLS. 13-18 OF THAT-
CN SAME CARD. ANY ISOTOPE NOT SPECIFICALLY REFERENCED WILL-
CN BE EDITED ACCORDING TO THE VALUE IN COLS. 13-18 ON THE-
CN FIRST TYPE 01 CARD (WHICH HAS COLS. 7-12 BLANK). IF-
CN COLS. 13-18 ON AN ADDITIONAL TYPE 01 CARD ARE -1, THE-
CN ISOTOPE NAMED IN COLS. 7-12 OF THAT CARD WILL NOT BE-
CN EDITED. IF THE FIRST TYPE 01 CARD IS NON-BLANK IN-
CN COLS. 7-12, ONLY THE ISOTOPES NAMED ON THE TYPE 01-
CN CARDS WILL BE EDITED, EACH ACCORDING TO THE FLAG IN-
CN COLS. 13-18 ON THE SAME CARD. IF DATA SET ACSE12 IS-
CN NOT SUPPLIED, THE ENTIRE SET IS EDITED AND ALL CROSS-
CN SECTION TYPES ARE EDITED FOR EACH ISOTOPE.
APPENDIX B. MC\textsuperscript{2}-2 BCD Input Files. ACSE12 (Contd.)

IF NO TYPE 01 CARDS ARE SUPPLIED, THE EDIT WILL
CORRESPOND TO HAVING PUT IN A SINGLE BLANK TYPE 01
CARD.

C

C-----------------------------

CR

BPOINTER EDIT OPTION (TYPE 02)

CL

FORMAT-----(I2,4X,16)

CD

COLUMNS CONTENTS...IMPLICATIONS, IF ANY

CD 1-2 02

CD 7-12 BPOINTER EDIT FLAG.
0...NO BPOINTER DEBUGGING PRINTS.
1...DEBUGGING DUMP PRINTOUT.
2...DEBUGGING TRACE PRINTOUT.
3...FULL DEBUGGING PRINTOUT.

C

C-----------------------------

CEOF
APPENDIX B. MC²-2 BCD Input Files. ACS009

**C**

*PREPARED 2/27/75 AT ANL*

**CF**

ACSO09

**BCD INPUT FOR EDITING ISOTXS DATA SET (CSFOC9)**

**CN**

THIS IS A USER SUPPLIED BCD DATA SET.

THE LIST FOR EACH RECORD IS GIVEN IN TERMS OF THE BCD FORMAT OF THAT DATA CARD.

COLUMNS 1-2 CONTAIN THE CARD TYPE NUMBER.

BLANK FIELDS PRODUCE THE DEFAULT OPTIONS.

**C**

**-----------------------------------T-----Z----------------------------------**

**CF**

COMPUTER CONTAINER ARRAY (TYPE 01)

**CC**

OPTIONAL CARD TYPE

**CL**

FORMAT——(I2,4X,3I6)

**CD**

COLUMNS CONTENTS...IMPLICATIONS, IF ANY

1-2 01

7-12 SIZE OF MAIN STORAGE ARRAY IN REAL*8 WORDS (DEFAULT=30000).

13-18 SIZE OF BULK CORE STORAGE ON REAL*8 WORDS (DEFAULT=0).

19-24 POINTR DEBUGGING EDIT.

0...NO DEBUGGING PRINTOUT (DEFAULT).

1...DEBUGGING DUMP PRINTOUT.

2...DEBUGGING TRACE PRINTOUT.

3...FULL DEBUGGING PRINTOUT.

**CN**

THIS CARD TYPE IS USED ONLY AFTER THE BPOINTER CONTAINER ARRAY CAN NOT BE ALLOCATED BY:

(1) ATTEMPTING TO CALCULATE THE SIZE OF THE CONTAINER ARRAY FROM THE FILE CONTROL RECORD OF THE ISOTXS DATA SET, OR

(2) OBTAINING THE SIZE OF THE CONTAINER ARRAY SPECIFIED IN DATA SET PRBSPC (IF IT EXISTS) WHICH CONTAINS THE SIZE OF THE CONTAINER ARRAY SPECIFIED BY THE DATA SET A.MCC2.
APPENDIX B. MC²-2 BCD Input Files. ACS009 (Contd.)

<table>
<thead>
<tr>
<th>Columns</th>
<th>Contents</th>
<th>Implications, if any</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-2</td>
<td>02</td>
<td></td>
</tr>
<tr>
<td>7-12</td>
<td>Isotope to be edited.</td>
<td></td>
</tr>
<tr>
<td>13-18</td>
<td>Isotope to be edited.</td>
<td></td>
</tr>
<tr>
<td>19-24</td>
<td>Isotope to be edited.</td>
<td></td>
</tr>
<tr>
<td>25-30</td>
<td>Isotope to be edited.</td>
<td></td>
</tr>
<tr>
<td>31-36</td>
<td>Isotope to be edited.</td>
<td></td>
</tr>
<tr>
<td>37-42</td>
<td>Isotope to be edited.</td>
<td></td>
</tr>
<tr>
<td>43-49</td>
<td>Isotope to be edited.</td>
<td></td>
</tr>
<tr>
<td>49-54</td>
<td>Isotope to be edited.</td>
<td></td>
</tr>
<tr>
<td>55-60</td>
<td>Isotope to be edited.</td>
<td></td>
</tr>
<tr>
<td>61-66</td>
<td>Isotope to be edited.</td>
<td></td>
</tr>
<tr>
<td>67-72</td>
<td>Isotope to be edited.</td>
<td></td>
</tr>
<tr>
<td>73-80</td>
<td>Isotope to be edited.</td>
<td></td>
</tr>
</tbody>
</table>

Isotope name must be left-justified in format field with imbedded blanks preserved. As many Type 02 cards as necessary may be used. No Type 02 card will result in all the isotopes in the isotope data set to be edited. A Type 02 card with no isotope names will result in only isotope independent data to be edited e.g., an edit of the first three or four records of data set isotope.
APPENDIX C

MC$^2$-2 BINARY INTERFACE FILES
APPENDIX C. MC\textsuperscript{2}-2 Binary Interface Files. ISOTXS

C******************************************************************************
C PREPARED 03/03/75
C
CF ISOTXS
CE MICROSCOPIC GROUP NEUTRON CROSS SECTIONS
CN THIS FILE PROVIDES A BASIC BROAD GROUP
CN LIBRARY, ORDERED BY ISOTOPE
C
C******************************************************************************

CD MULT 2 FOR IBM MACHINES, 1 OTHERWISE

C-----------------------------------------------------------------------
C FILE STRUCTURE
C-----------------------------------------------------------------------
CS RECORD TYPE PRESENT IF
CS =------------------------------ =---------------
CS FILE IDENTIFICATION ALWAYS
CS FILE CONTROL ALWAYS
CS FILE DATA ALWAYS
CS SET CHI DATA ICHIST.GT.1
CS ********** (REPEAT FOR ALL ISOTOPES)
CS * ISOTOPE CONTROL AND GROUP ALWAYS
CS * INDEPENDENT DATA
CS * PRINCIPAL CROSS SECTIONS ALWAYS
CS * ISOTOPE CHI DATA ICHI.GT.1
CS * ******** (REPEAT TO NSCMAX SCATTERING BLOCKS)
CS * * ***** (REPEAT FROM 1 TO NSBLOK)
CS * * * SCATTERING SUB-BLOCK LORD(N).GT.0
CS **********
C
C-----------------------------------------------------------------------
C FILE IDENTIFICATION (TYPE 1)
C HHNAME, (HUSE(I),I=1,2), IVERS
C 1+3*MULT
C HHNAME HOLLERITH FILE NAME - ISOTXS - (A6)
C HUSE HOLLERITH USER IDENTIFICATION (A6)
C IVERS FILE VERSION NUMBER

C-----------------------------------------------------------------------
APPENDIX C. MC²-2 Binary Interface Files. ISOTXS (Contd.)

FILE CONTROL (TYPE 2)

<table>
<thead>
<tr>
<th>NAME</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>NGROUP</td>
<td>Number of Energy Groups in Set</td>
</tr>
<tr>
<td>NISO</td>
<td>Number of Isotopes in Set</td>
</tr>
<tr>
<td>MAXUP</td>
<td>Maximum Number of Upscatter Groups</td>
</tr>
<tr>
<td>MAXDN</td>
<td>Maximum Number of Downscatter Groups</td>
</tr>
<tr>
<td>MAXORD</td>
<td>Maximum Number of Scattering Orders</td>
</tr>
<tr>
<td>ICHIST</td>
<td>Set Fission Spectrum Flag</td>
</tr>
<tr>
<td>NSCMAX</td>
<td>Maximum Number of Blocks of Scattering Data</td>
</tr>
<tr>
<td>NSBLOK</td>
<td>Blocking Control for Scattering Matrices. The</td>
</tr>
<tr>
<td></td>
<td>Records per Scattering Block</td>
</tr>
</tbody>
</table>

FILE DATA (TYPE 3)

<table>
<thead>
<tr>
<th>NAME</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>HSETID</td>
<td>Hollerith Identification of Set (A6)</td>
</tr>
<tr>
<td>HISONM</td>
<td>Hollerith Isotope Label for Isotope I (A6)</td>
</tr>
<tr>
<td>CHI (J)</td>
<td>Set Fission Spectrum (Present if ICHIST.EQ.1)</td>
</tr>
<tr>
<td>VEL (J)</td>
<td>Mean Neutron Velocity in Group J (cm/sec)</td>
</tr>
<tr>
<td>EMAX (J)</td>
<td>Maximum Energy Bound of Group J (eV)</td>
</tr>
<tr>
<td>EMIN</td>
<td>Minimum Energy Bound of Set (eV)</td>
</tr>
<tr>
<td>LOCA (I)</td>
<td>Number of Records to be Skipped to Read Data</td>
</tr>
<tr>
<td></td>
<td>For Isotope I. LOCA (1)=0</td>
</tr>
</tbody>
</table>

SET CHI DATA (TYPE 4)

<table>
<thead>
<tr>
<th>NAME</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>HSETID</td>
<td>Hollerith Identification of Set (A6)</td>
</tr>
</tbody>
</table>
APPENDIX C. MC\textsuperscript{2}-2 Binary Interface Files. ISOTXS (Contd.)

CC  PRESENT IF ICHIST.GT.1
C
CL  ((CHI(K,J), K=1, ICHIST), J=1,NGROUP), (ISSPEC(I), I=1,NGROUP)
C
CW  NGROUP*(ICHIST+1)
C
CD  CHI(K,J) FRACTION OF NEUTRONS EMITTED IN GROUP J AS A
CD  RESULT OF FISSION IN ANY GROUP USING SPECTRUM K-
CD  ISSPEC ISSPEC(I)=K IMPLIES THAT SPECTRUM K IS USED
CD  TO CALCULATE EMISSION SPECTRUM FROM FISSION
CD  IN GROUP I
C

-----------------------------------
C

CR  ISOTOPE CONTROL AND GROUP INDEPENDENT DATA (TYPE 5)
C
CL  HABSID,IDENT,MAT,AMASS,EFISS,ECAPT,TEMP,SIGPOT,ADENS,KBR,ICH1,
CL  IFIS,IALF,INP,IN2N,IND,INT,LTOT,LTRN,ISTRPD,
CL  2(IDSCT(N), N=1,NSCMAX), (LORD(N),N=1,NSCMAX),
CL  3((JBAND(J,N),J=1,NGROUP),N=1,NSCMAX),
CL  4((IJJ(J,N))=1,NGROUP),N=1,NSCMAX)
C
CW  (2*NGROUP+2)*NSCMAX+17+MULT*3
C
CD  HABSID HOLLIERITH ABSOLUTE ISOTOPE LABEL - SAME FOR
CD  ALL VERSIONS OF THE SAME ISOTOPE IN SET (A6)
CD  IDENT IDENTIFIER OF LIBRARY FROM WHICH BASIC DATA
CD  CAME (E.G. ENDF/B) (A6)
CD  MAT ISOTOPE IDENTIFICATION (E.G. ENDF/B MAT NO.)
CD  (A6)
CD  AMASS GRAM ATOMIC WEIGHT
CD  EFiSS TOTAL THERMAL ENERGY YIELD/FISSION (J.SEC/FISS)
CD  ECAPT TOTAL THERMAL ENERGY YIELD/CAPTURE (J.SEC/CAPT)
CD  TEMP ISOTOPE TEMPERATURE (DEGREES KELVIN)
CD  SIGPOT AVERAGE EFFECTIVE POTENTIAL SCATTERING IN
CD  RESONANCE RANGE (BARNES/ATOM)
CD  ADENS DENSITY OF ISOTOPE IN MIXTURE IN WHICH ISOTOPE
CD  CROSS SECTIONS WERE GENERATED (A/BARN.CM)
CD  KBR ISOTOPE CLASSIFICATION
CD  =1, FISSILE
CD  =2, FERTILE
CD  =3, OTHER ACTINIDE
CD  =4, FISSION PRODUCT
CD  =5, STRUCTURE
CD  =6, COOLANT
CD  =7, CONTROL
CD  ICH1 ISOTOPE FISSION SPECTRUM FLAG
APPENDIX C. MC\textsuperscript{2}-2 Binary Interface Files. ISOTXS (Contd.)

CD ICHI.EQ.0, USE SET CHI
CD ICHI.EQ.1, ISOPOKE CHI VECTOR
CD ICHI.GT.1, ISOPOKE CHI MATRIX
CD IF1S
CD IF1S=0, NO FISSION DATA IN PRINCIPAL CROSS
CD SECTION RECORD
CD =1, FISSION DATA PRESENT IN PRINCIPAL
CD CROSS SECTION RECORD
CD IALF
CD IALF=(N,ALPHA) CROSS SECTION FLAG
CD SAME OPTIONS AS IF1S
CD INP
CD INP=(N,P) CROSS SECTION FLAG
CD SAME OPTIONS AS IF1S
CD IN2N
CD IN2N=(N,2N) CROSS SECTION FLAG
CD SAME OPTIONS AS IF1S
CD IND
CD IND=(N,D) CROSS SECTION FLAG
CD SAME OPTIONS AS IF1S
CD INT
CD INT=(N,T) CROSS SECTION FLAG
CD SAME OPTIONS AS IF1S
CD LTOT
CD LTOT NUMBER OF MOMENTS OF TOTAL CROSS SECTION
CD PROVIDED IN PRINCIPAL CROSS SECTIONS RECORD
CD LTRN
CD LTRN NUMBER OF MOMENTS OF TRANSPORT CROSS SECTION
CD PROVIDED IN PRINCIPAL CROSS SECTIONS RECORD
CD ISTRPD
CD ISTRPD NUMBER OF COORDINATE DIRECTIONS FOR WHICH
CD COORDINATE DEPENDENT TRANSPORT CROSS SECTIONS
CD ARE GIVEN. IF ISTRPD=0, NO COORDINATE DEPENDENT
CD TRANSPORT CROSS SECTIONS ARE GIVEN
CD IDSCT(N)
CD IDSCT(N) SCATTERING MATRIX TYPE IDENTIFICATION FOR
CD SCATTERING BLOCK N. SIGNIFICANT ONLY IF
CD LORD(N).GT.0
CD IDSCT(N)=000 + NN, TOTAL SCATTERING
CD =100 + NN, ELASTIC SCATTERING
CD =200 + NN, INELASTIC SCATTERING
CD =300 + NN, (N,2N) SCATTERING PER
CD Emitted Neutron,
CD WHERE NN IS THE LEGENDRE EXPANSION INDEX OF
CD THE FIRST MATRIX IN BLOCK N
CD LORD(N)
CD LORD(N) NUMBER OF SCATTERING ORDERS IN BLOCK N. IF
CD LORD(N)=0, THIS BLOCK IS NOT PRESENT FOR THIS
CD ISOTOPE. IF NN IS THE VALUE TAKEN FROM
CD IDSCT(N), THEN THE MATRICES IN THIS BLOCK
CD HAVE LEGENDRE EXPANSION INDICES OF NN, NN+1,
CD NN+2, ..., NN+LORD(N)-1
CD JBAND(J,N)
CD JBAND(J,N) SCATTERING BANDWIDTH FOR GROUP J, SCATTERING
CD BLOCK N
CD IJ(J,N)
CD IJ(J,N) POSITION OF IN-GROUP SCATTERING CROSS SECTION
CD IN SCATTERING DATA FOR GROUP J, SCATTERING
CD BLOCK N, COUNTED FROM THE FIRST WORD OF
CD GROUP J DATA
APPENDIX C. MC²-2 Binary Interface Files. ISOTXS (Contd.)

CR---------------------------------
CR PRINCIPAL CROSS SECTIONS (TYPE 6)
CR---------------------------------
CL ((STRPL(J,L),J=1,NGROUP),L=1,LTRN),
CL 1 ((STOTPL(J,L),J=1,NGROUP),L=1,LTOT), (SNGAM(J),J=1,NGROUP),
CL 2 (SFIS(J),J=1,NGROUP), (SNUTOT(J),J=1,NGROUP),
CL 3 (CHISO(J),J=1,NGROUP), (SNALF(J),J=1,NGROUP),
CL 4 (SNP(J),J=1,NGROUP), (SN2N(J),J=1,NGROUP),
CL 5 (SND(J),J=1,NGROUP), (SNT(J),J=1,NGROUP),
CL 6 ((STRPD(J,I),J=1,NGROUP),I=1,ISTRPD).
C
CW (1+LTRN+LTOT+IALF+INP+IN2N+IND+INT+ISTRPD+2*IFTS+
CW ICHI*(2/(ICHI+1))]*NGROUP
C
CD STRPL PL WEIGHTED TRANSPORT CROSS SECTION
CD THE FIRST ELEMENT OF ARRAY STRPL IS THE
CD CURRENT (P1) WEIGHTED TRANSPORT CROSS SECTION
CD STOTPL PL WEIGHTED TOTAL CROSS SECTION
CD THE FIRST ELEMENT OF ARRAY STOTPL IS THE
CD FLUX (P0) WEIGHTED TOTAL CROSS SECTION
CD SNGAM (N,GAMMA)
CD SFIS (N,GAMMA) (PRESENT IF IFIS.GT.0)
CD SNUTOT TOTAL NEUTRON YIELD/ (PRESENT IF IFIS.GT.0)
CD FISSION
CD CHISO ISOTOPE CHI (PRESENT IF ICHI.EQ.1)
CD SNALF (N,ALPHA) (PRESENT IF IALF.GT.0)
CD SNP (N,P) (PRESENT IF INP.GT.0)
CD SN2N (N,2N) (PRESENT IF I2N.GT.0)
CD SND (N,D) (PRESENT IF IND.GT.0)
CD SNT (N,T) (PRESENT IF INT.GT.0)
CD STRPD COORDINATE DIRECTION (PRESENT IF ISTRPD.GT.0)
CD I TRANSPORT CROSS
CD SECTION
C

C---------------------------------
C ISOTOPE CHI DATA (TYPE 7)
C---------------------------------
CC PRESENT IF ICHI.GT.1
C
CL ((CHISO(K,J),K=1,ICHI),J=1,NGROUP), (ISOPEC(I),I=1,NGROUP)
C
CW NGROUP*(ICHI+1)
C
CD CHISO ISOTOPE FISSION SPECTRUM
CD ISOPEC FISSION SPECTRUM USED FOR A GIVEN SOURCE GROUP
APPENDIX C. MC²-2 Binary Interface Files. ISOTXS (Contd.)

C

C-----------------------------------------------

CR SCATTERING SUB-BLOCK (TYPE 8)

CC PRESENT IF LORD(N) .GT. 0

CC ((SCAT(K,L), K=1, KMAX), L=1, LORDN)

CC KMAX = SUM OVER J OF J BAND(J) WITHIN THE J-GROUP RANGE OF THIS
CC RANGE CONTAINED WITHIN THIS SUB-BLOCK IS
CC JL = (M-1) * ((NGROUP-1)/NSBLOK+1) + 1 TO JU = M * ((NGROUP-1)/NSBLOK+1)
CC LORDN = LORD(N)

CC KMAX * LORDN

CD SCAT(K,L) SCATTERING MATRIX OF SCATTERING ORDER L, FOR
CD REACTION TYPE IDENTIFIED BY IDSCT(N) FOR THIS
CD BLOCK. J BAND(J) VALUES FOR SCATTERING INTO
CD GROUP J ARE STORED AT LOCATIONS K = SUM FROM 1
CD TO (J-1) OF J BAND(I) PLUS 1 TO K+J BAND(J)-1.
CD THE SUM IS ZERO WHEN J=1. J-TO-J SCATTER IS
CD THE IJJ(J)-TH ENTRY IN THE RANGE J BAND(J).
CD VALUES ARE STORED IN THE ORDER (J+MAXUP),
CD (J+MAXUP-1), . . . , (J+1), J, (J-1), . . . , (J-MAXDN),
CD WHERE MAXUP = IJJ(J)-1 AND MAXDN = J BAND(J)-IJJ(J)

C

C-----------------------------------------------

CEOF
# APPENDIX C. MC\(^2\)-2 Binary Interface Files. MCC2F1

C****************************************************************************************************************************************************************************************************C
C PREPARED 2/11/75 AT ANL -
C
CF MCC2F1 -
CE ADMINISTRATIVE -
C
C****************************************************************************************************************************************************************************************************C

<table>
<thead>
<tr>
<th>CD</th>
<th>MMAT</th>
<th>NUMBER OF MATERIALS IN THE LIBRARY WITH INELASTIC AND/OR ((N, 2N)) DATA (C.F. DATA SET MCC2F6)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD</td>
<td>MULT</td>
<td>2 FOR IBM MACHINES, 1 OTHERWISE</td>
</tr>
<tr>
<td>CD</td>
<td>NMAT</td>
<td>NUMBER OF MATERIALS IN LIBRARY</td>
</tr>
<tr>
<td>CD</td>
<td>NMAX</td>
<td>MAXIMUM NUMBER OF GROUPS OF INELASTIC OR ((N, 2N)) DATA FOR ANY MATERIAL IN THE LIBRARY (\leq) (\text{MAX} (\text{NINEL}, \text{N2NTH})) WHERE NINEL AND N2NTH ARE THE THRESHOLD GROUP NUMBERS FOR INELASTIC AND ((N, 2N)) SCATTERING RESPECTIVELY</td>
</tr>
<tr>
<td>CD</td>
<td>NRFSMT</td>
<td>NUMBER OF MATERIALS IN LIBRARY WITH RESOLVED RESONANCE PARAMETERS (C.F. DATA SET MCC2F4)</td>
</tr>
<tr>
<td>CD</td>
<td>NUNRMT</td>
<td>NUMBER OF MATERIALS IN LIBRARY WITH UNRESOLVED RESONANCE PARAMETERS (C.F. DATA SET MCC2F3)</td>
</tr>
<tr>
<td>CD</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CR</td>
<td></td>
<td>SPECIFICATIONS (TYPE 1)</td>
</tr>
<tr>
<td>CC</td>
<td></td>
<td>ALWAYS PRESENT</td>
</tr>
<tr>
<td>CL</td>
<td>MMAT, NGROUP, NRESMT, NUNRMT, MSORS, NPASS, NPL, IPTMAX, ETOP, DELTAU, MANY1, MMAT, NMAX</td>
<td></td>
</tr>
<tr>
<td>CD</td>
<td>13</td>
<td></td>
</tr>
<tr>
<td>CD</td>
<td>NGROUP</td>
<td>NUMBER OF ENERGY GROUPS IN LIBRARY</td>
</tr>
<tr>
<td>CD</td>
<td>MSORS</td>
<td>NUMBER OF FISSION SPECTRA SPECIFIED IN LIBRARY (\leq) (\text{MAX} (\text{NINEL}, \text{N2NTH})) WHERE NINEL AND N2NTH ARE THE THRESHOLD GROUP NUMBERS FOR INELASTIC AND ((N, 2N)) SCATTERING RESPECTIVELY</td>
</tr>
<tr>
<td>CD</td>
<td>NPASS</td>
<td>NUMBER OF 'BLOCKS' OF LEGENDRE DATA IN LIBRARY (\leq) (\text{MAX} (\text{NINEL}, \text{N2NTH})) WHERE NINEL AND N2NTH ARE THE THRESHOLD GROUP NUMBERS FOR INELASTIC AND ((N, 2N)) SCATTERING RESPECTIVELY</td>
</tr>
<tr>
<td>CD</td>
<td>NPL</td>
<td>HIGHEST ORDER PERMITTED FOR EXTENDED TRANSPORT APPROXIMATION</td>
</tr>
<tr>
<td>CD</td>
<td>IPTMAX</td>
<td>MAXIMUM NUMBER OF LEGENDRE COMPONENTS PROVIDED IN THE LIBRARY</td>
</tr>
<tr>
<td>CD</td>
<td>ETOP</td>
<td>HIGHEST ENERGY POINT IN LIBRARY, I.E. ENERGY AT TOP OF FIRST ENERGY GROUP</td>
</tr>
</tbody>
</table>
APPENDIX C. MC²-2 Binary Interface Files. MCC2F1 (Contd.)

CD  DELTAU  GROUP LETHARGY WIDTH FOR ALL ENERGY GROUPS IN LIBRARY
CD  MANY1  NUMBER OF ENERGY LEVELS FOR EACH 'BLOCK'
CD C
C-----------------------------------------------
C
CR  MATERIAL NAMES (TYPE 2)
C C
C CL  ALWAYS PRESENT
C CW  MULT*NMAT
C CD  NAME DOUBLE PRECISION (R*8) MATERIAL IDENTIFICATION
C
C-----------------------------------------------
C
CR  MATERIAL IDENTIFICATION (TYPE 3)
C C
C CL  ALWAYS PRESENT
C CW  5*NMAT
C CD  A  MATERIAL MASS/NEUTRON MASS
CD  IZ  ATOMIC NUMBER OF MATERIAL
CD  MAT ENDF/B MATERIAL IDENTIFICATION NUMBER
CD  EFISS MEV/FISSION FOR EACH MATERIAL
CD  ECAPT MEV/CAPTURE FOR EACH MATERIAL WHERE CAPTURE
CD  REFERENCES TO NON-FISSION ABSORPTION
C
C-----------------------------------------------
C
CR  RESONANCE CONTROL INFORMATION (TYPE 4)
C C
C CL  PRESENT IF NRESMT.GT.0 OR IF NUNFMT.GT.0
C CL (NRES(I),I=1,NRESMT), (NREC(I),I=1,NRESMT),
CL 1(EMAXR(I),I=1,NRESMT), (EMAXU(I),I=1,NUNFMT),
CL 2(EMINU(I),I=1,NUNFMT)
C
C-----------------------------------------------
APPENDIX C. MC$^2$-2 Binary Interface Files. MCC2F1 (Contd.)

- C
  - CW
  - 3*NRESMT+2*NUNRMT
  - C
  - CD
  - NRES
  - NUMBER OF RESOLVED RESONANCES FOR EACH
  - CD
  - RESOLVED RESONANCE MATERIAL. NRES INCLUDES ALL
  - CD
  - RESONANCES FOR ALL ISOTOPES OF A MULTI-ISOTOPE
  - CD
  - MATERIAL
  - CD
  - NREC
  - NUMBER OF RECORDS FOR EACH RESOLVED RESONANCE
  - CD
  - MATERIAL
  - CD
  - EMAXR
  - ENERGY OF THE HIGHEST RESOLVED RESONANCE
  - CD
  - FOR EACH MATERIAL
  - CD
  - EMAXU
  - ENERGY OF THE HIGHEST POINT AT WHICH
  - CD
  - UNRESOLVED RESONANCE CALCULATIONS ARE
  - CD
  - PERFORMED, FOR EACH MATERIAL
  - CD
  - EMINU
  - ENERGY OF THE LOWEST POINT AT WHICH UNRESOLVED
  - CD
  - RESONANCE CALCULATIONS ARE PERFORMED,
  - CD
  - FOR EACH MATERIAL
  - C
  - CN
  - THE INFORMATION IN THIS RECORD REFERS TO THE
  - CN
  - STRUCTURE OF DATA SETS MCC2F3 AND MCC2F4
  - C
  - C

--

CR
INELASTIC AND N2N DISTRIBUTIONS CONTROL INFORMATION
CR
(TYPE 5)
C
CC
PRESENT IF MMAT.GT.0
C
CL
(NAME(I), I=1,MMAT), (NINEL(I), I=1,MMAT), (N2NTH(I), I=1,MMAT),
CL
1(NLEVLS(I), I=1,MMAT), (N2NLEV(I), I=1,MMAT), (MAX1(I), I=1,MMAT),
CL
2(MAX2(I), I=1,MMAT), (MAX3(I), I=1,MMAT), (MAX4(I), I=1,MMAT),
CL
3(NSINK1(I), I=1,MMAT), (NSINK2(I), I=1,MMAT),
CL
4(NUMREC(I), I=1,NMAX), MAXREC
C
C
10*MMAT+MULT*MMAT+1+NMAX
C
CD
NAME
DOUBLE PRECISION (R*8) MATERIAL IDENTIFICATION
CD
NINEL
THRESHOLD GROUP NUMBER FOR INELASTIC
CD
SCATTERING (=0 IF NO INELASTIC SCATTERING)
CD
N2NTH
THRESHOLD GROUP NUMBER FOR (N,2N)
CD
SCATTERING (=0 IF NO (N,2N) SCATTERING)
CD
NLEVLS
NUMBER OF DISCRETE INELASTIC SCATTERING
CD
LEVELS FOR EACH MATERIAL
CD
N2NLEV
NUMBER OF DISCRETE (N,2N) SCATTERING
CD
LEVELS FOR EACH MATERIAL
CD
MAX1
MAXIMUM NUMBER OF INELASTIC EVAPORATION
CD
SPECTRA FOR EACH MATERIAL
CD
MAX2
MAXIMUM NUMBER OF TABULATED INELASTIC
APPENDIX C. MC²-2 Binary Interface Files. MCC2FL (Contd.)

CD DISTRIBUTIONS FOR EACH MATERIAL
CD MAX2.EQ. ZERO OR ONE
CD MAX3 MAXIMUM NUMBER OF (N,2N) EVAPORATION SPECTRA FOR EACH MATERIAL
CD MAX4 MAXIMUM NUMBER OF TABULATED (N,2N) DISTRIBUTIONS FOR EACH MATERIAL
CD MAX4.EQ. ZERO OR ONE
CD NSINK1 NUMBER OF ENERGIES PROVIDED IN TABULATED INELASTIC DISTRIBUTIONS FOR EACH MATERIAL
CD IF MAX2.EQ.0 THEN NSINK1.EQ.0
CD NSINK2 NUMBER OF ENERGIES PROVIDED IN TABULATED (N,2N) DISTRIBUTIONS FOR EACH MATERIAL
CD IF MAX4.EQ.0 THEN NSINK2.EQ.0
CD MAXREC MAXIMUM RECORD LENGTH (WORDS) IN FILE MCC2F6
CD FOR ANY RECORD TYPE
CD NUMREC NUMBER OF RECORDS OF INELASTIC AND (N,2N) DATA FOR EACH GROUP. EQUAL TO 2 OR 3
CD FOR EACH GROUP
CD THE INFORMATION IN THIS RECORD REFERS TO
CD THE STRUCTURE OF DATA SET MCC2F6

C-----------------------------------------------------------------------

CP HARD SPHERE POTENTIAL SCATTERING CROSS SECTIONS (TYPE 6)
CP ALWAYS PRESENT
CP (SIGP(I), I=1,NMAT)
CW NMAT
CD SIGP HARD SPHERE POTENTIAL SCATTERING CROSS SECTIONS
CP THE SIGP ARE THE ENERGY INDEPENDENT VALUES
CP OBTAINED FROM THE NUCLEAR RADIUS USING
CP 4*PI*(RADIUS)**2
C
C-----------------------------------------------------------------------

CEOF
APPENDIX C. MC²-2 Binary Interface Files. MCC2F2

--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------

C** Real W Coarse (Type 1)

C Always Present

C

C

((WRC(I,J), I=1,41), J=1,27)

C 1107

C

C

WRC

REAL PART OF W(X,Y) TABULATED AT INCREMENTS OF

0.1 FOR -0.1.LE.X.LE.3.9 AND 0.4.LE.Y.LE.3.0

C

C--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------

C Imaginary W Coarse (Type 2)

C Always Present

C

C

((WIC(I,J), I=1,41), J=1,27)

C 1107

C

C

WIC

IMAGINARY PART OF W(X,Y) TABULATED AT

INCREMENTS OF 0.1 FOR -0.1.LE.X.LE.3.9 AND

0.4.LE.Y.LE.3.0

C

C--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------

C Real W Fine (Type 3)

C Always Present

C

C

((WRF(I,J), I=1,41), J=1,27)

C 1107

C
APPENDIX C. MC2-2 Binary Interface Files. MCC2F2 (Contd.)

CD       WRFF  REAL PART OF W(X,Y) TABULATED AT INCREMENTS
CD       OF 0.1 FOR -0.1.LE.X.LE.3.9 AND AT INCREMENTS
CD       OF 0.02 FOR -0.02.LE.Y.LE.0.5
C

CD       WIF  IMAGINARY PART OF W(X,Y) TABULATED AT
CD       INCREMENTS OF 0.1 FOR -0.1.LE.X.LE.3.9 AND
CD       AT INCREMENTS OF 0.02 FOR -0.02.LE.Y.LE.0.5
C

CD       E3  EXPONENTIAL INTEGRAL, E3(X), TABULATED AT
CD       INCREMENTS OF 0.01 FOR 0.0.LE.X.LE.10.0
C

CD       E      EXPONENTIAL FUNCTION (TYPE 6)
CD       ALWAYX PRESEN
C
CD       (EXPON(I),I=1,K1)
C
CD       2*NGROUP-1
C
CD       K1=2*NGROUP-1 WHERE NGROUP IS THE NUMBER OF LIBRARY
CD       ENERGY GROUPS AS SPECIFIED IN THE ADMINISTRATIVE FILE
C
CD       MCC2F1
APPENDIX C. MC²–2 Binary Interface Files. MCC2F2 (Contd.)

CD EXPO N
EXPON(I) = \( (1. + (1./C)^2 \times (\text{NGROUP}-I)) \times \exp(- (1./C)^2 \times (\text{NGROUP}-I)) \)
WHERE
C = \exp(-\text{DELTADU}) AND \text{DELTADU} IS THE LIBRARY GROUP LETHARGY WIDTH AS SPECIFIED IN THE ADMINISTRATIVE FILE MCC2F1

C

CR FIRST FLIGHT TRANSMISSION PROBABILITIES (TYPE 7)
ALWAYS PRESENT

CL \((T1(I, J), I = 1, 181), J = 1, 26), ((T2(I, J), I = 1, 181), J = 1, 51)\)

CV 13937

CD \(T1(I, J)\)
TRANSMISSION PROBABILITY, INNER TO OUTER SURFACE FOR ANNULAR REGION, FOR I-TH VALUE OF Z AND J-TH VALUE OF X, WHERE THE X INCREMENT IS 0.04

CD \(T2(I, J)\)
TRANSMISSION PROBABILITY, OUTER TO OUTER SURFACE FOR ANNULAR REGION, FOR I-TH VALUE OF Z AND J-TH VALUE OF X, WHERE THE X INCREMENT IS 0.02

Z = TOTAL CROSS SECTION * (OUTER RADIUS–INNER RADIUS), AND
X = (INNER RADIUS)/(OUTER RADIUS).
X TAKES ON VALUES BETWEEN 0.0 AND 1.0

<table>
<thead>
<tr>
<th>RANGE OF Z</th>
<th>Z INCREMENT</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0 TO 0.4</td>
<td>0.01</td>
</tr>
<tr>
<td>0.4 TO 1.0</td>
<td>0.02</td>
</tr>
<tr>
<td>1.0 TO 2.6</td>
<td>0.04</td>
</tr>
<tr>
<td>2.6 TO 5.0</td>
<td>0.06</td>
</tr>
<tr>
<td>5.0 TO 8.0</td>
<td>0.10</td>
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</tbody>
</table>

CR EXPONENTIAL INTEGRALS AND FUNCTIONS (TYPE 8)
ALWAYS PRESENT
APPENDIX C. MC²-2 Binary Interface Files. MCC2F2 (Contd.)

<table>
<thead>
<tr>
<th>CL</th>
<th>(EXPY(I), I=1,1023), (EXPM(I), I=1,1022), (E3(I), I=1,331),</th>
</tr>
</thead>
<tbody>
<tr>
<td>CL</td>
<td>1(E4(I), I=1,331)</td>
</tr>
<tr>
<td>C</td>
<td></td>
</tr>
<tr>
<td>C#</td>
<td>2707</td>
</tr>
<tr>
<td>C</td>
<td></td>
</tr>
<tr>
<td>CD</td>
<td>E3 EXPONENTIAL INTEGRAL, E3(X), TABULATED AT</td>
</tr>
<tr>
<td>CD</td>
<td>0 (0.01) 2 (0.02) 4 (0.08) 6.4.</td>
</tr>
<tr>
<td>CD</td>
<td>E4 EXPONENTIAL INTEGRAL, E4(X), TABULATED AT</td>
</tr>
<tr>
<td>CD</td>
<td>0 (0.01) 2 (0.02) 4 (0.08) 6.4.</td>
</tr>
<tr>
<td>CD</td>
<td>EXPY ORDINATES Y(I) FOR EXP(-X) = Y(I) - M(I) * X</td>
</tr>
<tr>
<td>CD</td>
<td>TABULATED FOR 0.0.LE.X.LE.18.0 WITH TABULAR</td>
</tr>
<tr>
<td>CD</td>
<td>INTERVAL 18.0/1022.</td>
</tr>
<tr>
<td>CD</td>
<td>EXPM SLOPES M(I) FOR EXP(-X) = Y(I) - M(I) * X</td>
</tr>
<tr>
<td>CD</td>
<td>TABULATED FOR 0.0.LE.Y.LE.18.0 WITH TABULAR</td>
</tr>
<tr>
<td>CD</td>
<td>INTERVAL 18.0/1022.</td>
</tr>
</tbody>
</table>

CEOF
APPENDIX C. MC²-2 Binary Interface Files. MCC2F3

C******************************************************************************C
C PREPARED 2/11/75 AT ANL
C
CF MCC2F3
CE UNRESOLVED RESONANCE DATA
C
C******************************************************************************C

CD JST  NUMBER OF CHANNEL SPIN STATES ASSOCIATED WITH
CD A PARTICULAR ANGULAR MOMENTUM STATE IN
CD UNRESOLVED RESONANCE CALCULATION
CD LST  NUMBER OF ANGULAR MOMENTUM STATES CONSIDERED
CD FOR A GIVEN ISOTOPE IN UNRESOLVED CALCULATION
CD MULT 2 FOR IBM MACHINES, 1 OTHERWISE
CD NISO NUMBER OF ISOTOPES IN MATERIAL
CD NPT  NUMBER OF ENERGIES AT WHICH UNRESOLVED
CD CALCULATION IS DONE
CD NUNRMT NUMBER OF MATERIALS WITH UNRESOLVED RESONANCE
CD PARAMETERS AS SPECIFIED IN THE ADMINISTRATIVE
CD FILE MCC2F1

C-------------------------------------
CS FILE STRUCTURE
CS
CS RECORD TYPE
CS -------------------------------
CS UNRESOLVED RESONANCE MATERIAL NAMES
CS ALWAYS
CS MATERIAL SPECIFICATIONS
CS ALWAYS
CS ******* (REPEAT FOR ALL MATERIALS WITH
CS * UNRESOLVED RESONANCE PARAMETERS)
CS * ISOTOPE CONTROL
CS ALWAYS
CS ******* (REPEAT FOR ALL ISOTOPES)
CS * * UNRESOLVED SPIN STATE AND
CS * * ENERGY DATA
CS * * STATISTICAL UNRESOLVED RESONANCE
CS * * INFORMATION
CS ******
C
C-------------------------------------
CR UNRESOLVED RESONANCE MATERIAL NAMES (TYPE 1)
C
CC ALWAYS PRESENT
C
CL (NAME(I), I=1, NUNRMT)
### APPENDIX C. MC²-2 Binary Interface Files. MCC2F3 (Contd.)

<table>
<thead>
<tr>
<th>C</th>
<th>MULT*NUNRMT</th>
<th>DOUBLE PRECISION (R*8) MATERIAL IDENTIFICATION</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>C</th>
<th>MATERIAL SPECIFICATIONS (TYPE 2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>ALWAYS PRESENT</td>
</tr>
<tr>
<td>C</td>
<td>(NISO(I), I=1,NUNRMT), (IFI(I), I=1,NUNRMT),</td>
</tr>
<tr>
<td>C</td>
<td>(ISK(I), I=1,NUNRMT), LSTMAX, JSTMAX, NPTMAX</td>
</tr>
<tr>
<td>C</td>
<td>3*NUNRMT+3</td>
</tr>
<tr>
<td>C</td>
<td>IFI</td>
</tr>
<tr>
<td>C</td>
<td>PESSILE ISOTOPE INDEX</td>
</tr>
<tr>
<td>C</td>
<td>IFI=0 FOR NON-FISSILE MATERIAL</td>
</tr>
<tr>
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<td>IFI=1 FOR FISSILE MATERIAL</td>
</tr>
<tr>
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<td>ISK</td>
</tr>
<tr>
<td>C</td>
<td>NUMBER OF LOGICAL RECORDS OF UNRESOLVED</td>
</tr>
<tr>
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<td>RESONANCE DATA FOR EACH MATERIAL</td>
</tr>
<tr>
<td>C</td>
<td>LSTMAX</td>
</tr>
<tr>
<td>C</td>
<td>MAXIMUM VALUE OF LST OVER ALL MATERIALS IN FILE</td>
</tr>
<tr>
<td>C</td>
<td>JSTMAX</td>
</tr>
<tr>
<td>C</td>
<td>MAXIMUM VALUE OF JST OVER ALL MATERIALS IN FILE</td>
</tr>
<tr>
<td>C</td>
<td>NPTMAX</td>
</tr>
<tr>
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<td>MAXIMUM VALUE OF NPT OVER ALL MATERIALS IN FILE</td>
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### ISOTOPE CONTROL DATA (TYPE 3)

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<tbody>
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</tr>
<tr>
<td>C</td>
<td>(LST(I), I=1,NISO), (NPT(I), I=1,NISO), (RPS(I), I=1,NISO)</td>
</tr>
<tr>
<td>C</td>
<td>6*NISO</td>
</tr>
<tr>
<td>C</td>
<td>ABUN</td>
</tr>
<tr>
<td>C</td>
<td>ABUNDANCE OF EACH ISOTOPE</td>
</tr>
<tr>
<td>C</td>
<td>A</td>
</tr>
<tr>
<td>C</td>
<td>ISOPTIC MASS/NEUTRON MASS</td>
</tr>
<tr>
<td>C</td>
<td>RPF</td>
</tr>
<tr>
<td>C</td>
<td>RPF=K*R/SQRT(E), K= WAVE NUMBER,</td>
</tr>
<tr>
<td>C</td>
<td>R=CHANNEL RADIUS, E=ENERGY. FOR USE IN</td>
</tr>
<tr>
<td>C</td>
<td>OBTAINING p AND D WAVE PENETRATION FACTOR</td>
</tr>
<tr>
<td>C</td>
<td>RPS</td>
</tr>
<tr>
<td>C</td>
<td>RPS=K*R/SQRT(E), K= WAVE NUMBER,</td>
</tr>
<tr>
<td>C</td>
<td>R=EFFECTIVE SCATTERING RADIUS, E=ENERGY. FOR USE-</td>
</tr>
<tr>
<td>C</td>
<td>IN OBTAINING THE S, P, AND D WAVE PHASE SHIFTS</td>
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APPENDIX C. MC^2-2 Binary Interface Files. MCC2F3 (Contd.)

CUNRESOLVED SPIN STATE AND ENERGY DATA (TYPE 4)
C
CALSAYS Present
C
C(ES(I),I=1,NPT),(DEL(I),I=1,NPT),(JST(I),I=1,LST)
C
C2*NPT+LST
C
ENERGIES AT WHICH UNRESOLVED CALCULATION
IS TO BE DONE, IN EV. AND ORDER OF DECREASING
ENERGY, ES(I).GT.ES(I+1)
C
CDEL
DOPPLER WIDTH/(SQUARE ROOT OF THE TEMPERATURE)
C

CSTASTRICAL UNRESOLVED RESONANCE INFORMATION (TYPE 5)
C
CALSAYS Present
C
C((GA(I,J,L),I=1,NPT),J=1,JST),L=1,LST),
C1((D(T,J,L),I=1,NPT),J=1,JST),L=1,LST),
C2(((GF(I,J,L),I=1,NPT),J=1,JST),L=1,LST),
C3(((SNO(I,J,L),I=1,NPT),J=1,JST),L=1,LST),
C4(((G(J,L),J=1,JST),L=1,LST),((NDFF(J,L),J=1,JST),L=1,LST),
C5((NDPM(J,L),J=1,JST),L=1,LST)
C
C(4*NPT+3)*(JST(1)+JST(2)+...+JST(LST))
C
GANERICAN RADIATION WIDTH, EV.,
CDDOPPER SPACING, EV., FOR EACH ENERGY ES
CDSFN AVERAGE FISSION WIDTH, EV., FOR EACH ENERGY ES
CDS2ZERED NEUTRON WIDTH, EV.,
CDSS FOR EACH ENERGY ES
CDSDFF NUMBER OF DEGREES OF FREEDOM IN FISSION WIDTH
CDSS DISTRIBUTION (1,2,3 OR 4)
CDSS STATISTICAL FACTOR
CDSDPN NUMBER OF DEGREES OF FREEDOM IN NEUTRON WIDTH
CDSS DISTRIBUTION (1 OR 2), NUMBER OF ENTRANCE
CDSS CHANNELS FOR NEUTRONS IN AN L,J SEQUENCE
C
CEND
APPENDIX C. \( MC^2 \)-2 Binary Interface Files. MCC2F4

CD
*
CD
*
PREPARED 1/13/76 AT ANL
*
CD
*
MCC2F4
*
CD
*
RESOLVED RESONANCE DATA
*

CD
*
************(REPEAT FOR ALL MATERIALS WITH
CD
*
RESOLVED RESONANCE PARAMETERS)
*
CD
*
ISOTYPE CONTROL
*
CD
*
************(REPEAT FOR ALL ISOTOPES)
*
CD
*
RESOLVED RESONANCE ENERGY DATA
*
CD
*
RESOLVED RESONANCE PEAK CROSS
*

CD
*
FILE STRUCTURE
*
CD
*
RECORD TYPE
*
CD
*
PRESENT IF
*
CD
*
RESOLVED RESONANCE MATERIAL NAMES
*
CD
*
ALWAYS
*
CD
*
MATERIAL SPECIFICATIONS
*
CD
*
ALWAYS
*
CD
*
************ (REPEAT FOR ALL MATERIALS WITH
*
CD
*
RESOLVED RESONANCE PARAMETERS)
*
CD
*
ISOTYPE CONTROL
*
CD
*
************ (REPEAT FOR ALL ISOTOPES)
*
CD
*
RESOLVED RESONANCE ENERGY DATA
*
CD
*
RESOLVED RESONANCE PEAK CROSS
*

CD
*
RESOLVED RESONANCE PARAMETER INDEX
CD
*
IWR
CD
*
IWR=1 MATERIAL HAS RESOLVED RESONANCE
CD
*
SINGLE-LEVEL BREIT-WIGNER PARAMETERS
CD
*
IWR=2 MATERIAL HAS MULTI-LEVEL ADLER-ADLER
CD
*
RESOLVED RESONANCE PARAMETERS
CD
*
IWR=3 MATERIAL HAS MULTI-LEVEL BREIT-WIGNER
CD
*
RESOLVED RESONANCE PARAMETERS
CD
*
MULT
CD
*
2 FOR IBM MACHINES, 1 OTHERWISE
CD
*
NTSO
CD
*
NUMBER OF ISOTOPES IN MATERIAL
CD
*
NRSHMT
CD
*
NUMBER OF MATERIALS WITH RESOLVED RESONANCE
CD
*
PARAMETERS AS SPECIFIED IN THE ADMINISTRATIVE
CD
*
FILE MCC2F1
CD
*
NRGYS
CD
*
NUMBER OF RESOLVED RESONANCES FOR AN ISOTOPE
CD
*
PHI
CD
*
S WAVE PHASE SHIFT EQUAL TO K*R. THE NEUTRON
CD
*
WAVE NUMBER K=2.196771E-3*(A/(A+1))*SQUARE
CD
*
ROOT OF RESONANCE ENERGY, A IS THE RATIO OF
CD
*
THE MASS OF THE PARTICULAR ISOTOPE TO THAT OF
CD
*
THE NEUTRON, AND R IS THE EFFECTIVE SCATTERING
CD
*
RADIUS. A AND R ARE SUPPLIED BY ENDF/B

CD
*
G'T, G'F, G'TC
CD
*
RESPECTIVELY, THE ASYMMETRICAL ADLER-ADLER
CD
*
TOTAL, FISSION, AND CAPTURE CROSS SECTION
CD
*
PARAMETERS SUPPLIED BY ENDF/B
CD
*
G'RT, G'RF, G'R'C
CD
*
RESPECTIVELY, THE SYMMETRICAL ADLER-ADLER
CD
*
TOTAL, FISSION, AND CAPTURE CROSS SECTION
CD
*
PARAMETERS SUPPLIED BY ENDF/B
CD
*
IWR
CD
*
RESOLVED RESONANCE PARAMETER INDEX
CD
*
IWR=1 MATERIAL HAS RESOLVED RESONANCE
CD
*
SINGLE-LEVEL BREIT-WIGNER PARAMETERS
CD
*
IWR=2 MATERIAL HAS MULTI-LEVEL ADLER-ADLER
CD
*
RESOLVED RESONANCE PARAMETERS
CD
*
IWR=3 MATERIAL HAS MULTI-LEVEL BREIT-WIGNER
CD
*
RESOLVED RESONANCE PARAMETERS
CD
*
MULT
CD
*
2 FOR IBM MACHINES, 1 OTHERWISE
CD
*
NTSO
CD
*
NUMBER OF ISOTOPES IN MATERIAL
CD
*
NRSHMT
CD
*
NUMBER OF MATERIALS WITH RESOLVED RESONANCE
CD
*
PARAMETERS AS SPECIFIED IN THE ADMINISTRATIVE
CD
*
FILE MCC2F1
CD
*
NRGYS
CD
*
NUMBER OF RESOLVED RESONANCES FOR AN ISOTOPE
CD
*
PHI
CD
*
S WAVE PHASE SHIFT EQUAL TO K*R. THE NEUTRON
CD
*
WAVE NUMBER K=2.196771E-3*(A/(A+1))*SQUARE
CD
*
ROOT OF RESONANCE ENERGY, A IS THE RATIO OF
CD
*
THE MASS OF THE PARTICULAR ISOTOPE TO THAT OF
CD
*
THE NEUTRON, AND R IS THE EFFECTIVE SCATTERING
CD
*
RADIUS. A AND R ARE SUPPLIED BY ENDF/B

CD
*
G'T, G'F, G'TC
CD
*
RESPECTIVELY, THE ASYMMETRICAL ADLER-ADLER
CD
*
TOTAL, FISSION, AND CAPTURE CROSS SECTION
CD
*
PARAMETERS SUPPLIED BY ENDF/B
CD
*
G'RT, G'RF, G'R'C
CD
*
RESPECTIVELY, THE SYMMETRICAL ADLER-ADLER
CD
*
TOTAL, FISSION, AND CAPTURE CROSS SECTION
CD
*
PARAMETERS SUPPLIED BY ENDF/B
CD
*
IWR
CD
*
RESOLVED RESONANCE PARAMETER INDEX
CD
*
IWR=1 MATERIAL HAS RESOLVED RESONANCE
CD
*
SINGLE-LEVEL BREIT-WIGNER PARAMETERS
CD
*
IWR=2 MATERIAL HAS MULTI-LEVEL ADLER-ADLER
CD
*
RESOLVED RESONANCE PARAMETERS
CD
*
IWR=3 MATERIAL HAS MULTI-LEVEL BREIT-WIGNER
APPENDIX C. MC\(^2\)-2 Binary Interface Files. MCC2F4 (Contd.)

CS * * SECTION
CS * * MODIFIED RESONANCE NATURAL TO. IWR.GF.1
CS * * DOPPLER WIDTH
CS * * INTERFERENCE SCATTERING FACTOR IWR.GF.1
CS * * RESOLVED RESONANCE TOTAL AND IWR.EQ.1
CS * * NEUTRON LINE WIDTHS
CS * * RESONANCE RADIATION LINE WIDTH IWR.EQ.1
CS * * RESONANCE FISSION LINE WIDTH IWR.EQ.1
CS * * S-MATRIX TOTAL LINE WIDTH IWR.EQ.2
CS * * SYMMETRIC PARAMETER FOR CAPTURE IWR.EQ.2
CS * * RESONANCE NATURAL TO.
CS * * SYMMETRIC PARAMETER FOR FISSION IWR.EQ.2
CS * * SYMMETRIC PARAMETER FOR TOTAL IWR.EQ.2
CS * * RADLER-ADLER FACTOR FOR J CAPTURE IWR.EQ.2
CS * * INTEGRAL
CS * * ADLER-ADLER FACTOR FOR J FISSION IWR.EQ.2
CS * * INTEGRAL
CS * * BREIT-WIGNER MULTI-LEVEL TOTAL LINE IWR.EQ.3
CS * * RESONANCE RADIATION LINE WIDTH
CS * * BREIT-WIGNER MULTI-LEVEL SYMMETRIC IWR.EQ.3
CS * * PARAMETER FOR CAPTURE REACTION
CS * * BREIT-WIGNER MULTI-LEVEL SYMMETRIC IWR.EQ.3
CS * * PARAMETER FOR FISSION REACTION
CS * * BREIT-WIGNER MULTI-LEVEL SYMMETRIC IWR.EQ.3
CS * * PARAMETER FOR TOTAL REACTION
CS * * BREIT-WIGNER MULTI-LEVEL RELATIVE IWR.EQ.3
CS * * ASYMMETRIC CONTRIBUTION TO CAPTURE IWR.EQ.3
CS * * REACTION
CS * * BREIT-WIGNER MULTI-LEVEL RELATIVE IWR.EQ.3
CS * * ASYMMETRIC CONTRIBUTION TO FISSION IWR.EQ.3
CS * * REACTION
CS ******

RESOLVED RESONANCE MATERIAL NAMES (TYPE 1)

ALWAYS PRESENT

(NAME(I), I=1, NRESMT)

MULT*NRESMT

NAME DOUBLE PRECISION (R*8) MATERIAL IDENTIFICATION
APPENDIX C. MC^2-2 Binary Interface Files. MCC2F4 (Contd.)

C
C MATERIAL SPECIFICATIONS (TYPE 2)
C
C ALWAYS PRESENT
C
C (NISO(I), I=1, NRESMT), (IWR(I), I=1, NRESMT), (EL(I), I=1, NRESMT),
C 1(FU(I), I=1, NRESMT)
C
C 4*NRESMT
C
C EL LOWEST ENERGY FOR WHICH RESONANCE PARAMETERS
C APPLY FOR ANY ISOTOPE OF EACH MATERIAL
C
C FU HIGHEST ENERGY FOR WHICH RESONANCE PARAMETERS
C APPLY FOR ANY ISOTOPE OF EACH MATERIAL
C
C
C ISOTOPE CONTROL DATA (TYPE 3)
C
C ALWAYS PRESENT
C
C (ABUN(I), I=1, NISO), (NRGYS(I), I=1, NISO)
C
C 2*NISO
C
C ABUN ABUNDANCE OF EACH ISOTOPE
C
C
C RESOLVED RESONANCE ENERGY DATA (TYPE 4)
C
C PRESENT IF IWR.GE.1
C
C (EN(J), J=1, NRGYS)
C
C NRGYS
C
C EN RESONANCE ENERGY EN(J).GT.FN(J+1)
C
C
C RESOLVED RESONANCE PEAK CROSS SECTION (TYPE 5)
APPENDIX C. MC²-2 Binary Interface Files. MCC2F4 (Contd.)

PRESENT IF IWR.GE.1

SIGO(J), J=1,NRGYS

NRGYS

CROSS SECTION AT RESONANCE

FOR IWR.EQ.1, SIGO IS 4*PI*G*LAMBDA-BAR SQUARED * ((GAMT-GAMGAM-GAP)/GAMT) *((A+1)/A) SQUARED.
(SEE RECORD TYPES 8, 9, AND 10)

FOR IWR.EQ.2, SIGO IS 4*PI*LAMBDA-BAR SQUARED* ((A+1)/A) SQUARED*ABS(GT)/(2*GAMS). (SEE RECORD TYPES 11 AND 14)

FOR IWR.EQ.3, SIGO IS THE VALUE COMPUTED FOR IWR.EQ.1 MULTIPLIED BY GT. (SEE RECORD TYPE 20)

RATIO OF RESONANCE NATURAL TO DOPPLER WIDTH (TYPE 6)

PRESENT IF IWR.GE.1

THETAP(J), J=1,NRGYS

NRGYS

THETAP

RATIO OF NATURAL WIDTH TO DOPPLER WIDTH *

SQRT(TEMPERATURE) IF IWR.EQ.1 OR IWR.EQ.3.

RATIO OF S-MATRIX TOTAL LINE WIDTH TO DOPPLER WIDTH*SQRT(TEMPERATURE) IF IWR.EQ.2

INTERFERENCE SCATTERING FACTOR (TYPE 7)

PRESENT IF IWR.GE.1

AFAC(J), J=1,NRGYS

NRGYS
### APPENDIX C. MC2-2 Binary Interface Files. MCC2F4 (Contd.)

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<tr>
<th>CD</th>
<th>AFAC</th>
<th>FACTOR TO MULTIPLY CHI TO OBTAIN INTERFERENCE SCATTERING</th>
</tr>
</thead>
<tbody>
<tr>
<td>CN</td>
<td></td>
<td>FOR IWR.EQ.1, AFAC IS THE SQUARE ROOT OF (G* ((GAMT-GAMGAM-GAF)/GAMT)* ATOM POTENTIAL SCATTERING CROSS SECTION /SIG0) G, THE STATISTICAL FACTOR, IS (2J+1)/(4J+2) WHERE J IS THE SPIN OF THE COMPOUND NUCLEUS RESONANCE AND I IS THE TARGET NUCLEUS SPIN. (SEE RECORD TYPES 5, 8, 9, AND 10) AFAC IS SET TO 0 FOR P AND D WAVE RESONANCES. FOR IWR.EQ.2, AFAC IS -0.5*(GRT<em>COS(2</em>PHI) - GRT<em>SIN(2</em>PHI))/(GRT<em>COS(2</em>PHI)+GRT<em>SIN(2</em>PHI)) - FOR IWR.EQ.3, AFAC IS THE VALUE COMPUTED FOR IWR.EQ.1 PLUS THE ASYMMETRIC LEVEL-LEVEL INTERFERENCE CONTRIBUTION, ALL DIVIDED BY GT. (SEE RECORD TYPE 20) AFAC IS SET TO 0 FOR P AND D WAVE RESONANCES.</td>
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<table>
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<tr>
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<td>CL</td>
<td>(GAMT(J), J=1, NRGYS), (GAMN(J), J=1, NRGYS)</td>
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<tr>
<td>CW</td>
<td>2*NRGYS</td>
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<tr>
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<td>GAMT</td>
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<td>GAMN</td>
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<th>RESONANCE RADIATION LINE WIDTH (TYPE 9)</th>
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<tr>
<td>CC</td>
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</tr>
<tr>
<td>CL</td>
<td>(GAMGAM(J), J=1, NRGYS)</td>
</tr>
<tr>
<td>CW</td>
<td>NRGYS</td>
</tr>
<tr>
<td>CD</td>
<td>GAMGAM</td>
</tr>
</tbody>
</table>

---
APPENDIX C. MC²-2 Binary Interface Files. MCC2F4 (Contd.)

-----------------------------------------------------------------------
RFSONANCE FISSION LINE WIDTH (TYPE 10)
-----------------------------------------------------------------------
PRESENT IF IWR.EQ.1
(GAP(J), J=1, NRGYS)
NRGYS
GAP
RESOLVED RESONANCE FISSION LINE WIDTH

-----------------------------------------------------------------------
S-MATRIX TOTAL LINE WIDTH (TYPE 11)
-----------------------------------------------------------------------
PRESENT IF IWR.EQ.2
(GAMS(J), J=1, NRGYS)
NRGYS
GAMS
S-MATRIX TOTAL LINE WIDTH FOR ADLER-ADLER FORMULATION (.EQ.2.0*NU)

-----------------------------------------------------------------------
SYMmetric PARAMETER FOR CAPTURE REACTION (TYPE 12)
-----------------------------------------------------------------------
PRESENT IF IWR.EQ.2
(GC(J), J=1, NRGYS)
NRGYS
GC
SYMmetric PARAMETER FOR CAPTURE REACTION
GC = (GRC*COS(2*PHI) + GIC*SIN(2*PHI)) * SQUARE ROOT OF THE RESONANCE ENERGY

-----------------------------------------------------------------------
APPENDIX C. MC²-2 Binary Interface Files. MCC2F4 (Contd.)

CR
SYMMETRIC PARAMETER FOR FISSION REACTION (TYPE 13)

CC PRESENT IF IWR.EQ.2

CL (GF(J), J=1, NRGYS)

CW NRGYS

CD GF

SYMmetric PARAMETER FOR FISSION REACTION

CN GF = (GRF*COS(2*PHI) + GIF*SIN(2*PHI)) * SQUARE
ROOT OF THE RESONANCE ENERGY

CR SYMMETRIC PARAMETER FOR TOTAL REACTION (TYPE 14)

CC PRESENT IF IWR.EQ.2

CL (GT(J), J=1, NRGYS)

CW NRGYS

CD GT

SYMmetric PARAMETER FOR TOTAL REACTION

CN GT = (GRT*COS(2*PHI) + GIT*SIN(2*PHI)) * SQUARE
ROOT OF THE RESONANCE ENERGY

CR ADLER-ADLER FACTOR FOR J CAPTURE INTEGRAL (TYPE 15)

CC PRESENT IF IWR.EQ.2

CL (BC(J), J=1, NRGYS)

CW NRGYS

CD BC

-0.5*(GIC*COS(2*PHI) - GRC*SIN(2*PHI)) * SQUARE
ROOT OF THE RESONANCE ENERGY/GC, WHERE GC IS
DEFINED IN RECORD TYPE 12
APPENDIX C. MC²-2 Binary Interface Files. MCC2F4 (Contd.)

CR
ADLER-ADLER FACTOR FOR J FISSION INTEGRAL (TYPE 16)
 CC PRESENT IF IWR.EQ.2
 C CL (BP(J), J=1,NRGYS)
 C CW NRGYS
 CD BF
   -0.5*(GIF*Cos(2*PHI)-GRF*Sin(2*PHI))*SQUARE
   ROOT OF THE RESONANCE ENERG/MF, WHERE MF IS
   DEFINED IN RECORD TYPE 13
 C CN BF IS SET TO ZERO FOR UNFISSIONABLE
 CN MULTI-LEVEL MATERIALS
 C

C——

CR
BREIT-WIGNER MULTI-LEVEL TOTAL LINE WIDTH (TYPE 17)
 CC PRESENT IF IWR.EQ.3
 C CL (GAMS(J), J=1,NRGYS)
 C CW NRGYS
 CD GAMS BREIT-WIGNER MULTI-LEVEL TOTAL LINE WIDTH
 C

C——

CR
BREIT-WIGNER MULTI-LEVEL SYMMETRIC PARAMETER FOR
 CR CAPTURE REACTION (TYPE 18)
 CC PRESENT IF IWR.EQ.3
 C CL (GC(J), J=1,NRGYS)
 C CW NRGYS
 CD GC BREIT-WIGNER MULTI-LEVEL SYMMETRIC PARAMETER
 CD FOR CAPTURE REACTION, THE RATIO OF GAMGAM TO
 CD GAMS. (SEE RECORD TYPE 9 AND 17)
 C
## APPENDIX C. $\text{MC}^2-2$ Binary Interface Files. MCC2F4 (Contd.)

<table>
<thead>
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<th>CR</th>
<th>BREIT-WIGNER MULTI-LEVEL SYMMETRIC PARAMETER FOR</th>
</tr>
</thead>
<tbody>
<tr>
<td>CR</td>
<td>FISSION REACTION (TYPE 19)</td>
</tr>
<tr>
<td>C</td>
<td>PRESENT IF IWR.EQ.3</td>
</tr>
<tr>
<td>CL</td>
<td>$(GP(J), J=1, NRGYS)$</td>
</tr>
<tr>
<td>CW</td>
<td>NRGYS</td>
</tr>
<tr>
<td>CD</td>
<td>GP</td>
</tr>
<tr>
<td></td>
<td>BREIT-WIGNER MULTI-LEVEL SYMMETRIC PARAMETER</td>
</tr>
<tr>
<td></td>
<td>FOR FISSION REACTION, THE RATIO OF GAF TO GAMS.</td>
</tr>
<tr>
<td></td>
<td>(SEE RECORD TYPE 10 AND 17)</td>
</tr>
<tr>
<td>C</td>
<td></td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>CR</th>
<th>BREIT-WIGNER MULTI-LEVEL SYMMETRIC PARAMETER FOR</th>
</tr>
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<tbody>
<tr>
<td>CR</td>
<td>TOTAL REACTION (TYPE 20)</td>
</tr>
<tr>
<td>C</td>
<td>PRESENT IF IWR.EQ.3</td>
</tr>
<tr>
<td>CL</td>
<td>$(GT(J), J=1, NRGYS)$</td>
</tr>
<tr>
<td>CW</td>
<td>NRGYS</td>
</tr>
<tr>
<td>CD</td>
<td>GT</td>
</tr>
<tr>
<td></td>
<td>BREIT-WIGNER MULTI-LEVEL SYMMETRIC PARAMETER</td>
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<tr>
<td></td>
<td>FOR TOTAL REACTION, 1 PLUS THE SYMMETRIC</td>
</tr>
<tr>
<td></td>
<td>LEVEL-LEVEL INTERFERENCE CONTRIBUTION</td>
</tr>
<tr>
<td>C</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>CR</th>
<th>BREIT-WIGNER MULTI-LEVEL RELATIVE ASYMMETRIC CONTRIBUTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>CR</td>
<td>TO CAPTURE REACTION (TYPE 21)</td>
</tr>
<tr>
<td>C</td>
<td>PRESENT IF IWR.EQ.3</td>
</tr>
<tr>
<td>CL</td>
<td>$(BC(J), J=1, NRGYS)$</td>
</tr>
<tr>
<td>CW</td>
<td>NRGYS</td>
</tr>
<tr>
<td>CD</td>
<td>BC</td>
</tr>
<tr>
<td></td>
<td>BREIT-WIGNER MULTI-LEVEL RELATIVE ASYMMETRIC CONTRIBUTION</td>
</tr>
<tr>
<td></td>
<td>CONTRIBUTION TO CAPTURE REACTION</td>
</tr>
<tr>
<td>CN</td>
<td>NOTE THAT BC IS IDENTICALLY 0.0 FOR BREIT-</td>
</tr>
<tr>
<td>CN</td>
<td>WIGNER MULTI-LEVEL FORMALISM</td>
</tr>
</tbody>
</table>
APPENDIX C. MC²-2 Binary Interface Files. MCC2F4 (Contd.)

C---------------
CR             BREIT-WIGNER MULTI-LEVEL RELATIVE ASYMMETRIC CONTRIBUTION
CC TO FISSION REACTION (TYPE 22)
C
CC            PRESENT IF IFR.EQ.3
C
CL   (BF (J), J=1,NRGYS)
C
CW   NRGYS
C
CD    BF             BREIT-WIGNER MULTI-LEVEL RELATIVE ASYMMETRIC
CD CONTRIBUTION TO FISSION REACTION
C
CN               NOTE THAT BF IS IDENTICALLY 0.0 FOR BREIT-
CN WIGNER MULTI-LEVEL FORMALISM
C
C---------------

CEOF
-315-

APPENDIX C. MC^2-2 Binary Interface Files. MCC2F5

C**************************************************************
C
C PREPARED 2/11/75 AT ANL
C
C MCC2F5
C SMOOTH (TABULATED) NON-RESONANT DATA
C
C**************************************************************

CD MULT 2 FOR IBM MACHINES, 1 OTHERWISE
CD NREAC NREAC=NUMBER OF REACTION TYPES FOR A
       GIVEN MATERIAL

C**************************************************************

CS FILE STRUCTURE
CS
CS RECORD TYPE
       PRPSNT IP

CS ****** (REPEAT FOR ALL MATERIALS)
CS  * MATERIAL NAME ALWAYS
CS  * SPECIFICATIONS ALWAYS
CS  * ****** (REPEAT FOR NREAC REACTION TYPES)
CS  * * CROSS SECTIONS NREAC.GT.0
CS  ******

C**************************************************************

CR MATERIAL NAME (TYPE 1)
C
CC ALWAYS PRESENT
C
CL NAME
C
CW MULT*1
C
CD NAME DOUBLE PRECISION (R*8) MATERIAL IDENTIFICATION

C**************************************************************

CR SPECIFICATIONS (TYPE 2)
C
CC ALWAYS PRESENT
C
L NREAC, NEL, NF, NSAM, NP, ND, NH3, NHE3, NALPHA, NTOT, A0, A1, A2, A3

C**************************************************************
APPENDIX C. MC²-2 Binary Interface Files. MCC2F5 (Contd.)

<table>
<thead>
<tr>
<th>CD</th>
<th>NC</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD</td>
<td>14</td>
<td>FLAG FOR ELASTIC CROSS SECTIONS</td>
</tr>
<tr>
<td>CD</td>
<td>NEL</td>
<td>FLAG FOR FISSION CROSS SECTIONS</td>
</tr>
<tr>
<td>CD</td>
<td>NF</td>
<td>FLAG FOR (N, GAMMA) CROSS SECTIONS</td>
</tr>
<tr>
<td>CD</td>
<td>NP</td>
<td>FLAG FOR (N, P) CROSS SECTIONS</td>
</tr>
<tr>
<td>CD</td>
<td>ND</td>
<td>FLAG FOR (N, D) CROSS SECTIONS</td>
</tr>
<tr>
<td>CD</td>
<td>NH3</td>
<td>FLAG FOR (N, H3) CROSS SECTIONS</td>
</tr>
<tr>
<td>CD</td>
<td>NZ+3</td>
<td>FLAG FOR (N, HE3) CROSS SECTIONS</td>
</tr>
<tr>
<td>CD</td>
<td>NAT</td>
<td>FLAG FOR (N, ALPHA) CROSS SECTIONS</td>
</tr>
<tr>
<td>CD</td>
<td>NTO</td>
<td>FLAG FOR TOTAL CROSS SECTIONS</td>
</tr>
</tbody>
</table>

For each of the above reaction types the flags are zero if no cross section data are given and equal to the highest energy group number (lowest energy) for which cross section data are given.

CD | AO, A1, A2, A3 | COEFFICIENTS FOR CALCULATION OF \( \nu(E) \), THE NUMBER OF NEUTRONS PER FISSION. IF THE ISOTOPE IS NOT FISSIONABLE, THEN THE COEFFICIENTS WILL BE SET TO ZERO.

CROSS SECTIONS (TYPE 3)

Present if NREA.C.GT.0

(\( \text{XSIG}(J), J=1, \text{NLAST} \))

CROSS SECTION ASSOCIATED WITH ULTRAFINE GROUP J FOR A GIVEN REACTION TYPE.

FLAG FOR REACTION TYPE IN QUESTION. (THAT IS, NEL, NF, ETC.)

NUMBER OF ENERGY GROUPS IN LIBRARY.

The cross section records for the different reaction types which are present will be in the following order: ELASTIC, FISSION, (N, GAMMA), (N, P), (N, D), (N, H3), (N, HE3), (N, ALPHA), and TOTAL.

The total cross section for ultra-fine group J = ELASTIC SCATTERING + INELASTIC SCATTERING + (N, 2N) SCATTERING + FISSION + (N, GAMMA) +
APPENDIX C. MC²-2 Binary Interface Files. MCC2F5 (Contd.)

```
(N,P) + (N,D) + (N,H3) + (N,HE3) + (N,ALPHA). THE
ELASTIC SCATTERING=SMOOTH (TABULATED) ELASTIC
SCATTERING+UNRESOLVED RESONANCE SCATTERING+
RESOLVED RESONANCE SCATTERING. THE ELASTIC
SCATTERING DOES NOT INCLUDE THE UNRESOLVED
RESONANCE SCATTERING AND RESOLVED RESONANCE
SCATTERING CONTRIBUTIONS FOR MATERIALS WITH
'HIGH' MASSES. A 'HEAVY' MASS MATERIAL IS
DESIGNATED BY THE USER. ELASTIC SCATTERING
EXPLICITLY INCLUDES THE POTENTIAL SCATTERING
CROSS SECTION

ONE CROSS SECTION RECORD IS PRESENT FOR EACH
NON-ZERO FLAG
```
APPENDIX C. MC²-2 Binary Interface Files. MCC2F6

C*****************************************************************************C
C PREPARED 10/27/75 AT ANL
C
CF MCC2F6
CE INELASTIC AND N2N DISTRIBUTIONS
C
C*****************************************************************************C
CD    MMAT NUMBER OF MATERIALS IN THE LIBRARY WITH
CD INELASTIC AND/OR (N,2N) DATA AS SPECIFIED IN
CD THE ADMINISTRATIVE FILE MCC2F1
CD    MMAT1 NUMBER OF MATERIALS THAT HAVE INELASTIC AND/OR
CD (N,2N) DATA FOR THE ENERGY GROUP BEING
CD PROCESSED. IF THE VALUE OF NINEL OR N2NTH
CD FOR A MATERIAL IS LESS THAN THE ENERGY GROUP
CD NUMBER BEING PROCESSED, THEN NO DATA ARE
CD PRESENT FOR THIS MATERIAL. THE CONTROL
CD INFORMATION NINEL AND N2NTH ARE SPECIFIED IN
CD RECORD TYPE 5 OF MCC2F1
CD    NEND1 NUMBER OF LAST SINK ENERGY POINT (EIN) FOR
CD WHICH THE TABULATED INELASTIC PROBABILITY
CD IS NON-ZERO FOR THE SOURCE GROUP IN QUESTION
CD    NEND2 NUMBER OF LAST SINK ENERGY POINT (EN2N) FOR
CD WHICH THE TABULATED (N,2N) PROBABILITY
CD IS NON-ZERO FOR THE SOURCE GROUP IN QUESTION
CD    NINEVP NUMBER OF TABULATED INELASTIC EVAPORATION SPECTRA
CD FOR ENERGY GROUP IN QUESTION
CD    NINTAB NUMBER OF TABULATED INELASTIC DISTRIBUTIONS
CD FOR ENERGY GROUP IN QUESTION
CD NINTAB.EQ.ZERO OR ONE
CD    NLVS NUMBER OF DISCRETE INELASTIC SCATTERING LEVELS
CD FOR EACH MATERIAL FOR THE ENERGY GROUP IN
CD QUESTION
CD    NMAX MAXIMUM NUMBER OF GROUPS OF INELASTIC OR
CD (N,2N) DATA FOR ANY MATERIAL IN THE LIBRARY
CD (.EQ.MAX(NINEL,N2NTH) AS SPECIFIED IN THE
CD ADMINISTRATIVE FILE MCC2F1)
CD    NSINK1 NUMBER OF ENERGIES PROVIDED IN TABULATED
CD INELASTIC DISTRIBUTIONS FOR EACH MATERIAL
CD AS SPECIFIED IN THE ADMINISTRATIVE FILE MCC2F1
CD    NSINK2 NUMBER OF ENERGIES PROVIDED IN TABULATED
CD (N,2N) DISTRIBUTIONS FOR EACH MATERIAL
CD AS SPECIFIED IN THE ADMINISTRATIVE FILE MCC2F1
CD    NSTRT1 NUMBER OF FIRST SINK ENERGY POINT (EIN) FOR
CD WHICH THE TABULATED INELASTIC PROBABILITY
CD IS NON-ZERO FOR THE SOURCE GROUP IN QUESTION
CD    NSTRT2 NUMBER OF FIRST SINK ENERGY POINT (EN2N) FOR
CD WHICH THE TABULATED (N,2N) PROBABILITY
APPENDIX C. MC²-2 Binary Interface Files. MCC2F6 (Contd.)

CD N2NEVP
    IS NON-ZERO FOR THE SOURCE GROUP IN QUESTION
CD N2NEVP
    NUMBER OF \((N,2N)\) EVAPORATION SPECTRA
CD N2NEV
    FOR ENERGY GROUP IN QUESTION
CD N2NLV
    NUMBER OF DISCRETE \((N,2N)\) SCATTERING LEVELS
CD N2NLV
    FOR EACH MATERIAL FOR THE ENERGY GROUP IN
CD N2NLV
    QUESTION
CD N2NTAB
    NUMBER OF TABULATED \((N,2N)\) DISTRIBUTIONS
CD N2NTAB
    FOR ENERGY GROUP IN QUESTION
CD N2NTAB
    EQ. ZERO OR ONE

CS FILE STRUCTURE
CS RECORD TYPE
CS -----------------------------------------------
CS GROUP INDEPENDENT INELASTIC
CS AND \((N,2N)\) DATA
CS ********** (REPEAT FOR NMAX GROUPS)
CS * CONTROL INFORMATION AND CROSS
CS * SECTION DATA
CS * SECONDARY DISTRIBUTION DATA
CS * (NLVS.GT.0) OR
CS * (N2NLV.GT.0) OR
CS * (N2NEVP.GT.0) OR
CS * (N2NEVP.GT.0) OR
CS * FOR ANY MATERIAL
CS * TABULATED INELASTIC AND \((N,2N)\)
CS * PROBABILITIES
CS * \((NINTAB.GT.0) OR
CS * \((N2NTAB.GT.0) OR
CS * \((N2NTAB.GT.0) OR
CS * FOR ANY MATERIAL
CS **********

CS GROUP INDEPENDENT INELASTIC AND \((N,2N)\) DATA (TYPE 1)
CS PRESENT IF MMAT.GT.0
CL ((EGAM(I,J), I=1, NLSJ), (U(I,J), I=1, MAX1J),
CL 1(GAMN2N(I,J), I=1, N2NLJ), (EIN(I,J), I=1, NSK1J),
CL 2(EN2N(I,J), I=1, NSK2J), J=1, MMAT)
CS SUMJ
CS EGAM
    GAMMA RAY ENERGY ASSOCIATED WITH THE L'TH
CS EGAM
    RESOLVED SCATTERING LEVEL. IF Q IS THE
CS EGAM
    ASSOCIATED Q-VALUE OF THE REACTION, THEN
CS EGAM=-Q (EGAM.GT.0)
CS EGAM IS ORDERED SUCH THAT EGAM(1).LE.EGAM(2)...
APPENDIX C. MC\textsuperscript{2}-2 Binary Interface Files. MCC2F6 (Contd.)

CD U DEFINES INELASTIC UPPER ENERGY LIMIT FOR THE -
CD SECONDARY NEUTRON ENERGY E\textprime\ such that -
CD 0 \leq E\textprime\ \leq E - U (GIVEN IN THE LABORATORY) WHERE -
CD E IS THE INCOMING NEUTRON ENERGY -
CD GAMN2N GAMMA RAY ENERGY ASSOCIATED WITH THE L\textsuperscript{TH} -
CD (N,2N) RESOLVED SCATTERING LEVEL. IF Q IS THE -
CD ASSOCIATED Q-VALUE OF THE REACTION, THEN -
CD GAMN2N= -Q (GAMN2N.GT.0) -
CD GAMN2N IS ORDERED SUCH THAT -
CD GAMN2N(1).LE.GAMN2N(2).LE.GAMN2N(3).... -
CD EIN SINK ENERGIES FOR WHICH TABULATED INELASTIC -
CD SCATTERING PROBABILITIES ARE GIVEN -
CD EIN?N SINK ENERGIES FOR WHICH TABULATED (N,2N) -
CD SCATTERING PROBABILITIES ARE GIVEN -
CD SUMJ SUM OF (NLSJ+MAX1J+N2NLJ+NSNK1J+NSNK2J) OVER -
CD ALL MMAT MATERIALS -
CD NLSJ = NLEVLS(J) FOR CURRENT MATERIAL J -
CD MAX1J = MAX1(J) FOR CURRENT MATERIAL J -
CD N2NLJ = N2NLEV(J) FOR CURRENT MATERIAL J -
CD NSNK1J = NSINK1(J) FOR CURRENT MATERIAL J -
CD NSNK2J = NSINK2(J) FOR CURRENT MATERIAL J -
C THE INELASTIC AND (N,2N) CONTROL INFORMATION -
C NLEVLS, MAX1, N2NLEV, NSINK1, AND NSINK2 ARE -
C SPECIFIED IN RECORD TYPE 5 OF MCC2F1 -
C DATA ARE PRESENT ONLY FOR MATERIALS THAT HAVE -
C EITHER INELASTIC OR (N,2N) DATA -
C
C-------------------------
C
CR CONTROL INFORMATION AND CROSS SECTION DATA (TYPE 2) -
C CC PRESENT IF NMAX.GT.0 -
C CL (SIGN(I),SIGN2N(I),NINEVP(I),NINTAB(I),N2NEVP(I),N2NTAB(I), -
CL 1NSTR1(I),NEND1(I),NSTR12(I),NEND2(I),KT1(I),KT2(I), -
CL 2NLVS(I),N2NLV(I),I=1,MMAT1) -
C CW SUMJ -
C
CD STGIN GROUP TOTAL INELASTIC SCATTERING CROSS SECTION -
CD SIGN2N GROUP (N,2N) SCATTERING CROSS SECTION -
CD KT1 INTERPOLATION LAW FOR CALCULATING GROUP TO -
CD GROUP TABULATED INELASTIC SCATTERING -
CD KT=0 CONSTANT PROBABILITY
| CD | KT=1 | LN(ENERGY) VS. LN(PROBABILITY) |
| CD | KT=2 | LN(ENERGY) VS. PROBABILITY     |
| CD | KT=3 | ENERGY VS. PROBABILITY         |
| CD | KT=4 | ENERGY VS. LN(PROBABILITY)     |
| CD | KT2  | INTERPOLATION LAW FOR CALCULATING GROUP TO |
|     |      | GROUP TABULATED \((N,2N)\) SCATTERING |
| CD |      | PROBABILITIES FROM THE GROUP TO ENERGY \((?NNTAB)\) |
| CD |      | PROBABILITIES GIVEN IN RECORD TYPE 4 |
| CD |      | KT=0  CONSTANT PROBABILITY      |
| CD |      | KT=1  LN(ENERGY) VS. LN(PROBABILITY) |
| CD |      | KT=2  LN(ENERGY) VS. PROBABILITY |
| CD |      | KT=3  ENERGY VS. PROBABILITY    |
| CD |      | KT=4  ENERGY VS. LN(PROBABILITY) |
| CD | SUM1 | SUM OVER I FOR ALL 14 ARRAYS FOR ALL |
| CD |      | MMAT1 MATERIALS                |
| C  |      | CROSS SECTION DATA AND CONTROL INFORMATION |
| CN |      | DATA ARE PRESENT FOR A MATERIAL ONLY IF THE |
| CN |      | MATERIAL HAS THESE DATA PRESENT AS SPECIFIED |
| CN |      | IN RECORD TYPE 5 OF MCC2F1. ALSO THESE DATA |
| CN |      | ARE PRESENT ONLY IF THE GROUP BEING PROCESSED |
| CN |      | IS ABOVE THE THRESHOLD ENERGY OF THE REACTION |
| CN |      | BEING CONSIDERED                |
| CN |      | SIGN2N IS PRESENT FOR MATERIALS THAT HAVE |
| CN |      | INELASTIC DATA FOR THE ENERGY GROUP BEING |
| CN |      | PROCESSED. NINEVP IS PRESENT FOR ALL MATERIALS |
| CN |      | THAT HAVE MAX1.GT.0. NLVS IS PRESENT FOR ALL |
| CN |      | MATERIALS THAT HAVE NLEVLS.GT.0. IN ADDITION |
| CN |      | SIGN, NINEVP, AND NLVS ARE PRESENT ONLY FOR |
| CN |      | GROUPS.LE.NINEL                 |
| CN |      | SIGN2N IS PRESENT FOR MATERIALS THAT HAVE |
| CN |      | \((N,2N)\) DATA FOR THE ENERGY GROUP BEING |
| CN |      | PROCESSED. N2NEVP IS PRESENT FOR ALL MATERIALS |
| CN |      | THAT HAVE MAX3.GT.0. N2NLV IS PRESENT FOR ALL |
| CN |      | MATERIALS THAT HAVE N2NLEV.GT.0. IN ADDITION |
| CN |      | STIGN2N, N2NEVP, AND N2NLV ARE PRESENT ONLY |
| CN |      | FOR GROUPS.LE.N2NTH             |
| CN |      | NINTAB3, NSTRT1, NEND1, AND KT1 ARE PRESENT FOR |
| CN |      | ALL MATERIALS THAT HAVE MAX2.GT.0. DATA |
| CN |      | PRESENT FOR ALL GROUPS.LE.NINEL |
| CN |      | N2NTAB, NSTRT2, NEND2, AND KT2 ARE PRESENT |
| CN |      | FOR ALL MATERIALS THAT HAVE MAX4.GT.0. DATA |
| CN |      | PRESENT FOR ALL GROUPS.LE.N2NTH |
| CN |      | NINEL, N2NTH, NLEVLS, N2NLEV, MAX1, MAX2, |
| CN |      | MAX3, AND MAX4 ARE PRESENT IN RECORD 5 |
APPENDIX C. MC$^2$-2 Binary Interface Files. MCC2F6 (Contd.)

OF MCC2F1

SECONDARY DISTRIBUTION DATA (TYPE 3)

PRESENT IF (NLVS.GT.0) OR (N2NLV.GT.0) OR (NINEVP.GT.0) OR (N2NEVP.GT.0) FOR ANY MATERIAL

((SIGLEV(I,J),I=1,NLVSJ), (AVGMU(I,J),I=1,NLVSJ),
1(SIGN(I,J),I=1,N2NLVJ), (TSTAT(I,J),I=1,NINEVPJ),
2(PIN(I,J),I=1,NINEVPJ), (TN2N(I,J),I=1,N2NVPJ),
3(PN2N(I,J),I=1,N2NVPJ), J=1,MMAT1)

SUMJ

SIGLEV  GROUP CROSS SECTION ASSOCIATED WITH THE L' TH RESOLVED INELASTIC SCATTERING LEVEL
SIGN   GROUP CROSS SECTION ASSOCIATED WITH THE L' TH RESOLVED (N,2N) SCATTERING LEVEL
AVGMU  AVERAGE COSINE OF THE SCATTERING ANGLE IN THE CENTER OF MASS SYSTEM FOR THE GROUP IN QUESTION FOR DISCRETE INELASTIC SCATTERING
TSTAT  GROUP AVERAGED "STATISTICAL" INELASTIC TEMPERATURE
PIN    FRACTIONAL PROBABILITY THAT THE I' TH INELASTIC EVAPORATION LAW CAN BE USED FOR THE GROUP IN QUESTION
TN2N   AVERAGE GROUP TEMPERATURE ASSOCIATED WITH A STATISTICAL CALCULATION OF (N,2N) SCATTERING FOR THE I' TH DISTRIBUTION
PN2N   FRACTIONAL PROBABILITY THAT THE I' TH (N,2N) EVAPORATION LAW CAN BE USED FOR THE GROUP IN QUESTION
SUMJ   SUM OF (2*(NLVSJ+NINVPJ+N2NVPJ)+N2NLVJ) OVER ALL MMAT MATERIALS
NLVSJ  = NLVS(J) FOR CURRENT MATERIAL J
N2NLVJ = N2NLV(J) FOR CURRENT MATERIAL J
NINEVPJ = NINEVP(J) FOR CURRENT MATERIAL J
N2NVPJ = N2NVP(J) FOR CURRENT MATERIAL J

APPENDIX C. MC\textsuperscript{2}-2 Binary Interface Files: MCC2F6 (Contd.)

DATA IN THE ARRAY IN QUESTION ARE NOT PRESENT -

CR -------------------------------

CR TABULATED INELASTIC AND (N,2N) PROBABILITIES (TYPE 4)

CC PRESENT IF (NINTAB.GT.0) OR (N2NTAB.GT.0)

CC FOR ANY MATERIAL

CL ((PINTAB(I,J),I=1,K1), (PNNTAB(I,J),I=1,K2), J=1,MMAT1)

CL (K1+K2)*MMAT1

CD PINTAB TABULATED PROBABILITY OF A NEUTRON BEING

CD INELASTICALLY SCATTERED FROM THE GROUP IN

CD QUESTION TO ALL POSSIBLE SINK ENERGIES (EN1).

CD PINTAB(1)=PROBABILITY OF SCATTERING FROM

CD GROUP IN QUESTION TO ENERGY EN1(NSTRT1)

CD PINTAB(K1)=PROBABILITY OF SCATTERING FROM GROUP

CD IN QUESTION INTO ENERGIES EN1(NEND1)

CD PINTAB IS CALCULATED AS THE SUM OVER ALL

CD (ENDF/R) GIVEN TABULATED INELASTIC

CD DISTRIBUTIONS OF THE PARTIAL ENERGY

CD DISTRIBUTION*FRACTIONAL PROBABILITY

CD K1

CD PNNTAB TABULATED PROBABILITY OF A NEUTRON BEING

CD (N,2N) SCATTERED FROM THE GROUP IN

CD QUESTION INTO ALL POSSIBLE SINK ENERGIES (EN2N).

CD PNNTAB(1)=PROBABILITY OF SCATTERING FROM

CD GROUP IN QUESTION TO ENERGY EN2N(NSTRT2)

CD PNNTAB(K2)=PROBABILITY OF SCATTERING FROM GROUP

CD IN QUESTION INTO ENERGIES EN2N(NEND2)

CD PNNTAB IS CALCULATED AS THE SUM OVER ALL

CD (ENDF/B) GIVEN TABULATED (N,2N)

CD DISTRIBUTIONS OF THE PARTIAL ENERGY

CD DISTRIBUTION*FRACTIONAL PROBABILITY

CD K2

CD PNNTAB IS PRESENT ONLY IF NINTAB.GT.0

CD PNNTAB IS PRESENT ONLY IF N2NTAB.GT.0

CD NEND1, NSTRT1, NEND2, NSTRT2, NINTAB, AND

CD N2NTAB ARE SPECIFIED IN RECORD TYPE 2

CD OF MCC2F6

:"EOF
APPENDIX C. MC²-2 Binary Interface Files. MCC2F7

C**************************************************************************
C
PREPARED 2/11/75 AT ANL
C
C
C**************************************************************************

CD   ICHI
     FLAG INDICATING WHETHER PARAMETERS IN
     GENERALIZED FISSION SPECTRUM ARE ENERGY
     (GROUP) DEPENDENT OR NOT
     ICHI=1 PARAMETERS NOT ENERGY DEPENDENT
     ICHI=NGROUP PARAMETERS ARE ENERGY DEPENDENT
     AND NGROUP, THE NUMBER OF GROUPS
     IN THE LIBRARY IS SPECIFIED IN THE
     ADMINISTRATIVE FILE MCC2F1

CD   MSORS
     NUMBER OF FISSION SPECTRA IN LIBRARY
     AS SPECIFIED IN THE ADMINISTRATIVE
     FILE MCC2F1

CD   MULT
     2 FOR IBM MACHINES, 1 OTHERWISE

CS
FILE STRUCTURE
CS
RECORD TYPE PRESENT IF
CS
MATERIAL NAMES MATERIAL NAMES
CS
SPECIFICATIONS ALWAYS
CS
** (REPEAT MSORS TIMES)
CS
FISSION SPECTRA ALWAYS
CS
**
CS

CS
MATERIAL NAMES (TYPE 1)
CS
ALWAYS PRESENT
CS
(NAME(I),I=1,MSORS)
CS
MULT*MSORS
CS
NAME DOUBLE PRECISION (R*8) MATERIAL IDENTIFICATION
CS
ASSOCIATED WITH THE GIVEN FISSION SPECTRUM
CS
PARAMETERS
APPENDIX C. MC^2-2 Binary Interface Files. MCC2F7 (Contd.)

C
C
C---------------------------------------------------------------
C
CR SPECIFICATIONS (TYPE 2)
C
CC ALWAYS PRESENT
C
CL (ICH (I), I=1, MSORS)
C
CW MSORS
C
C---------------------------------------------------------------
C
CR FISSION SPECTRA (TYPE 3)
C
CC ALWAYS PRESENT
C
CL (BETA (I), I=1, ICH), (ALPHA (I), I=1, ICH), (TAU (I), I=1, ICH)
C
CW 3*ICHI
C
CD BETA, ALPHA, TAU PARAMETERS IN GENERALIZED FISSION SPECTRUM
C
C---------------------------------------------------------------
C
CPOF
APPENDIX C. MC²-2 Binary Interface Files. MCC2F8

PREPARED 2/11/75 AT ANL

MCC2F8

LEGENDRE DATA

C*****************************

IL

NUMBER OF BLOCKS OF DATA FOR A GIVEN MATERIAL
NO DATA ARE PROVIDED FOR ENERGIES BELOW
WHICH SCATTERING IS ISOTROPIC
NUMBER OF LEGENDRE COEFFICIENTS PROVIDED FOR
EACH BLOCK OF DATA BY MATERIAL
NUMBER OF INTERPOLATION REGIONS FOR LEGENDRE
DATA RECORD
2 FOR IBM MACHINES, 1 OTHERWISE
HIGHEST ORDER PERMITTED FOR EXTENDED TRANSPORT
APPROXIMATION AS SPECIFIED IN THE
ADMINISTRATIVE FILE MCC2F1

---

FILE STRUCTURE

RECORD TYPE
SPECIFICATIONS
********* (REPEAT FOR ALL MATERIALS)
* MATERIAL IDENTIFICATION
* T MATRIX AND INTERPOLATION DATA
* *** (REPEAT IL TIMES)
* * LEGENDRE COEFFICIENTS
*********

---

SPECIFICATIONS (TYPE 1)
ALWAYS PRESENT

LGTH(I), I=1,NMAT), (IR(I), I=1,NMAT), (IL(I), I=1,NMAT),
(IPT(I), J=1,NMAT), J=1,NMAT)
NMAT*(3+NPASS)
LENGTH (IN WORDS) OF
APPENDIX C. MC\(^{2}\)-2 Binary Interface Files. MCC2F8 (Contd.)

CD T MATRIX AND INTERPOLATION DATA RECORD
CD NMAT NUMBER OF MATERIALS IN LIBRARY AS SPECIFIED IN THE ADMINISTRATIVE FILE MCC2F1
CD NPASS NUMBER OF 'BLOCKS' OF LEGENDRE DATA AS SPECIFIED IN THE ADMINISTRATIVE FILE MCC2F1

---

CR MATERIAL IDENTIFICATION (TYPE 2)
CC ALWAYS PRESENT
CL NAME
CW MULT*1
CD NAME DOUBLE PRECISION (R*8) MATERIAL IDENTIFICATION

---

CR T MATRIX AND INTERPOLATION DATA (TYPE 3)
CC ALWAYS PRESENT
CL (KT(I), I=1, IR), (NG(I), I=1, IR),
CL 1 ((TLJ(L, J), L=1, NPL), J=1, MAX(IPT) + 1),
CL 2 ((TLJ(L, J), L=1, 2), J=1, MAX(IPT) + 1),
CL 3 ((TLJ2(L, J), L=1, 2), J=1, 6), ((FACK(I, J), I=1, 6), J=1, 6),
CL 4 ((FAC(I, J), I=1, 4), J=1, MAX(IPT) + 1)
CW 2*TP*MULT*(54+MAX(IPT)*(NPL+6)+NPL) FOR DELTAU.GE.Q (SEE BELOW)
CW 2*TP*MULT*(50+MAX(IPT)*(NPL+2)+NPL) FOR DELTAU.LT.Q (SEE BELOW)
CD KT INTERPOLATION LAW USED TO OBTAIN HYPERFINE
CD GROUP VALUES OF THE LEGENDRE COEFFICIENTS, F1, F2, ..., FN, IN THE INTERPOLATION REGION I
CD KT=0 CONSTANT
CD KT=1 LN E VS. LN FN
CD KT=2 LN E VS. FN
CD KT=3 E VS. FN
CD KT=4 E VS. LN FN
CD NG LOWEST ENERGY GROUP NUMBER (HIGHEST ENERGY)
CD FOR WHICH INTERPOLATION LAW APPLIES
CD TLJ STANDARD ZERO ORDER T MATRIX ELEMENTS
CD TLJ1 STANDARD FIRST ORDER T MATRIX ELEMENTS
APPENDIX C. MC^2-2 Binary Interface Files. MCC2F8 (Contd.)

| CD   | TLJ2                  | STANDARD SECOND ORDER T MATRIX ELEMENTS |
| CD   | FACK                  | MASS DEPENDENT CONSTANTS USED IN CALCULATION |
| CD   | FAC                   | OF CONTINUOUS SLOWING DOWN MODERATING |
| CD   |                       | PARAMETERS |
| CD   |                       | 'INCOMPLETE' T MATRIX ELEMENTS |
| CD   |                       | THE ARRAY FAC IS PRESENT ONLY FOR THOSE |
| CD   | DELTAU GE Q           | ELEMENTS THAT HAVE |
| CD   |                       | WHERE Q = \log\left(\frac{(A+1)}{(A-1)}\right)^2/3. |
| CD   |                       | DELTAU AND A ARE THE GROUP LETHARGY |
| CD   |                       | WIDTH AND MATERIAL MASS/NEUTRON MASS |
| CD   |                       | RESPECTIVELY. BOTH ARE SPECIFIED IN THE |
| CD   |                       | ADMINISTRATIVE FILE MCC2F1 |
| CN   |                       | ALL REAL ARRAYS, TLJ, TLJ1, TLJ2, FACK, AND FAC |
| CN   |                       | ARE WRITTEN IN DOUBLE PRECISION (REAL*8) |

GR   | LEGENDRE COEFFICIENTS (TYPE 4) |
CN   | PRESENT IF IL.GT.0 |
CN   | (F1(J), F2(J), ..., FN(J), J=1, MANY1) |
CN   | MANY1*TPT |
CN   | F1, F2, ..., FN |
CD   | FIRST, SECOND, ..., N'TH ORDER EXPANSION |
CD   | COEFFICIENT AT THE ENERGY LEVEL SPECIFIED |
CD   | BY THE INDEX J. FOR EXAMPLE, ON THE THIRD |
CD   | PASS, THE THIRD BLOCK OF DATA, F1(1) WOULD |
CD   | BE THE FIRST ORDER COEFFICIENT FOR ENERGY |
CD   | LEVEL 2*MANY1-1 |
CD   | THE NUMBER OF COEFFICIENTS (N) FOR A GIVEN |
CD   | 'BLOCK' OF DATA IS GIVEN BY THE ARRAY TPT |
CD   | IN THE TABLE OF CONTENTS. NOTE THAT |
CD   | F0(J) = 1.0 AND IS THEREFORE NOT TABULATED. THIS |
CD   | RECORD IS NOT PROVIDED FOR THOSE ENERGY BLOCKS |
CD   | CORRESPONDING TO ENERGIES BELOW WHICH |
CD   | SCATTERING IS ISOTROPIC IN THE CENTER OF |
CD   | MASS SYSTEM. |
CD   | MANY1 |
CD   | NUMBER OF ENERGY LEVELS FOR EACH 'BLOCK' OF |
CD   | DATA (EXCEPT THE LAST) AS SPECIFIED IN THE |
CD   | ADMINISTRATIVE FILE MCC2F1 |
CD   | RECOMMENDED MAXIMUM VALUE FOR MANY1 WOULD BE |
CD   | MANY1=126 |

CEO
APPENDIX C. $M_C^2$-2 Binary Interface Files. XS.ISO

C**********************************************************************************************************
C PREPARED 3/11/76 AT ANL
C
CF XS.ISO
CE MICROSCOPIC GROUP CROSS SECTIONS, FILE 1
C
CN THIS IS FILE 1 OF A TWO-FILE DATA SET CONTAINING MICROSCOPIC GROUP CROSS SECTIONS.
C
C**********************************************************************************************************

CD NGROUP NUMBER OF BROAD ENERGY GROUPS IN SET.
CD NISO NUMBER OF ISOTOPES IN SET.
CD MULT 2 FOR IBM MACHINES, 1 OTHERWISE.

CR FILE SIZE (TYPE 1)
CC ALWAYS PRESENT
C
CL NGROUP, NISO, MAXUP, MAXDN, MAXORD, IPREC
C
CW 6

CD MAXUP MAXIMUM NUMBER OF GROUPS OF UPSCATTER IN THE SET.
CD MAXDN MAXIMUM NUMBER OF GROUPS OF DOWNSCATTER IN THE SET.
CD MAXORD (MAXIMUM OF LEL, LIN, OR LN2N FOR THE SET)-1
CD (SEE ISOTOPE HEADING RECORD OF DATA SET XS.ISO, FILE 2).
CD IPREC 0 FOR DOUBLE PRECISION VERSION OF DATA SET XS.ISO, 1 FOR SINGLE PRECISION VERSION OF THE DATA SET.

CR ISOTOPE NAMES (TYPE 2)
CC ALWAYS PRESENT
C
CL (ISONAM(I), I=1,NISO), (LOCA(I), I=1,NISO), (TEMP(I), I=1,NISO),
CL (TNAME(I), I=1,NISO), (AMASS(I), I=1,NISO)
C
:NISO1=NISO+1
APPENDIX C. MC²-2 Binary Interface Files. XS.ISO (Contd.)

C
C W NTSO+1+2*MULT*NISO+2*NISO*(2-IPREC)
C
C D ISONAM(I) LOCAL NAME OF I-TH ISOTOPE (REAL*8).
C D LOCA(I) NUMBER OF RECORDS IN FILE 2 OF XS.ISO TO BE
C D TEMP(I) SKIPPED TO READ DATA FOR ISOTOPE I. LOCA(1)=0.
C D TNAME I-TH ISOTOPE NAME AS GIVEN IN ENDF/B FILES.
C D AMASS GRAM ATOMIC WEIGHTS OF THE ISOTOPE.
C
C-----------------------------------------------

CR

GROUP STRUCTURE (TYPE 3)

CC

ALWAYS PRESENT

CC

Ichi, (E(I),I=1,NGP1), (U(I),I=1,NGP1), (Vel(I),I=1,NGROUP)

CC

NGP1=NGROUP+1

C

CW

1+(3*NGROUP+2)*(2-IPREC)

C

CD ICHI FISSION SPECTRUM FLAG FOR SET.
C D =0, NO SET CHI.
C D =1, SET CHI VECTOR.
C
C D E(I) ENERGY BOUNDARIES OF GROUPS. E(1) IS
C D THE MAXIMUM ENERGY.
C D U(I) LETHARGY BOUNDARIES OF GROUPS. U(1)=0.
C D Vel(I) NEUTRON SPEED FOR GROUP I,
C D SPEED 1./(1./V).

C-----------------------------------------------

CR

SET FISSION SPECTRUM (TYPE 4)

CC

PRESENT IF ICHI.NE.0

CC

((CHI(I,J),I=1,ICHI),J=1,NGROUP)

C W

ICHI*NGROUP*(2-IPREC)

C

CD CHI(I,J) PROMPT FISSION FRACTION INTO GROUP J
C D FROM GROUP I.

C

CEOF
APPENDIX C. MC²-2 Binary Interface Files. XS.ISO (Contd.)

PREPARED 3/11/76 AT ANL

XS.ISO2
MICROSCOPIC GROUP CROSS SECTIONS, FILE 2
THIS IS FILE 2 OF A TWO-FILE DATA SET CONTAINING MICROSCOPIC GROUP CROSS SECTIONS.

FILE STRUCTURE

RECORD TYPE   PRESENT IF

********* (REPEAT FOR ALL ISOTOPES)  
* ISOTOPE NAME  ALWAYS
* ISOTOPE HEADING  ALWAYS
* ISOTOPE FISSION SPECTRUM  ICHI.GT.0
********* (REPEAT FOR ALL GROUPS)
* * PRINCIPAL CROSS SECTIONS  ALWAYS

*********

********* (REPEAT FOR EACH SCATTERING ORDER)
* * L=1, LMAX, WHERE LMAX IS THE
* * LARGEST OF LIN, LEL, AND LN2N.
* * SEE ISOTOPE HEADING RECORD.)
********* (REPEAT FOR ALL GROUPS)
* * * INDEX FOR SCATTERING GROUP  ALWAYS
* * * INELASTIC SCATTERING  LIN.GP.L
* * * ELASTIC SCATTERING  LEL.GP.L
* * * (N,2N) SCATTERING  LN2N.GP.L

**********

CD LELDN  NUMBER OF ELASTIC DOWNSCATTER GROUPS.
CD LELUP  NUMBER OF ELASTIC UPSCATTER GROUPS.
CD LINDN  NUMBER OF INELASTIC DOWNSCATTER GROUPS.
CD LINUP  NUMBER OF INELASTIC UPSCATTER GROUPS.
CD LN2NLDN  NUMBER OF (N,2N) DOWNSCATTER GROUPS.
CD LN2NUP  NUMBER OF (N,2N) UPSCATTER GROUPS.
CD NGROUP  NUMBER OF ENERGY GROUPS IN THE SET.
CD MULT  2 FOR IBM MACHINES, 1 OTHERWISE.
CD IPREC  0 FOR DOUBLE PRECISION VERSION OF DATA SET
CD XS.ISO, 1 FOR SINGLE PRECISION VERSION OF THE
APPENDIX C. MC²-2 Binary Interface Files. XS.ISO (Contd.)

CD DATA SET.

CR ISOTOPE NAME (TYPE 1)
CC ALWAYS PRESENT
CL ISONAM
CW MULT
CD ISONAM ISOTOPE NAME (REAL*8).

CR ISOTOPE HEADING RECORD (TYPE 2)
CC ALWAYS PRESENT
CL ICHI,LIN,LEL,LN2N,EFISS,ECAPT
CW 4+2*(2-IPREC)
CD ICHI ISOTOPE FISSION SPECTRUM FLAG.
CD ICHI=-1, ISOTOPE USES PROMPT FISSION SPECTRUM
CD FOR SET.
CD =0, ISOTOPE IS NOT FISSIONABLE.
CD =1, ISOTOPE USES OWN PROMPT FISSION
CD SPECTRUM WHICH IS NOT INCIDENT-ENERGY-
CD DEPENDENT (VECTOR).
CD =NGROUP, ISOTOPE USES OWN PROMPT FISSION
CD SPECTRUM WHICH IS INCIDENT-ENERGY-
CD DEPENDENT (MATRIX).
CD LIN MAXIMUM ORDER OF INELASTIC SCATTERING.
CD LIN=0, NO SCATTERING.
CD =1, ISOTROPIC SCATTERING.
CD =2, LINEAR ANISOTROPIC SCATTERING.
CD =N, ORDER N-1 ANISOTROPIC SCATTERING.
CD LEL MAXIMUM ORDER OF ELASTIC SCATTERING.
CD LEL=0, NO SCATTERING.
CD =1, ISOTROPIC SCATTERING.
CD =2, LINEAR ANISOTROPIC SCATTERING.
CD =N, ORDER N-1 ANISOTROPIC SCATTERING.
CD LN2N MAXIMUM ORDER OF (N,2N) SCATTERING.
CD LN2N=0, NO SCATTERING.
CD =1, ISOTROPIC SCATTERING.
CD =2, LINEAR ANISOTROPIC SCATTERING.
APPENDIX C. MC\textsuperscript{2}-2 Binary Interface Files. XS_ISO (Contd.)

\begin{verbatim}
CD EFiSS = N, ORDER N-1 ANISOTROPIC SCATTERING.
CD ECAFT = WATT-SECONDS/FISSION.
CD ECAPT = WATT-SECONDS/CAPTURE WHERE CAPTURE REFERS TO
CD NON-FISSION ABSORPTION.

C-----------------------------------------------

CR ISOTOPE FISSION SPECTRUM (TYPE 3)
CC PRESENT IF ICHI.GT.0 (SEE ISOTOPE HEADING RECORD)
CC
CL (CHI(I,J), I=1, ICHI), J=1, NGROUP).
CW ICHI*NGROUP*(2-IPREC)
CD CHI(I,J) FISSION SPECTRUM INCIDENT IN GROUP J, BORN
CD IN GROUP I.

C-----------------------------------------------

CR PRINCIPAL CROSS SECTIONS (TYPE 4)
CC ALWAYS PRESENT
CC
CL J,STR,SCAP,SNALF,SNP,ANISO,SFIS,FISNU
CW 1+7*(2-IPREC) IF ICHI.NE.0
CW 1+5*(2-IPREC) IF ICHI.EQ.0
CD J GROUP INDEX.
CD STR TRANSPORT CROSS SECTION.
CD SCAP RADIATIVE CAPTURE (N,GAMMA) CROSS SECTION.
CD SNALF (N,ALPHA) CROSS SECTION.
CD SNP (N,P) CROSS SECTION.
CD ANISO ISOTROPIC ELASTIC SELF-SCATTERING CONSISTENT
CD WITH ANISOTROPIC TOTAL CROSS SECTION.
CD ANISO, WHEN ADDED TO THE SUM OF ALL EVENTS
CD WHICH REMOVE A NEUTRON FROM THE GROUP,
CD YIELDS THE TOTAL GROUP CROSS SECTION.
CD SFIS FISSION CROSS SECTION, PRESENT IF ICHI.NE.0.
CD FTSNU NUMBER OF FISSION NEUTRONS PER FISSION TIMES
CD FISSION CROSS SECTION, PRESENT IF ICHI.NE.0.

C-----------------------------------------------
\end{verbatim}
APPENDIX C. MC²-2 Binary Interface Files. XS.ISO (Contd.)

C IND t FOR SCATTERING GROUP (TYPE 5)
C
CC PRESENT IF LIN+LEL+LN2N.NE.0
CC (SEE ISOTOPE HEADING RECORD)
C
CL LINUP, LINDN, LELUP, LELDN, LN2NUP, LN2NDN
C
CW 6
C

C INELASTIC SCATTERING (TYPE 6)
C
CC PRESENT IF LIN. GE. CURRENT SCATTERING ORDER
CC (SEE ISOTOPE HEADING RECORD)
C
CL SINL(J+LINUP), SINL(J+LINUP-1), ..., SINL(J), ..., SINL(J-LINDN)
C
CW (LINUP+LINDN+1)*(2-IPREC)
C
CD SINL(K) INELASTIC SCATTERING, GROUP K TO GROUP J.
C

C ELASTIC SCATTERING (TYPE 7)
C
CC PRESENT IF LEL. GE. CURRENT SCATTERING ORDER
CC (SEE ISOTOPE HEADING RECORD)
C
CL SELT(J+LELUP), SELT(J+LELUP-1), ..., SELT(J), ..., SELT(J-LELDN)
C
CW (LELUP+LELDN+1)*(2-IPREC)
C
CD SELT(K) ELASTIC SCATTERING, GROUP K TO GROUP J.
C

C (N,2N) SCATTERING (TYPE 8)
C
CC PRESENT IF LN2N. GE. CURRENT SCATTERING ORDER
CC (SEE ISOTOPE HEADING RECORD)
C
CL SN2N(J+LN2NUP), SN2N(J+LN2NUP-1), ..., SN2N(J), ..., SN2N(J-LN2NDN)
APPENDIX C. MC2-2 Binary Interface Files. XS.ISO (Contd.)

C

\[ C_W = (L_2^{N_{UP}} + L_2^{N_{DN}} + 1) \times (2 - IPREC) \]

C

\[ C_D = S_{2N}(K) \] (n,2n) SCATTERING, GROUP K TO GROUP J.

C

CEOFT
APPENDIX D

\textit{MC^2-2 BINARY FILES}
APPENDIX D. MC²-2 Binary Files. ATNUAT

*-------------------------------------------------------------------*
| CD   | IFI  | FISSILE MATERIAL INDEX. |
| CD   | JL   | IPI=0 FOR NON-FISSILE MATERIAL |
| CD   | MULT | IPI=1 FOR FISSILE MATERIAL |
| CD   | NREG | NUMBER OF SPIN STATES FOR CURRENT ISOTOPE |
| CD   | NUMRES | 2 FOR IBM MACHINES, 1 OTHERWISE |
| CD   | NUNRES | NUMBER OF FIXED ENERGY MESH POINTS |
| CD   | NREG   | NUMBER OF REGIONS |
| CD   | NUNRES | NUMBER OF UNRESOLVED RESONANCE MATERIALS |
| CD   | NREG   | NREG=1 FOR HOMOGENEOUS PROBLEMS (NGEOM=0) |
| CD   | NREG   | NREG=2 FOR PIN CELLS (NGEOM=2) AND IF |
| CD   | NREG   | MAXHTM.GT.0 |
| CD   | NREG   | NREG=1 + NUMBER OF SLAB REGIONS FOR SLAB |
| CD   | NREG   | (MAXHTM IS THE MAXIMUM NUMBER OF MATERIALS IN |
| CD   | NREG   | ANY HETEROGENEOUS REGION) |
| CD   | NUMRES | NUMBER OF UNRESOLVED RESONANCE MATERIALS |
| CD   | NUNRES | NUNRES=0 IF UNRESOLVED RESONANCE CROSS SECTIONS |
| CD   | NUNRES | NUNRES=1 IF UNRESOLVED RESONANCE |
| CD   | NUNRES | INTEGRALS ARE GENERATED |

C-------------------

FILE STRUCTURE

<table>
<thead>
<tr>
<th>RECORD TYPE</th>
<th>PRESENT IF</th>
</tr>
</thead>
<tbody>
<tr>
<td>SPECIFICATIONS</td>
<td>ALWAYS</td>
</tr>
<tr>
<td>MATERIAL NAMES</td>
<td>ALWAYS</td>
</tr>
<tr>
<td>FIXED UNRESOLVED RESONANCE</td>
<td>ALWAYS</td>
</tr>
<tr>
<td>ENERGY MESH</td>
<td></td>
</tr>
<tr>
<td>**************** (REPEAT FOR NUMRES MATERIALS)</td>
<td></td>
</tr>
<tr>
<td>* MATERIAL SPECIFICATIONS</td>
<td>ALWAYS</td>
</tr>
<tr>
<td>* ******** (REPEAT FOR NISO ISOTOPES)</td>
<td></td>
</tr>
<tr>
<td>* * SPIN STATE DATA</td>
<td>ALWAYS</td>
</tr>
<tr>
<td>* * LEVEL SPACING</td>
<td>ALWAYS</td>
</tr>
<tr>
<td>* * * (REPEAT FOR 1+NO. OF REGIONS</td>
<td></td>
</tr>
<tr>
<td>* * * IN WHICH MATERIAL IS TREATED</td>
<td></td>
</tr>
<tr>
<td>* * * HETEROGENEously)</td>
<td></td>
</tr>
</tbody>
</table>
APPENDIX D. MC²-2 Binary Files. ATNUAT (Contd.)

CS * * * CAPTURE J INTEGRAL ALWAYS
CS * * * TOTAL J INTEGRAL ALWAYS
CS * * * FISSION J INTEGRAL IFI.EQ.1
CS ********** TOTAL FLUX CORRECTION FACTOR ALWAYS

C

C SPECIFICATIONS (TYPE 1)
C
C ALWAYS PRESENT

CL NUMRES, NRESF, NREG, JLMAX, MAXISO
C
CW 5

CD JLMAX LSTMAX*JSTMAX WHERE LSTMAX IS THE MAXIMUM
CD VALUE OF THE NUMBER OF ANGULAR MOMENTUM
CD STATES OVER ALL MATERIALS IN THE FILE AND
CD JSTMAX IS THE MAXIMUM VALUE OF THE NUMBER OF
CD CHANNEL SPIN STATES ASSOCIATED WITH A
CD PARTICULAR ANGULAR MOMENTUM STATE OVER ALL
CD MATERIALS IN THE FILE
CD MAXISO MAXIMUM NUMBER OF ISOTOPES IN THE MIXTURE

C

C MATERIAL NAMES (TYPE 2)
C
C ALWAYS PRESENT

CL (UNRMAT (I), I=1, NUMRES)
C CW MULT*NUMRES
C
CD UNRMAT DOUBLE PRECISION (R*8) UNRESOLVED RESONANCE
CD MATERIAL NAMES

C

C FIXED UNRESOLVED RESONANCE ENERGY MESH (TYPE 3)
C
C ALWAYS PRESENT

C
APPENDIX D. MC²-2 Binary Files. ATNUAT (Contd.)

CL (ESF(I), I=1,NESF)  

CW NESF

CD ESF  FIXED ENERGY MESH POINTS GIVEN IN ORDER OF DECREASING ENERGY

CR  MATERIAL SPECIFICATIONS (TYPE 4)

CC  ALWAYS PRESENT

CL NISO,IFI

CW 2

CD NISO  NUMBER OF ISOTOPES

CR  SPIN STATE DATA (TYPE 5)

CC  ALWAYS PRESENT

CL JL

CW 1

CR  LEVEL SPACING (TYPE 6)

CC  ALWAYS PRESENT

CL ((D(I,J), I=1,NESF), J=1,JL)

CW NESF*JL

CD D  AVERAGE LEVEL SPACING
APPENDIX D. MC²-2 Binary Files. ATNUAT (Contd.)

Capture J Integral (Type 7)

\[ (\text{UCJ}(I,J), I=1, \text{NESP}) \]

Unresolved Resonance Capture Integral

Total J Integral (Type 8)

\[ (\text{UTJ}(I,J), I=1, \text{NESP}) \]

Unresolved Resonance Total Integral

Fission J Integral (Type 9)

\[ (\text{UFJ}(I,J), I=1, \text{NESP}) \]

Unresolved Resonance Fission Integral

Total Flux Correction Factor (Type 10)
APPENDIX D. MC^2-2 Binary Files. ATNUAT (Contd.)
APPENDIX D. MC²-2 Binary Files. BC

C***********************************************************************************************
C                                                                                           
C                                                                                           
C PREPARED 6/13/75 AT ANL                                                                 
C                                                                                           
C BC                                                                                         
C BOUNDARY CONDITION SPECIFICATIONS                                                           
C                                                                                           
C THIS IS AN ABBREVIATED VERSION OF THE DATA SET BC. IT IS USED FOR MC²-2-II                  
C CALCULATIONS.                                                                              
C                                                                                           
C***********************************************************************************************

CR                                                                                           
C SPECIFICATIONS (TYPE 1)                                                                      
C                                                                                           
CL                                                                                           
C NBCL, NBCF                                                                                   
C                                                                                           
CW                                                                                           
C 2                                                                                           
CD                                                                                           
C NBCL  BOUNDARY CONDITION TYPE NUMBER FOR LEFT                                                
C                                                                                           
CD                                                                                           
C NBCR  BOUNDARY CONDITION TYPE NUMBER FOR RIGHT                                               
C                                                                                           
CD                                                                                           
C                                                                                           
CD                                                                                           
C TYPE DESCRIPTION                                                                             
CD                                                                                           
C 8  REFLECTIVE                                                                               
CD                                                                                           
C 9  PERIODIC                                                                                 
CD                                                                                           
C 10 WHITE                                                                                    
C                                                                                           
C******************************************************************************
CEOF
APPENDIX D. MC\textsuperscript{2}-2 Binary Files. BIGXS(I)

PREPARED 3/10/75 AT ANL

BIGXS1 THROUGH BIGXSP
MACROSCOPIC ELASTIC SCATTERING

THESE FILES ARE WRITTEN BY MC\textsuperscript{2}-2-II AREA 7 (CSC008)

CD NDOWN
NUMBER OF SOURCE GROUPS OF DATA REPRESENTED IN EACH CROSS SECTION RECORD
CD NDOWN1
NUMBER OF GROUPS OF DOWNSCATTER CHARACTERISTIC OF THE PROBLEM ISOTOPE OF LIGHTEST MASS

CR SPECIFICATIONS (TYPE 1)

ALWAYS PRESENT FOR FILE BIGXS1
NEVER PRESENT FOR FILES BIGXS2 THROUGH BIGCSP

NDOWN, NDOWN1, NUMSPC

NUMSPC

C CROSS SECTION (TYPE 2)

ALWAYS PRESENT

((SIGS(I), I=1, NORD), (SIG0(I), I=1, NDN1), (SIG1(I), I=1, NDN1), 1J=1, NDOWN)
APPENDIX D. \(MC^2\)-2 Binary Files. \(BIGXS(I)\) (Contd.)

\[C\]
\[CD\]  \(NDOWN\ast (NORD1+ISP*NDN1)\)
\[CD\]  \(ISP=1\) FOR INCONSISTENT SPECTRUM OPTIONS (\(ISPOPT.LE.2\))
\[CD\]  \(ISP=2\) FOR CONSISTENT SPECTRUM OPTIONS (\(ISPOPT.GE.3\))
\[CD\]  \(NORD1\) ORDER OF EXTENDED TRANSPORT APPROXIMATION+1
\[CD\]  \(NDN1=NDOWN1+1\)
\[CD\]  \(SIGS\) LEGENDRE MOMENTS OF MACROSCOPIC SCATTERING
\[CD\]  \(I=1\) CORRESPONDS TO THE NORDER COMPONENT
\[CD\]  \(I=NORDER\) CORRESPONDS TO THE \(P1\) COMPONENT
\[CD\]  \(I=NORD1\) CORRESPONDS TO THE \(P0\) COMPONENT
\[CD\]  \(SIG0\) MACROSCOPIC \(P0\) SCATTERING MATRIX ORDERED AS
\[CD\]  \(J\) TO \(J+I-1\) SO THAT \(I=1\) IS THE IN-GROUP TERM
\[CD\]  \(SIG1\) MACROSCOPIC \(P1\) SCATTERING MATRIX ORDERED AS
\[CD\]  \(J\) TO \(J+I-1\) SO THAT \(I=1\) IS THE IN-GROUP TERM
\[CN\]  THE \(J\)'TH GROUP IN THE ABOVE LISTS CORRESPONDS
\[CN\]  TO A PARTICULAR ULTRA-FINE-GROUP IN THE
\[CN\]  PROBLEM. THAT IS, FOR \(BIGXS1\) THE \(J\)'TH
\[CN\]  GROUP CORRESPONDS TO THE \(J\)'TH ULTRA-FINE GROUP.
\[CN\]  FOR \(BIGXS2\) THE \(J\)'TH GROUP CORRESPONDS TO THE
\[CN\]  ULTRA-FINE-GROUP IN THE PROBLEM OF \(J+NDOWN\),
\[CN\]  AND SO ON THROUGH \(BIGXSP\).
\[CN\]  THE ARRAY \(SIG1\) IS PRESENT ONLY FOR \(ISP=2\)

CEOF
APPENDIX D. MC²-2 Binary Files. GEOM1

PREPARED 6/13/75 AT ANL

GEOM1

GEOMETRY DATA

THIS IS AN ABBREVIATED VERSION OF THE DATA SET GEOM. IT IS USED FOR MC**2-II CALCULATIONS.

ALL NON-INTEGER QUANTITIES IN THIS FILE ARE REAL*8.

MULT 2 FOR IBM MACHINES, 1 OTHERWISE.
NCMP NUMBER OF COMPOSITIONS.
NINTI NUMBER OF MESH INTERVALS.
NPTI NUMBER OF MESH INTERVAL LINES.
NREG NUMBER OF REGIONS.

NDIM, NGEOM, NPTI, NDM, NINTI, NDM, NREG, NCMP, NDM, NDM, NDM, NDM, 1NDM, NDM, NDM

14

NDIM NUMBER OF DIMENSIONS=1.
NGEOM GEOMETRY.
NGEOM=1, ONE-DIMENSIONAL SLAB.
NGEOM=2, ONE-DIMENSIONAL CYLINDER.
NDUM DUMMY VARIABLE SET TO 0.

(MESH INTERVAL BOUNDARIES (TYPE 2))

(XMESH (I), I=1, NPTI)
MULT*NPTI

XMESH MESH BOUNDARIES (REAL*8).
APPENDIX D. \( \text{MC}^2 \)-2 Binary Files. GEOnl (Contd.)

---

**REGION-INTERVAL CORRESPONDENCE (TYPE 3)**

\[
\text{MP} (I), I = 1, N\text{INTI} \quad \text{MR}
\]

REGION INDEX. IF \( \text{MR} (I) = N \), THEN \( \text{REG} (N) \) IS THE REGION LABEL IN INTERVAL \( I \) (SEE LABELS RECORD BELOW).

---

**COMPOSITION-INTERVAL CORRESPONDENCE (TYPE 4)**

\[
\text{MC} (I), I = 1, N\text{INTI} \quad \text{MC}
\]

COMPOSITION INDEX. IF \( \text{MC} (I) = N \), THEN \( \text{CNAME} (N) \) IS THE COMPOSITION LABEL IN INTERVAL \( I \) (SEE LABELS RECORD BELOW).

---

**COMPOSITION-REGION CORRESPONDENCE (TYPE 5)**

\[
\text{NC} (I), I = 1, N\text{REG} \quad \text{NC}
\]

COMPOSITION INDEX. IF \( \text{MC} (I) = N \), THEN \( \text{CNAME} (N) \) IS THE COMPOSITION LABEL IN REGION \( I \) (SEE LABELS RECORD BELOW).

---

**LABELS (TYPE 6)**

\[
\text{REG} (I), I = 1, N\text{REG}, \quad \text{CNAME} (I), I = 1, N\text{CMP} \quad \text{MULT} \ast (N\text{REG} + N\text{CMP})
\]
APPENDIX D. MC²-2 Binary Files. GEOML (Contd.)

C
CD REG       REGION LABELS (REAL*8).
CD CNAME     COMPOSITION LABELS (REAL*8).
C

C-----------------------------------------------

C
CR REGION VOLUMES (TYPE 7)
C
CL (VOL(I), I=1,NREG)
C
CW MULT*NREG
C
CD VOL       VOLUME OF REGION REG(I) (REAL*8) (SEE LABELS RECORD ABOVE). VOL EQUALS THE VOLUME PER UNIT HEIGHT IN THE TRANSVERSE DIRECTION.
CD
C
C-----------------------------------------------

CEOF
APPENDIX D. $^{235}$U Binary Files. IRESCS

PREPARED 4/26/76 AT ANL

BROAD GROUP RESONANCE CAPTURE, FISSION, ScATTERING AND TRANSFER CROSS SECTIONS AS CALLED IN $^{235}$U AREA 10 (CRC011)

INTEGRAL TRANSPORT THEORY

FILE STRUCTURE

RECORD TYPE

SPECIFICATIONS

MATERIAL NAMES

REGION NAMES

****** (REPEAT NBR'OAD TIMES)

* DOWNSCATTERS

* RESONANCE CROSS SECTIONS

* TRANSFER CROSS SECTIONS

******

CELL CROSS SECTIONS

GROUPS SCATTERED

CELL TRANSFER CROSS SECTIONS

MULT = 2 FOR IBM MACHINES, 1 OTHERWISE

NBR'OAD = NUMBER OF BROAD GROUPS IN THE RABANL (CRC011)

ENERGY RANGE

NCNTM = NUMBER OF RESOLVED RESONANCE MATERIALS IN THE PROBLEM MIXTURE EXCLUDING ANY UNIQUE FOIL MATERIALS

NGEOM = GEOMETRY TYPE

NGEOM = 0 FOR HOMOGENEOUS PROBLEM

NGEOM = 1 FOR SLAB GEOMETRY

NGEOM = 2 FOR CYLINDRICAL GEOMETRY

NREG = NUMBER OF REGIONS IN THE CELL. NREG = 1 FOR HOMOGENEOUS PROBLEMS
APPENDIX D. MC²—2 Binary Files. IRESCS (Contd.)

CR       SPECIFICATIONS (TYPE 1)
C        ALWAYS PRESENT
C
CL       NCNTM, NREG, NBROAD, NGEOM
C
CW       4
C

CR       MATERIAL NAMES (TYPE 2)
C
CC       ALWAYS PRESENT
C
CL       RESNAM(M), M=1, NCNTM
C
CW       MULT*NCNTM
C
CD       RESNAM        REAL*8 NAMES OF RESONANCE MATERIALS HAVING AN INTEGRAL TRANSPORT TREATMENT BY AREA 10 (CSC011)
CD
C

CR       REGION NAMES (TYPE 3)
C
CC       PRESENT IF NGEOM.GT.0
C
CL       RLABEL(N), N=1, NREG
C
CW       MULT*NREG
C
CD       RLABEL        REAL*8 NAMES OF REGIONS
C

CR       DOWNSCATTERS (TYPE 4)
C
CC       ALWAYS PRESENT
C
CL       NEBMAX(M), M=1, NCNTM
C
CW       NCNTM
APPENDIX D. MC²-2 Binary Files. IRESCS (Contd.)

CD  NBG\text{MAX}  \text{MAXIMUM NUMBER OF BROAD GROUPS DOWN-SCATTERED}
CD  \hspace{1cm} \text{FOR EACH MATERIAL AND CURRENT BROAD GROUP}

\begin{verbatim}

CP  \text{RESONANCE CROSS SECTIONS (TYPE 5)}
CC  \text{ALWAYS PRESENT}
CL  \{(RES\text{CAP}(M,K), M=1, NC\text{NTM}), K=1, N\text{REG}), (RESF\text{IS}(M,K), M=1, NC\text{NTM}),
CL  1, J=1, N\text{REG}), (RESS\text{CT}(M,K), M=1, NC\text{NTM}), K=1, N\text{REG})
CW  3*NC\text{NTM}N\text{REG}
CD  \text{RESCAP}(M,K)  \text{RESONANCE CAPTURE CROSS SECTION FOR MATERIAL M}
CD  \hspace{1cm} \text{AND REGION K FOR THE CURRENT BROAD GROUP}
CD  \text{RESFIS}(M,K)  \text{RESONANCE FISSION CROSS SECTION FOR MATERIAL M}
CD  \hspace{1cm} \text{AND REGION K FOR THE CURRENT BROAD GROUP}
CD  \text{RESSCT}(M,K)  \text{RESONANCE SCATTERING CROSS SECTIONS FOR}
CD  \hspace{1cm} \text{MATERIAL M AND REGION K FOR THE CURRENT BROAD GROUP}

\end{verbatim}

\begin{verbatim}

CR  \text{TRANSFER CROSS SECTIONS (TYPE 6)}
CC  \text{ALWAYS PRESENT}
CL  \{(TR\text{NSFR}(M,K, J), M=1, NC\text{NTM}), K=1, N\text{REG}), J=1, N\text{MAX})
CW  NC\text{NTM}N\text{REG}N\text{MAX}
CD  \text{TRANSFR}(M,K,J)  \text{RESONANCE MATERIAL M TRANSFER CROSS SECTION}
CD  \hspace{1cm} \text{FOR REGION K FROM THE CURRENT BROAD GROUP, SAY}
CD  \hspace{1cm} I, TO BROAD GROUP I+J
CD  \text{NMAX}  \text{LARGEST OF THE NBG\text{MAX} FOR THE CURRENT BROAD}
CD  \hspace{1cm} \text{GROUP FOR ANY OF THE NC\text{NTM MATERIALS}

\end{verbatim}

\begin{verbatim}

CR  \text{CELL CROSS SECTIONS (TYPE 7)}
CC  \text{PRESENT IF N\text{GEOM}.GT.0}
\end{verbatim}
APPENDIX D. MC²-2 Binary Files. IRESCS (Contd.)

\[
\begin{align*}
&\text{CL} \quad ((\text{CELCAP}(M,K), M=1, NCNTM), K=1, NBROAD), ((\text{CELFIS}(M,K), M=1, NCNTM), K=1, NBROAD) \\
&\text{C} \quad 3*NCNTM*NBROAD \\
&\text{CD} \quad \text{CELCAP}(M,K) \quad \text{CELL AVERAGED RESOLVED RESONANCE CAPTURE} \\
&\text{CD} \quad \text{CELFIS}(M,K) \quad \text{CELL AVERAGED RESOLVED RESONANCE FISSION} \\
&\text{CD} \quad \text{CELSCT}(M,K) \quad \text{CELL AVERAGED RESOLVED RESONANCE SCATTERING} \\
&\text{CD} \quad \text{CROSS SECTION FOR MATERIAL M AND BROAD GROUP K} \\
&\text{C} \quad \text{GROUPS SCATTERED (TYPE 8)} \\
&\text{C} \quad \text{PRESENT IF NGEOM.GT.0} \\
&\text{C} \quad ((\text{NGRPDN}(M,K), M=1, NCNTM), K=1, NBROAD) \\
&\text{C} \quad \text{NGRPDN}(M,K) \quad \text{NUMBER OF BROAD GROUPS DOWNSCATTERED BY} \\
&\text{C} \quad \text{MATERIAL M IN BROAD GROUP K} \\
&\text{C} \quad \text{CELL TRANSFER CROSS SECTIONS (TYPE 9)} \\
&\text{C} \quad \text{PRESENT IF NGEOM.GT.0} \\
&\text{C} \quad ((\text{CELTPR}(M,K,J), M=1, NCNTM), K=1, NBROAD), J=1, MOST) \\
&\text{C} \quad \text{CELTPR}(M,K,J) \quad \text{CELL AVERAGED TRANSFER CROSS SECTION FOR} \\
&\text{C} \quad \text{MATERIAL M FROM BROAD GROUP K TO BROAD GROUP K+J} \\
&\text{C} \quad \text{MOST} \quad \text{LARGEST OF THE NBGMAX FOR ANY BROAD GROUP} \\
&\text{C} \quad \text{CEOF}
\end{align*}
\]
APPENDIX D. MC^2-2 Binary Files. LORENZ

C**********************************************************************************************
C
C PREPARED 3/05/75 AT ANL
C
CF LORENZ
CE LORENTZIAN SHAPE RESONANCE INTEGRALS
C
CN THIS INTERFACE DATA SET IS WRITTEN
CN BY MC**2-II AREA 6 (CSC005)
CN THIS DATA SET IS PRESENT ONLY IF MAXNOL.GT.0
C
C**********************************************************************************************

CD NOLINT NUMBER OF ULTRA FINE GROUPS HAVING
CD LORENTZIAN SHAPE RESONANCE INTEGRALS FOR
CD EACH RESONANCE SO TREATED
CD NOLRES NUMBER OF RESONANCES GIVEN A LORENTZIAN SHAPE
CD TREATMENT FOR EACH REGION
CD NREG1 1 FOR HOMOGENEOUS PROBLEMS, 2 FOR CYLINDRICAL
CD PROBLEMS, 1+THE NUMBER OF SLAB REGIONS FOR
CD SLAB GEOMETRY PROBLEMS

C----------------------------------------------------------------------
CS FILE STRUCTURE
CS
CS
CS RECORD TYPE
CS =============== PRESENT IF
CS SPECIFICATIONS
CS ALWAYS
CS ***** (REPEAT NREG1 TIMES)
CS * RESONANCE SPECIFICATIONS
CS * RESONANCE NUMBERS
CS * ***** (REPEAT NOLRES TIMES)
CS * * ULTRA FINE GROUP NUMBERS
CS * * LORENTZIAN RESONANCE INTEGRALS
CS ********
C
C----------------------------------------------------------------------

C SPECIFICATIONS (TYPE 1)
C CC ALWAYS PRESENT
C CL MAXNOL, MAXGRP, MAXGPH
C CW 3
APPENDIX D. MC²-2 Binary Files. LORENZ (Contd.)

CD MAXNOI. MAXIMUM VALUE OF NOLRES OVER ALL REGIONS
CD MAXGRP MAXIMUM VALUE OF NOLINT OVER ALL REGIONS
CD MAXGPH MAXIMUM VALUE OF NOLINT OVER THE HOMOGENEOUS MIXTURE (REGION 1)

CR RESONANCE SPECIFICATIONS (TYPE 2)
CC ALWAYS PRESENT
CL NOLRES, N1MIN, N2MAX
CW 3
CD N1MIN HIGHEST ENERGY ULTRA FINE GROUP HAVING LORENTZIAN SHAPE RESONANCE INTEGRALS
CD N2MAX LOWEST ENERGY ULTRA FINE GROUP HAVING LORENTZIAN SHAPE RESONANCE INTEGRALS

CR RESONANCE NUMBERS (TYPE 3)
CC PRESENT ONLY IF NOLRES > 0
CL LRFSNO(I), I=1, NOLRES
CW NOLRES
CD LRFSNO RESOLVED RESONANCE NUMBERS FOR RESONANCES HAVING A LORENTZIAN SHAPE TREATMENT

CR ULTRA FINE GROUP NUMBERS (TYPE 4)
CC PRESENT ONLY IF NOLRES > 0
CL NOLINT, N1, N2
CW 3
CD N1 HIGHEST ENERGY ULTRA FINE GROUP HAVING
<table>
<thead>
<tr>
<th>CD</th>
<th>LORENTZIAN SHAPE RESONANCE INTEGRALS</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD</td>
<td>LOWEST ENERGY ULTRA FINE GROUP HAVING</td>
</tr>
<tr>
<td>CD</td>
<td>LORENTZIAN SHAPE RESONANCE INTEGRALS</td>
</tr>
<tr>
<td>C</td>
<td></td>
</tr>
<tr>
<td>C-----</td>
<td>--------------------------------------</td>
</tr>
<tr>
<td>CP</td>
<td>LORENTZIAN RESONANCE INTEGRALS (TYPE 5)</td>
</tr>
<tr>
<td>C</td>
<td>PRESENT ONLY IF NORES.GT.0</td>
</tr>
<tr>
<td>C</td>
<td></td>
</tr>
<tr>
<td>CL</td>
<td>CJINTL(I), I=1, NOLINT</td>
</tr>
<tr>
<td>C</td>
<td>NOLINT</td>
</tr>
<tr>
<td>C</td>
<td></td>
</tr>
<tr>
<td>CD</td>
<td>CJINTL</td>
</tr>
<tr>
<td>C</td>
<td>LORENTZIAN SHAPE RESONANCE INTEGRALS</td>
</tr>
<tr>
<td>C</td>
<td></td>
</tr>
<tr>
<td>C-----</td>
<td>--------------------------------------</td>
</tr>
</tbody>
</table>

CEOF
## APPENDIX D. MC²-2 Binary Files. MACTOT

<table>
<thead>
<tr>
<th>CD</th>
<th>NREC</th>
<th>Number of Records in the Data Set</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD</td>
<td>NREC=1 FOR HOMOGENEOUS PROBLEMS</td>
<td></td>
</tr>
<tr>
<td>CD</td>
<td>NREC=3 FOR CYLINDRICAL GEOMETRY</td>
<td></td>
</tr>
<tr>
<td>CD</td>
<td>NREC=1 + THE NUMBER OF SLAB REGIONS FOR SLAB GEOMETRY</td>
<td></td>
</tr>
</tbody>
</table>

### File Structure

<table>
<thead>
<tr>
<th>CS</th>
<th>Record Type</th>
<th>Present If</th>
</tr>
</thead>
<tbody>
<tr>
<td>CS</td>
<td>-----------------------------</td>
<td>-----------------------------</td>
</tr>
<tr>
<td>CS</td>
<td><em><strong>(REPEAT NREC TIMES)</strong></em></td>
<td></td>
</tr>
<tr>
<td>CS</td>
<td>* MACROSCOPIC TOTAL CROSS SECTION</td>
<td>ALWAYS</td>
</tr>
</tbody>
</table>

### Macroscopic Total Cross Section (Type 1)

| CL   | (SIGMAT(I),I=1,NGROUP)       |                                |
| CL   | NGROUP                       |                                |
| CD   | SIGMAT                       | Macrossopic Total Cross Section (1/CY) |
| CD   | NGROUP                       | Number of Energy Groups        |
APPENDIX D. MC²-2 Binary Files. MACTOT (Contd.)

PREPARED 3/10/75 AT ANL

MACTOT

ULTRA FINE GROUP TOTAL CROSS SECTIONS

BOTH CONFIGURATIONS OF THIS SCRATCH DATA SET MACTOT ARE WRITTEN BY MC²-2-II AREA 10 (CSCO11). THE FIRST CONFIGURATION CONTAINS ULTRA FINE GROUP MICROSCOPIC TOTAL CROSS SECTIONS. THE SECOND CONFIGURATION CONTAINS ULTRA FINE GROUP MACROSCOPIC TOTAL CROSS SECTIONS.

FIRST ULTRA FINE GROUP READ FOR CURRENT PASS
LAST ULTRA FINE GROUP READ FOR CURRENT PASS
NUMBER OF TYPE 1 RECORDS PRESENT IN THE FILE.
IF NULTRA.GT.NUPGRD*NPASS, THERE WILL BE ONE ADDITIONAL RECORD READ FOR THE REMAINING NULOCTRA-NPASS*NUPGRD ULTRA FINE GROUPS
NUMBER OF MATERIALS IN THE PROBLEM MIXTURE WHICH HAVE TABULATED TOTAL CROSS SECTIONS IN THE AREA 10 (CSCO11) ENERGY RANGE
NUMBER OF ULTRA FINE GROUPS READ PER PASS. NUPGRD=I2-I1+1

FILE STRUCTURE

RECORD TYPE

PRESENT IF

(REPEAT NPRMT0 TIMES)
THE CURRENT MATERIAL HAS TOTAL CROSS SECTIONS IN THE AREA 10 (CSCO11) ENERGY RANGE
APPENDIX D. MC²-2 Binary Files. MACTOT (Contd.)

ULTRA FINE GROUP TOTAL CROSS SECTIONS (TYPE 1)
ALWAYS PRESENT

(SIGTOT(I), I=NIUF, NG)
NGROUP-NIUF+1

SIGTOT(I) ULTRA FINE GROUP MICROSCOPIC TOTAL CROSS
SECTION FOR ULTRA FINE GROUP I
NIUF HIGHEST ENERGY ULTRA FINE GROUP ON THE AREA 10
(CSC01) ENERGY RANGE
NGROUP LOWEST ENERGY ULTRA FINE GROUP IN THE PROBLEM

FILE STRUCTURE

RECORD TYPE

****** (REPEAT NPASS TIMES)
*
ULTRA FINE GROUP MACROSCOPIC TOTAL
*
CROSS SECTIONS

******

ULTRA FINE GROUP MACROSCOPIC TOTAL CROSS SECTIONS
NULTRA.GT.
NUFGRD*NPASS

ULTRA FINE GROUP MACROSCOPIC TOTAL CROSS SECTIONS (TYPE 1)
ALWAYS PRESENT
APPENDIX D. MC\(^2\)-2 Binary Files. MACTOT (Contd.)

C
CL  \((\text{SIGTOT}(M,I), M=1, \text{NCMPFL}), I=I1, I2)\)
C
CW \text{NCMPFL*NUFGRD}
C
CD \text{SIGTOT}(M,I) \quad \text{ULTRA FINE GROUP MACROSCOPIC TOTAL CROSS SECTION FOR COMPOSITION M AND ULTRA FINE GROUP I}
CD \text{NCMPFL} \quad \text{NUMBER OF COMPOSITIONS PLUS NUMBER OF FOILS IN THE PROBLEM}
C
CN \text{NUFGRD ULTRA FINE GROUPS ARE READ FOR EACH PASS WHERE NUFGRD}=I2-I1+1. THERE WILL BE ONE ADDITIONAL RECORD AFTER THE NPASS RECORDS WHICH CONTAINS NULTRA-NPASS*NUFGRD ULTRA FINE GROUPS IF NULTRA IS NOT AN INTEGRAL MULTIPLE OF NUFGRD. NULTRA IS THE NUMBER OF ULTRA FINE GROUPS IN THE AREA 10 (CSC011) ENERGY RANGE
C
C---

CEOF
APPENDIX D. MC²-2 Binary Files. MICROT

C******************************************************************************
C
C PREPARED 3/06/75 AT ANL
C
C CF MICROT
CN MICROSCOPIC TOTAL CROSS SECTIONS
CN
CN THIS DATA SET IS WRITTEN BY MC**2-II AREA 5
CN (CSC004), AREA 6 (CSC005) AND/OR AREA 6.5
CN (CSC006)
C
C******************************************************************************

CD NPRMAT NUMBER OF PROBLEM MATERIALS

C----------------------
CS FILE STRUCTURE
CS
CS RECORD TYPE
CS =-----------------
CS =-----------------
CS =-----------------
CS =-----------------
CS * (REPEAT FOR NPRMAT MATERIALS)
CS * MICROSCOPIC TOTAL CROSS SECTION ALWAYS
C
C----------------------

CR MICROSCOPIC TOTAL CROSS SECTION (TYPE 1)
C
CC ALWAYS PRESENT
C
CL (SIGMAT(I),I=1,NGROUP)
C
CW NGROUP
C
CD SIGMAT MICROSCOPIC TOTAL CROSS SECTION (BARKS)
CD NGROUP NUMBER OF ENERGY GROUPS
C
C
CEOFS


APPENDIX D. MC$^2$-2 Binary Files. OLDSGS.

C******************************************************************************
C
C PREPARED 3/19/75 AT ANL
C
CF OLDSGS
CE MICROSCOPIC ELASTIC SCATTERING
C
CN THIS FILE IS READ BY MC$^2$-II AREA 7 (CSC008).
CN THE FORMAT OF THIS DATA SET IS IDENTICAL TO THAT OF DATA SET SMSIGS
C
C******************************************************************************

CEOF
APPENDIX D. MC²-2 Binary Files. OPTICL

PREPARED 3/06/75 AT ANL

SLAB GEOMETRY OPTICAL THICKNESSES

THIS DATA SET IS WRITTEN BY MC²-II AREA 5 (CSCO04), AREA 6 (CSCO05) AND/OR AREA 6.5 (CSCO06) AND IS PRESENT IF NGEOM.EQ.1

********** (REPEAT FOR NREG SLAB REGIONS)
*C
SIGLXL SIGRXR
ALWAYS

**********

FILE STRUCTURE

RECORD TYPE

=====

******* (REPEAT FOR NREG SLAB REGIONS)
CS
UTILITY

C

SIGNAL XL SIGMA XR (TYPE 1)
ALWAYS PRESENT

((SIGLXL(I,K), I = 1, MAXHTM), K = 1, NGROUP),

1((SIGRXR(I,K), I = 1, MAXHTM), K = 1, NGROUP)

MAXHTM*NGROUP*2

SIGLXL

OPTICAL THICKNESS TO THE LEFT OF THE CURRENT SLAB REGION FOR MATERIAL I AND GROUP K. THE CONNECTION BETWEEN I AND PROBLEM MATERIAL IS DETERMINED BY THE ARRAY MATHET (SEE DATA SET PRBSPC)

SIGRXR

OPTICAL THICKNESS TO THE RIGHT OF THE CURRENT SLAB REGION FOR MATERIAL I AND GROUP K. THE CONNECTION BETWEEN I AND PROBLEM MATERIAL IS DETERMINED BY THE ARRAY MATHET (SEE DATA SET PRBSPC)
APPENDIX D. MC^2-2 Binary Files. OPTICL (Contd.)

<table>
<thead>
<tr>
<th>CD</th>
<th>MAXHTM</th>
<th>MAXIMUM NUMBER OF MATERIALS IN ANY HETEROGENEOUS REGION</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD</td>
<td>NGROUP</td>
<td>NUMBER OF ENERGY GROUPS</td>
</tr>
<tr>
<td>C</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CN</td>
<td></td>
<td>SOME REGIONS WILL HAVE SIGLXL AND SIGRXR FILLED OUT WITH ZEROS IF THERE ARE FEWER MATERIALS THAN MAXHTM TREATED HETEROGENEOUSLY</td>
</tr>
<tr>
<td>CN</td>
<td></td>
<td>IN THAT REGION</td>
</tr>
<tr>
<td>C</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
APPENDIX D. MC²-2 Binary Files. PRBCHI

**************************************************************************************
PREPARED 3/12/75 AT ANL

PRBCHI
FISSION SPECTRUM DATA

THIS FILE IS WRITTEN BY MC**2-II AREA 7 (CSC008)

**************************************************************************************

CD    NCHI
FISSION SPECTRUM VECTOR OR MATRIX FLAG
NCHI=1 FOR VECTOR CHI
NCHI.GT.1 FOR MATRIX CHI

CD    NGROUP
NUMBER OF UFG IN MC**2 LIBRARY

CD    NGRP
NUMBER OF UPG IN PROBLEM

CD    NUMCHI
NUMBER OF FISSION SPECTRA IN PROBLEM

C FILE STRUCTURE

C RECORD TYPE PRESENT IF
C ==---------------------------------==
C SPECIFICATIONS ALWAYS
C PROBLEM MATERIAL CORRESPONDENCE ALWAYS
C FISSION SPECTRUM FLAG ALWAYS
C FISSION SPECTRUM USE COUNT ALWAYS
C ******** (REPEAT FOR NUMCHI SPECTRA)
C * FISSION SPECTRUM VALUES NCHI.EQ.1
C * FISSION SPECTRUM PARAMETERS NCHI.GT.1
C * *** (REPEAT FOR ALL ISOTOPES USING
C * SPECTRUM)
C * * FISSION CROSS SECTIONS NUMCHI.GT.1
C ********

C SPECIFICATIONS (TYPE 1)
ALWAYS PRESENT
NUMCHI
1
APPENDIX D. MC²-2 Binary Files. PRBCHI (Contd.)

---

CR                  PROBLEM MATERIAL CORRESPONDENCE (TYPE 2)
CR                  ALWAYS PRESENT
CR                  (IFIS(I), I=1,NPRMAT)
CW                  NPRMAT
CD                  IFIS                  FISSION SPECTRUM IDENTIFICATION
CD                  IFIS=0 PROBLEM MATERIAL IS NOT FISSIONABLE
CD                  IFIS=N PROBLEM MATERIAL USES THE N'TH FISSION SPECTRUM

---

CR                  FISSION SPECTRUM FLAG (TYPE 3)
CR                  ALWAYS PRESENT
CR                  (NCHI(I), I=1,NUMCHI)
CW                  NUMCHI

---

CR                  FISSION SPECTRUM USE COUNT (TYPE 4)
CR                  ALWAYS PRESENT
CR                  (LCHI(I), I=1,NUMCHI)
CW                  NUMCHI
CD                  LCHI                  NUMBER OF PROBLEM MATERIALS USING A GIVEN FISSION SPECTRUM DISTRIBUTION

---

CR                  FISSION SPECTRUM VALUES (TYPE 5)
C
APPENDIX D. MC²-2 Binary Files. PRBCHI (Contd.)

CC PRESENT IF NCHI.EQ.1
CL (CHI(I),I=1,NGRP)
CW NGRP
CD CHI FRACTION OF FISSION NEUTRONS BORN IN GROUP

CR FISSION SPECTRUM PARAMETERS (TYPE 6)
CC PRESENT IF NCHI.GT.1
CL (BETA(I),I=1,NGROUP), (ALPHA(I),I=1,NGROUP),
CL 1(TAU(I),I=1,NGROUP), (ANORM(I),I=1,NGRP)
CW 3*NGROUP+NGRP.
CD ALPHA FRACTIONAL PROBABILITY OF USING EVAPORATION
CD SPECTRUM LAW. 1-ALPHA IS FRACTIONAL
CD PROBABILITY OF USING FISSION DISTRIBUTION LAW.
CD BETA NUCLEAR TEMPERATURE (EV.) FOR EVAPORATION
CD SPECTRUM LAW
CD TAU NUCLEAR TEMPERATURE (EV.) FOR FISSION
CD DISTRIBUTION LAW
CD ANORM FISSION SPECTRUM NORMALIZATION FACTOR

CR FISSION CROSS SECTIONS (TYPE 7)
CC PRESENT IF NUMCHI.GT.1
CL (BSIGF(I),I=1,NGRP)
CW NGRP
CD BSIGF ISOTOPIC ATOM DENSITY*NUMBER OF NEUTRONS
CD PER FISSION*MICROSCOPIC FISSION CROSS SECTION

'CEOF
APPENDIX D. MC\(^2\)-2 Binary Files. PRBSPC

C*******************************************************************************
C PREPARED 10/29/75 AT ANL
C
CF PRBSPC
CE BINARY VERSION OF MC\(^2\)-II BCD INPUT DATA
C
C*******************************************************************************

CD BSQ1 FIXED OR FIRST GUESS FOR BUCKLING
CD ICHI ICHI=0, USE LIBRARY FISSION SPECTRA FOR ALL
CD MATERIALS IN THE PROBLEM
CD =1, USE FISSION SPECTRUM OF MATERIAL
CD IDENTIFIED IN FISSION SPECTRUM RECORD
CD FOR ALL MATERIALS IN THE PROBLEM
CD =NPRMAT, USE FISSION SPECTRUM OF MATERIAL
CD GIVEN IN FISSION SPECTRUM RECORD
CD FOR THE PROBLEM MATERIAL I
CD MAXHTM MAXIMUM NUMBER OF MATERIALS TREATED
CD HETEROGENEOUSLY IN ANY REGION. FOR
CD CYLINDRICAL PROBLEMS, ONLY REGION 1 IS
CD CONSIDERED
CD MULT 2 FOR IBM MACHINES, 1 OTHERWISE
CD NRG1 1+THE NUMBER OF EPI-THermal BROAD GROUPS
CD NCMP NUMBER OF COMPOSITIONS FOR USE IN HETEROGEOUS
CD REGIONS AS DEFINED ON DATA SET A.MIP TYPE 14
CD CARDS
CD NE3P NUMBER OF POINTS IN THE FIXED UNRESOLVED
CD RESONANCE ENERGY MESH
CD NFLMAT NUMBER OF MATERIALS USED IN FOILS IN THE
CD INTEGRAL TRANSPORT THEORY CALCULATION
CD NFOTLS NUMBER OF FOILS TO BE EDITED IN THE INTEGRAL
CD TRANSPORT THEORY CALCULATION
CD NGROUP NUMBER OF UPG IN THE PROBLEM
CD NPRMAT NUMBER OF MATERIALS IN THE HOMOGENEOUS
CD MIXTURE OF THE PROBLEM
CD NREG NUMBER OF HETEROGENEOUS REGIONS. NREG=1 FOR
CD A HOMOGENEOUS PROBLEM (NGEOM=0), NREG=2 FOR
CD CYLINDRICAL GEOMETRY (NGEOM=2), AND NREG EQUALS
CD THE NUMBER OF PLATES FOR SLAB GEOMETRY (NGEOM=1)

CD SPECIFICATIONS (TYPE 1)
CD
CC ALWAYS PRESENT
C
CL NPRMAT,NGROUP,NGCSD,NGROP,NORDER,ISPOPT,ICSOPT,ITRANS,NGEOM,
APPENDIX D. MC$^2$-2 Binary Files. PRSPC (Contd.)

CL 1NREG, NHFP, ICHI, IBSQ, MAXSIZ, MAXBLK, THETA, CAPSQR, AMIN, MAXHTM, -
CL 2MATSIB, NOHET, WISEF, NUNRES, NBG, NOVRLP, NCAND, IPRINT, NCSD, NCMP, -
CL 3A1, A2, IZORS, NITBG, NUFGIG, NHFGDW, NFOILS, NINGRP, NLEAK, NFLMAT, -
CL 4RESTST, HOMTEM, INELAS, NHYDRO -
C C -
C CW 43 -
C CD MGCSD UFG NUMBER AT WHICH THE CONTINUOUS SLOWING -
CD CALCULATION BEGINS -
CD NGROP LIBRARY UFG NUMBER CORRESPONDING TO THE -
CD HIGHEST UFG OF THE PROBLEM -
CD NORDER ORDER OF THE EXTENDED TRANSPORT APPROXIMATION -
CD ISPOPT SPECTRUM OPTION -
CD ISPOPT=1, P1 -
CD =2, B1 -
CD =3, CONSISTENT P1 -
CD =4, CONSISTENT B1 -
CD ICSOPT CONTINUOUS SLOWING DOWN PARAMETER OPTION -
CD ICSOPT=0, IMPROVED GOERTZEL-GREULING -
CD =1, ORDINARY GOERTZEL-GREULING -
CD ITRANS TRANSPORT APPROXIMATION -
CD ITRANS=0, USE ALL LEGENDRE COMPONENTS -
CD =1, USE STANDARD TRANSPORT APPROXIMATION -
CD =2, USE IMPROVED TRANSPORT APPROXIMATION -
CD NGEOM GEOMETRY OPTION -
CD NGEOM=0, HOMOGENEOUS -
CD =1, SLAB GEOMETRY -
CD =2, CYLINDRICAL GEOMETRY -
CD NHFG MAXIMUM NUMBER OF HYPER FINE GROUPS PER -
CD ULTRA FINE GROUP TO BE USED IN CALCULATING -
CD ELASTIC SCATTERING MATRICES -
CD IBSQ BUCKLING OPTION -
CD IBSQ=-1, DO NOT ITERATE ON BUCKLING AND -
CD BUCKLING IS NOT ENERGY DEPENDENT -
CD =0, ITERATE ON BUCKLING AND BUCKLING IS -
CD NOT ENERGY DEPENDENT -
CD =1, DO NOT ITERATE ON BUCKLING AND -
CD BUCKLING IS GROUP DEPENDENT -
CD MAXSIZ NUMBER OF REAL*8 WORDS ASSIGNED TO THE MAIN -
CD CORE CONTAINER ARRAY -
CD MAXBLK NUMBER OF REAL*8 WORDS ASSIGNED TO THE BULK -
CD CORE CONTAINER ARRAY -
CD THETA CONTINUOUS SLOWING DOWN INTEGRATING FACTOR -
CD CAPSQR KAPPA SQUARED, THE BUCKLING USED IN -
CD CALCULATING THE EXTENDED TRANSPORT CROSS -
CD SECTION AND THE LEAKAGE TERM FOR THE -
CD RESONANCE INTEGRAL CALCULATIONS -
CD AMIN MASS OF MATERIAL USED IN DETERMINATION OF THE -
CD DATA MANAGEMENT STRATEGY FOR THE SPECTRUM -
CD CALCULATION. AMIN.LE. THE MASS OF THE -
<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>MATSLB</td>
<td>Lightest material in the problem (excluding H)</td>
</tr>
<tr>
<td>NOHET</td>
<td>Includes overlap calculation for upper to NCAND neighboring resonances</td>
</tr>
<tr>
<td>NUNRES</td>
<td>Number of resolved resonances to be tested for overlap on each side of each resolved resonance. NCAND will be 1 if NUNRES=1</td>
</tr>
<tr>
<td>NOVRLP</td>
<td>Unresolved resonance self-overlap option</td>
</tr>
<tr>
<td>NCAND</td>
<td>Number of resolved resonances</td>
</tr>
<tr>
<td>IPRINT</td>
<td>Bpointer debugging print flag</td>
</tr>
<tr>
<td>NCSD</td>
<td>Number of ultra fine groups per continuous slowing down group</td>
</tr>
<tr>
<td>A1</td>
<td>Constant used in the equivalence principle</td>
</tr>
<tr>
<td>A2</td>
<td>Constant used in the equivalence principle</td>
</tr>
<tr>
<td>ISORS</td>
<td>If 0, no external sources are used. If 1, external sources are used</td>
</tr>
<tr>
<td>NITBG</td>
<td>Highest energy broad group number for which integral transport theory resolved resonance cross sections may be calculated. If NITBG=0, the integral transport theory calculation will not be invoked</td>
</tr>
<tr>
<td>NUFSGIG</td>
<td>Number of ultra fine groups per intermediate group for the integral transport calculation</td>
</tr>
<tr>
<td>NHFGRDN</td>
<td>Number of hyper fine groups per Doppler width used for the integral transport calculation</td>
</tr>
<tr>
<td>NINGRP</td>
<td>Ingroup scattering option</td>
</tr>
<tr>
<td>NLEAK</td>
<td>Transverse leakage option</td>
</tr>
<tr>
<td>NESTST</td>
<td>Criterion used for selection of resonances to be included in the integral transport calculation</td>
</tr>
<tr>
<td>HOMTEM</td>
<td>Temperature of homogeneous mixture for integral transport calculations</td>
</tr>
<tr>
<td>INELAS</td>
<td>Inelastic and (n,2n) ultra-fine-group treatment</td>
</tr>
</tbody>
</table>

**APPENDIX D. MC²-2 Binary Files. PRBSPC (Contd.)**

- LATEST MATERIAL IN THE PROBLEM (EXCLUDING H) -
- MATSLB=NPRMAT IF NGEOM.EQ.1. OTHERWISE MATSLB=1 -
- NOHET=NPRMAT IF NGEOM.GT.0. OTHERWISE NOHET=1 -
- RESOLVED RESONANCE OVERLAP OPTION  -
- NUNRES=0, INCLUDE OVERLAP CALCULATION FOR UP TO NCAND NEIGHBORING RESONANCES -
- NOVRLP UNRESOLVED RESONANCE SELF-OVERLAP OPTION -
- NOVRLP=0, INCLUDE SELF-OVERLAP CALCULATION -
- NCAND NUMBER OF RESOLVED RESONANCES TO BE TESTED FOR OVERLAP ON EACH SIDE OF EACH RESOLVED RESONANCE. NCAND WILL BE 1 IF NUNRES=1 -
- IPRINT BPOINTER DEBUGGING PRINT FLAG -
- IPRINT=0, NO DEBUGGING PRINTOUT -
- IPRINT=1, DEBUGGING DUMP PRINTOUT -
- IPRINT=2, DEBUGGING TRACE PRINTOUT -
- IPRINT=3, FULL DEBUGGING PRINTOUT -
- NCSD NUMBER OF ULTRA FINE GROUPS PER CONTINUOUS SLOWING DOWN GROUP -
- A1 CONSTANT USED IN THE EQUIVALENCE PRINCIPLE -
- A2 CONSTANT USED IN THE EQUIVALENCE PRINCIPLE -
- ISORS IF 0, NO EXTERNAL SOURCES ARE USED. IF 1, EXTERNAL SOURCES ARE USED -
- NITBG HIGHEST ENERGY BROAD GROUP NUMBER FOR WHICH INTEGRAL TRANSPORT THEORY RESOLVED RESONANCE CROSS SECTIONS MAY BE CALCULATED. IF NITBG=0, THE INTEGRAL TRANSPORT THEORY CALCULATION WILL NOT BE INVOKED -
- NUFSGIG NUMBER OF ULTRA FINE GROUPS PER INTERMEDIATE GROUP FOR THE INTEGRAL TRANSPORT CALCULATION -
- NHFGRDN NUMBER OF HYPER FINE GROUPS PER DOPPLER WIDTH USED FOR THE INTEGRAL TRANSPORT CALCULATION -
- NINGRP INGROUP SCATTERING OPTION -
- NINGRP=0, INCLUDE INGROUP SCATTERING IN THE INTEGRAL TRANSPORT CALCULATION -
- NINGRP=1, OMIT THE INGROUP SCATTERING -
- NLEAK TRANSVERSE LEAKAGE OPTION -
- NLEAK=0, OMIT THE TRANSVERSE LEAKAGE CORRECTION IN THE INTEGRAL TRANSPORT CALCULATION -
- NLEAK=1, INCLUDE TRANSVERSE LEAKAGE CORRECTION USING CAPSQR FOR THE BUCKLING -
- NESTST CRITERION USED FOR SELECTION OF RESONANCES TO BE INCLUDED IN THE INTEGRAL TRANSPORT CALCULATION -
- HOMTEM TEMPERATURE OF HOMOGENEOUS MIXTURE FOR INTEGRAL TRANSPORT CALCULATIONS -
- INELAS INELASTIC AND (N,2N) ULTRA-FINE-GROUP TREATMENT -
- INELAS=0, RIGOROUS TREATMENT -
- INELAS=1, APPROXIMATE TREATMENT -
APPENDIX D. MC\(^2\)-2 Binary Files. PRBS (Contd.)

**CD** NHYDRO HYDROGEN TREATMENT

**CD** NHYDRO=0, HYDROGEN IS NOT IN THE PROBLEM MIXTURE

**CD** =1, HYDROGEN IS PRESENT IN THE PROBLEM MIXTURE

---------------------------------------------------------------------

**CR** PROBLEM NAMES (TYPE 2)

**CC** ALWAYS PRESENT

**CL** (PRBNAM(I), I=1, NPRMAT), (ALIAS(I), I=1, NPRMAT),

**CL** 1 (IEDIT(I), I=1, NPRMAT), (ISTYPE(I), I=1, NPRMAT),

**CL** 2 (EFISS(I), I=1, NPRMAT), (ECAP(I), I=1, NPRMAT)

**CW** 2*MULT*NPRMAT+4*NPRMAT

**CD** PRBNAM REAL*8 NAMES OF LIBRARY NUCLIDES CORRESPONDING TO PROBLEM MATERIALS

**CD** ALIAS REAL*8 ALIAS NAMES OF PROBLEM MATERIALS

**CD** IEDIT(I) 0 IF MATERIAL I IS TO BE ADDED TO THE OUTPUT CROSS SECTION DATA SET, 1 IF MATERIAL I IS NOT TO BE ADDED TO THE OUTPUT DATA SET

**CD** ISTYPE MATERIAL TYPES

**CD** ISTYPE=1, FISSILE

**CD** =2, FERTILE

**CD** =3, OTHER ACTINIDE

**CD** =4, FISSION PRODUCT

**CD** =5, STRUCTURAL

**CD** =6, COOLANT

**CD** =7, CONTROL

**CD** EFISS ENERGY RELEASE FOR FISSION (MEV/FISSION)

**CD** ECAP ENERGY RELEASE FOR CAPTURE (MEV/CAPTURE)

---------------------------------------------------------------------

**CR** HOMOGENEOUS ATOM DENSITIES (TYPE 3)

**CC** ALWAYS PRESENT

**CL** (ATMDEN(I), I=1, NPRMAT)

**CW** NPRMAT

**CD** ATMDEN ATOMIC DENSITIES OF PROBLEM MATERIALS IN THE
APPENDIX D. MC²-2 Binary Files. PRBSPC (Contd.)

HOMOGENOUS MIXTURE

TEMPERATURES (TYPE 4)
Always present

(TEMP(I), I=1, NPRMAT), (CHITEM(I), I=1, NPRMAT)

2*NPRMAT

TEMPERATURES OF PROBLEM MATERIALS, DEGREES K
FISSION SPECTRUM TEMPERATURES IN E.V. FOR THE
PROBLEM MATERIALS. CHITEM(I)=0.0 IF MATERIAL I WAS NOT SPECIFIED ON THE DATA SET A.MCC2
TYPE 23 CARDS

HETEROGENOUS ATOM DENSITIES (TYPE 5)
Present only if MAXHTM.GT.0

((HETDEN(I,K), I=1, NPRMAT), K=1, NREG)

NPRMAT*NREG

HETDEN ATOMIC DENSITIES OF MATERIALS IN HETEROGENOUS REGIONS

HETEROGENOUS MATERIAL DESIGNATIONS (TYPE 6)
Present only if NGEOM.GT.0

((MATHT(I,K), I=1, NPRMAT), K=1, NREG1)

NPRMAT*NREG1

MATHT MATHT(I,K) IS .GT.0 IF MATERIAL I IS A RESONANCE MATERIAL AND IS TREATED HETEROGENOUSLY IN REGION K. OTHERWISE MATHT=( 
APPENDIX D. MC²-2 Binary Files. PRBSPC (Contd.)

CD MATHET(I,K) IS INDEXED BY 1 FOR EACH MATERIAL I TO BE TREATED HETEROGENEously IN EACH REGION K. ANY MATERIAL HAVING MATHET=0 WILL NOT BE INVOLVED IN THE CALCULATION OF RESONANCE OVERLAP FOR ANY OTHER MATERIAL IN THAT REGION.

CD NREG1 1 IF NGEOM=2, NREG IF NGEOM=1

---------------------------------------------------------------

CR ATOM DENSITIES TIMES LEFT SLAB THICKNESSES (TYPE 7)
CC PRESENT ONLY IF NGEOM.EQ.1 AND MAXHTM.GT.0
CL (((SXL(I,J,K),I=1,MAXHTM),J=1,NPRMAT),K=1,NREG)
CW MAXHTM*NPRMAT*NREG
CD SXL SUM OF ATOM DENSITY*THICKNESS OF SLAB REGIONS FOR EACH MATERIAL I IN SLAB REGION K, FOR ALL MATERIALS J IN ALL SLAB REGIONS TO THE LEFT OF REGION K. SXL IS FILLED WITH ZEROS IN REGIONS K IN WHICH THERE ARE FEWER THAN MAXHTM MATERIALS TREATED HETEROGENEOUSLY.

---------------------------------------------------------------

CR ATOM DENSITIES TIMES RIGHT SLAB THICKNESSES (TYPE 8)
CC PRESENT ONLY IF NGEOM.EQ.1 AND MAXHTM.GT.0
CL (((SXR(I,J,K),I=1,MAXHTM),J=1,NPRMAT),K=1,NREG)
CW MAXHTM*NPRMAT*NREG
CD SXR SUM OF ATOM DENSITY*THICKNESS OF SLAB REGIONS FOR EACH MATERIAL I IN SLAB REGION K, FOR ALL MATERIALS J IN ALL SLAB REGIONS TO THE RIGHT OF REGION K. SXR IS FILLED WITH ZEROS IN REGIONS K IN WHICH THERE ARE FEWER THAN MAXHTM MATERIALS TREATED HETEROGENEOUSLY.
APPENDIX D. MC2-2 Binary Files. PRBSPC (Contd.)

CR    REGION OUTER BOUNDARIES (TYPE 9)
C
CC    PRESENT ONLY IF MAXHOT.GT.0
C
CL    (R(I),I=1,NREG)
C
CW    NREG
C
CD    R
CD    OUTER DIMENSIONS ARE MEASURED RELATIVE TO THE CENTER OF REGION 1 FOR CYLINDERS, AND RELATIVE TO THE LEFT BOUNDARY OF REGION 1 FOR SLABS
C

CR    FISSION SPECTRUM (TYPE 10)
C
CC    PRESENT IF ICHI.GE.1
C
CL    (CHINAM(I),I=1,ICHI)
C
CW    MULT*ICHI
C
CD    CHINAM(I)
CD    REAL*8 LIBRARY NUCLIDE IDENTIFICATION LABEL
CD    WHOSE FISSION SPECTRUM WILL BE USED FOR PROBLEM MATERIAL I. IF ONLY ONE VALUE IS GIVEN, THE FISSION SPECTRUM OF THE GIVEN NUCLIDE WILL BE USED FOR ALL FISSIONABLE MATERIALS IN THE PROBLEM
C

CR    FIXED UNRESOLVED RESONANCE ENERGY MESH (TYPE 11)
C
CC    ALWAYS PRESENT
C
CL    (ESP(I),I=1,NESF)
C
CW    NESF
C
CD    ESP
CD    FIXED ENERGY MESH FOR UNRESOLVED RESONANCE CALCULATIONS. (ES(I).GT.ES(I+1))
APPENDIX D. MC2-2 Binary Files. PRBSFC (Contd.)

C
C-----------------------------------------------------------------------
C
C HETEROGENOUS MATERIAL EDITS (TYPE 12)
C
C PRESENT ONLY IF MAXHTM.GT.0
C
C ((LOCHET(I,K),I=1,NPRMAT),K=1,NREG)
C
C NPRMAT*NREG
C
C LOCHET(I,K) LOCHET(I,K)=0, IF MATERIAL I IS NOT A RESONANCE-
C MATERIAL OR IS NOT PRESENT IN
C REGION K
C =-1, IF MATERIAL I IN REGION K USES
C THE HOMOGENEOUS CROSS SECTIONS
C FOR MATERIAL I
C =L, IF MATERIAL I IN REGION K USES
C THE HETEROGENOUS CROSS SECTIONS
C FOR MATERIAL I IN REGION L
C
C IF LOCHET(I,K).NE.K THEN MATHET(I,K).EQ.0
C NOTE ALSO THAT FOR NGEOM=2, LOCHET(I,2) IS
C EQUAL TO 0 OR -1. MATHET IS NOT DEFINED FOR
C K=2 IN THIS CASE
C
C
C FIXED BUCKLING GUESS (TYPE 13)
C
C PRESENT ONLY IF IBSQ=-1
C
C BSQ1
C
C 1
C
C
C VARIABLE BUCKLING GUESSES (TYPE 14)
C
C PRESENT ONLY IF IBSQ=0
C
C BSQ1,BSQ2,EPS
**APPENDIX D. MC²-2 Binary Files. PRBSPC (Contd.)**

**C W** 3

**C D** BSQ2

SECOND GUESS FOR BUCKLING

**C D** EPS

CONVERGENCE CRITERION FOR BUCKLING ITERATION

**C**

**C R**

GROUP DEPENDENT BUCKLINGS (TYPE 15)

**C C**

PRESENT ONLY IF BSQ=1

**C L** (BSQ(I), I=1, NGROUP)

**C W** NGROUP

**C D** BSQ

BUCKLINGS FOR ULTRA FINE GROUPS

**C**

**C R**

COMPOSITION DENSITIES (TYPE 16)

**C C**

PRESENT ONLY IF NCMP.GT.0

**C L**

((COMDEN(I,K), I=1, NPRMAT), K=1, NCMP), (COMTEM(K), K=1, NCMP)

**C W** (NPRMAT+1)*NCMP

**C D** COMDEN(I,K)

ATOM DENSITY OF MATERIAL I IN COMPOSITION K

**C D** COMTEM(K)

COMPOSITION TEMPERATURES IN DEGREES K

**C N**

COMTEM IS USED ONLY BY THE INTEGRAL TRANSPORT THEORY CALCULATION. ALL MATERIALS IN A REGION CONTAINING A PARTICULAR COMPOSITION ARE ASSIGNED THE TEMPERATURE OF THAT COMPOSITION. NOTE THAT NOT ALL DEFINED COMPOSITIONS NEED BE ASSIGNED TO REGIONS IN A GIVEN PROBLEM. THE COMPOSITION-REGION ASSIGNMENTS ARE GIVEN IN DATA SET GEOM

**C**

**C R**

EXTERNAL SOURCES (TYPE 17)

**C C**

PRESENT ONLY IF ISORS.GT.0
APPENDIX D. MC\textsuperscript{2}-2 Binary Files. PRBSFC (Contd.)

\begin{verbatim}
C CL (SOURCE(I),I=1,NGROUP)
C CW NGROUP
C CD SOURCE EXTERNAL SOURCES FOR EACH ULTRA FINE GROUP

C------------------------------'---------------------------------------------
C------------------------------------------------------------------------
C CR BROAD-GROUP ENERGIES (TYPE 18)
C CC ALWAYS PRESENT
C CL (EBG(I),I=1,NBG1)
C CW NBG1
C CD EBG(I) UPPER ENERGY OF BROAD GROUP I. EBG(NBG1) IS THE
CD ENERGY AT THE INTERFACE BETWEEN THE THERMAL
CD GROUP AND LOWEST EPI-THERMAL BROAD GROUP

C------------------------------'---------------------------------------------
C------------------------------------------------------------------------
C CR THERMAL GROUP CROSS SECTIONS (TYPE 19)
C CC ALWAYS PRESENT
C CL (SIGCAP(I),I=1,NPRMAT),(SIGFIS(I),I=1,NPRMAT),
CL 1(GNU(I),I=1,NPRMAT),(SIGTOT(I),I=1,NPRMAT),
CL 2(SIGNA(I),I=1,NPRMAT),(SIGNP(I),I=1,NPRMAT),
CL 3(SIGND(I),I=1,NPRMAT),(SIGNH3(I),I=1,NPRMAT),
CL 4(SIGHE3(I),I=1,NPRMAT),RECVEL)
C CW 9*NPRMAT+1
C CD SIGCAP THERMAL GROUP CAPTURE CROSS SECTIONS
CD SIGFIS THERMAL GROUP FISSION CROSS SECTIONS
CD GNU THERMAL GROUP NUMBER OF NEUTRONS PER FISSION
CD SIGTOT THERMAL GROUP TOTAL CROSS SECTIONS
CD SIGNA THERMAL GROUP N-ALPHA CROSS SECTIONS
CD SIGNP THERMAL GROUP N-P CROSS SECTIONS
CD SIGND THERMAL GROUP N-D CROSS SECTIONS
CD SIGNH3 THERMAL GROUP N-H3 CROSS SECTIONS
CD SIGHE3 THERMAL GROUP N-HE3 CROSS SECTIONS
CD RECVEL THERMAL GROUP RECIPROCAL VELOCITY
\end{verbatim}
APPENDIX D. MC²-2 Binary Files. PRBSPC (Contd.)

**CN**

ANY QUANTITY HAVING THE VALUE -1.0E-20 WILL BE ASSIGNED THE CORRESPONDING LAST EPI-THERMAL GROUP VALUE FOR THE THERMAL GROUP.

**CR**

HOMOGENEOUS INFINITELY DILUTE SPECIFICATIONS (TYPE 20)

ALWAYS PRESENT

**CL**

(INFINT(I), I=1, NPRMAT)

**CW**

NPRMAT

**CD**

INFINT

IF 0, MATERIAL I IS NOT INFINITELY DILUTE.

IF 1, MATERIAL I IS ASSUMED TO BE INFINITELY DILUTE FOR THE HOMOGENEOUS RESOLVED RESONANCE CALCULATION. MATERIALS HAVING INFINT=1 ARE NOT INVOLVED IN THE OVERLAP CALCULATION OF ANY OTHER RESONANCES. THEIR RESONANCE INTEGRALS WILL BE SET TO THE INFINITELY DILUTE LIMIT OF PI/(2.*BETA)

**CR**

EDIT OPTIONS (TYPE 21)

ALWAYS PRESENT

**CL**

KUNRES, KATNUA, KRESIN, KSIGMA, KLORNZ, KUFGCS, KUFGMP, KUFGPL, KRESED, KSPEC, KGRES, KBGR, KUFGCS

**CW**

12

**CD**

KUNRES

IF 0, DO NOT EDIT DATA SET UNRES. OTHERWISE EDIT THE DATA SET

KATNUA

IF 0, DO NOT EDIT DATA SET ATNUA. OTHERWISE EDIT THE DATA SET

KRFSIN

IF 0, DO NOT EDIT DATA SET RESINT. OTHERWISE EDIT THE DATA SET

KSIGMA

IF 0, DO NOT EDIT DATA SET SIGMAP. OTHERWISE EDIT THE DATA SET

KLORNZ

IF 0, DO NOT EDIT DATA SET LORFZ. OTHERWISE EDIT THE DATA SET

KUFGCS

IF 0 EDIT ULTRA FINE GROUP MACROSCOPIC FISSION, TOTAL, TRANSPORT, AND SCATTERING CRO
APPENDIX D. MC²-2 Binary Files. PRBSFC (Contd.)

- SECTIONS. OTHERWISE DO NOT EDIT THESE DATA
- IF 0 EDIT ULTRA FINE GROUP MACROSCOPIC MODEMITING PARAMETERS. OTHERWISE DO NOT EDIT THESE DATA
- IF 0, DO NOT EDIT ULTRA FINE GROUP MICROSCOPIC SCATTERING CROSS SECTIONS, P₀ AND P₁
- ELASTIC TRANSFER MATRICES. OTHERWISE EDIT THESE DATA
- IF 0, RESONANCE CROSS SECTIONS ARE ADDED TO THE BROAD GROUP OUTPUT DATA SET. IF 1, RESONANCE CROSS SECTIONS ARE OMITTED FROM THE BROAD GROUP CROSS SECTIONS. IF 2, RESONANCE CAPTURE AND FISSION CROSS SECTIONS ARE OMITTED FROM THE BROAD GROUP CROSS SECTIONS
- IF 0, EDIT ULTRA-FINE-GROUP FLUX, CURRENT AND SLOWING DOWN DENSITIES. OTHERWISE DO NOT EDIT THESE DATA
- IF 0, DO NOT EDIT BROAD GROUP RESONANCE CROSS SECTIONS. OTHERWISE EDIT THESE DATA
- IF 0, EDIT BROAD GROUP REACTION RATES. OTHERWISE DO NOT EDIT THESE DATA

- FOIL SPECIFICATIONS (TYPE 22)
- PRESENT IF NFOILS.GT.0
- (FOILNM(K), K=1,NFOILS), (FOILMT(I), I=1,NFLMAT),
- 1 (FOILDX(K), K=1,NFOILS), (FOILDN(I,K), I=1,NFLMAT), K=1,NFOILS),
- 2 (FOILTM(K), K=1,NFOILS)
- (NFLMAT+2) *NFOILS+MULT*(NFOILS*NFLMAT)
- REAL*8 LABELS OF FOILS
- REAL*8 LABELS OF LIBRARY NUCLIDES USED IN FOILS
- FOIL THICKNESSES IN CM
- ATOMIC DENSITY OF MATERIAL I IN FOIL K
- (ATOMS/CC*1.E-24)
- FOIL TEMPERATURES IN DEGREES K

- NON-CELL AVERAGED CROSS SECTION SPECIFICATIONS (TYPE 23)
- PRESENT IF NGEOM .GT. 0
APPENDIX D. MC²-2 Binary Files. PRBSPC (Contd.)

C
CL  ((ALEDIT(N,I), N=1, NREG2), I=1, NPRMAT)
CW  NREG2*NPRMAT*MULT
CD  ALEDIT(N,T)  REAL*8 ALIAS NAME FOR PROBLEM MATERIAL I TO
CD  NREG2  BE EDITED FOR REGION N
CD  NREG+1
C
CEOF
APPENDIX D. MC²-2 Binary Files. RESDAT

C**************************************************************************************************************
C PREPARED 3/07/75 AT ANL
C RESDAT
C RESOLVED RESONANCE DATA
C THIS DATA SET IS WRITTEN BY MC**2-II AREA 6
(CSC005)
C**************************************************************************************************************

<table>
<thead>
<tr>
<th>CD</th>
<th>NRES</th>
<th>TOTAL NUMBER OF RESOLVED RESONANCES IN THE PROBLEM. THE RESONANCES ARE ORDERED ACCORDING TO DECREASING ENERGY</th>
</tr>
</thead>
</table>

C----------------- RESONANCE ENERGY - TOTAL WIDTH RATIOS (TYPE 1) -----------------------------------------------
C ALWAYS PRESENT
C (X(I), I=1, NRES)
C
<table>
<thead>
<tr>
<th>CD</th>
<th>NRES</th>
<th>2.0*RESONANCE ENERGY/GAMMA, WHERE GAMMA IS THE TOTAL LINE WIDTH FOR SINGLE LEVEL RESONANCES OR THE S-MATRIX TOTAL LINE WIDTH FOR ADLER-ADLER MULTILEVEL RESONANCES</th>
</tr>
</thead>
</table>

C----------------- TOTAL TO NEUTRON LINE WIDTH RATIOS (TYPE 2) -----------------------------------------------
C ALWAYS PRESENT
C (GAMTN(I), I=1, NRES)
C
<table>
<thead>
<tr>
<th>CD</th>
<th>NRES</th>
<th>GAMTN</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD</td>
<td>GAMTN</td>
<td>IF A EQUALS ZERO, WHERE A IS THE FACTOR WHICH MULTIPLIES CHI TO OBTAIN THE INTERFERENCE SCATTERING (SEE RECORD TYPE 4), THEN GAMTN EQUALS ZERO FOR SINGLE LEVEL RESONANCES</td>
</tr>
</tbody>
</table>
APPENDIX D. MC²-2 Binary Files. RESDAT (Contd.)

CD
CD
CD
CD
CD
CD
CD
CD
CD
CD

GAMTN = GAMT/GAMN, WHERE GAMT AND GAMN ARE RESPECTIVELY THE TOTAL AND NEUTRON LINE WIDTHS FOR ADLER-ADLER MULTILEVEL RESONANCES,

GAMTN = -0.5*(HT-HC-HF)/(A*(GT-GC-GF)), WHERE HT, HC, AND HF ARE ASYMMETRIC ADLER-ADLER PARAMETERS FOR TOTAL, CAPTURE, AND FISSION, AND GT, GC, AND GF ARE THE CORRESPONDING SYMMETRIC PARAMETERS

CR
CC
CL
CD

RESOLVED RESONANCE PEAK CROSS SECTION (TYPE 3)
ALWAYS PRESENT
(SIGO(I), I=1, NRES)
NRES
SIG0
RESOLVED RESONANCE CROSS SECTION AT RESONANCE

CR
CC
CL
CD

INTERFERENCE SCATTERING FACTOR (TYPE 4)
ALWAYS PRESENT
(A(I), I=1, NRES)
NRES
A
FACTOR TO MULTIPLY CHI TO OBTAIN INTERFERENCE SCATTERING
APPENDIX D. MC²-2 Binary Files. RESINT

PREPARED 3/05/75 AT ANL

RESINT INTERFACE DATA SET

THIS INTERFACE DATA SET IS WRITTEN BY MC²-2-IT AREA 6 (CSC005)

CD NREG

NUMBER OF REGIONS

NREG = 1 FOR HOMOGENEOUS PROBLEMS

NREG = 2 FOR CYLINDRICAL PIN PROBLEMS AND IF MAXHTM.GT.0

NREG = 1 + THE NUMBER OF SLAB REGIONS FOR SLAB PROBLEMS AND IF MAXHTM.GT.0

CD NRES

NUMBER OF RESOLVED RESONANCES

FILE STRUCTURE

RECORD TYPE

SPECIFICATIONS

RESOLVED RESONANCE GROUPS

RESOLVED RESONANCE MATERIALS

RESOLVED RESONANCE ENERGIES

(Repeat NREG times)

RESOLVED CAPTURE INTEGRALS

RESOLVED FISSION INTEGRALS

TOTAL RESONANCE INTEGRALS

(Repeat NREG times)

UNRESOLVED OVERLAP CORRECTED

CAPTURE INTEGRALS

UNRESOLVED OVERLAP CORRECTED

FISSION INTEGRALS

UNRESOLVED OVERLAP CORRECTED

TOTAL INTEGRALS

TOTAL INTEGRALS

SPECIFICATIONS (TYPE 1)
APPENDIX D. MC²-2 Binary Files. RESINT (Contd.)

<table>
<thead>
<tr>
<th>Field</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>CC</td>
<td>ALWAYS PRESENT</td>
</tr>
<tr>
<td>CL</td>
<td>NRES, NREG, NRESMT</td>
</tr>
<tr>
<td>CW</td>
<td>3</td>
</tr>
<tr>
<td>CD</td>
<td>NRESMT</td>
</tr>
<tr>
<td></td>
<td>NUMBER OF RESOLVED RESONANCE PROBLEM MATERIALS</td>
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<th>Field</th>
<th>Description</th>
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<tbody>
<tr>
<td>CR</td>
<td>RESOLVED RESONANCE GROUPS (TYPE 2)</td>
</tr>
<tr>
<td>CC</td>
<td>ALWAYS PRESENT</td>
</tr>
<tr>
<td>CL</td>
<td>NGPRES(I), I=1, NRES</td>
</tr>
<tr>
<td>CW</td>
<td>NRES</td>
</tr>
<tr>
<td>CD</td>
<td>NGPRES</td>
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<tr>
<td></td>
<td>NUMBER OF RESOLVED RESONANCE GROUPS</td>
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<th>Description</th>
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<tbody>
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<tr>
<td>CL</td>
<td>MATRES(I), I=1, NRES</td>
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<tr>
<td>CW</td>
<td>NRES</td>
</tr>
<tr>
<td>CD</td>
<td>MATRES(I)</td>
</tr>
<tr>
<td></td>
<td>PROBLEM MATERIAL NUMBER CORRESPONDING TO RESONANCE I</td>
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<table>
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<th>Field</th>
<th>Description</th>
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<tbody>
<tr>
<td>CR</td>
<td>RESOLVED RESONANCE ENERGIES (TYPE 4)</td>
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<td>ALWAYS PRESENT</td>
</tr>
<tr>
<td>CL</td>
<td>EN(I), I=1, NRES</td>
</tr>
<tr>
<td>CW</td>
<td>NRES</td>
</tr>
</tbody>
</table>
APPENDIX D. MC²-2 Binary Files. RESINT (Contd.)

CD EN RESOLVED RESONANCE ENERGIES

CR

RESOLVED CAPTURE INTEGRALS (TYPE 5)

CC ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE. ALSO PRESENT

CC FOR EACH HETEROGENEOUS REGION

CL (CJ (I), I=1, NRES)

CW NRES

CD CJ RESOLVED CAPTURE INTEGRALS

CR

RESOLVED FISSION INTEGRALS (TYPE 6)

CC ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE. ALSO PRESENT

CC FOR EACH HETEROGENEOUS REGION

CL (FJ (I), I=1, NRES)

CW NRES

CD FJ RESOLVED FISSION INTEGRALS

CR

TOTAL RESONANCE INTEGRALS (TYPE 7)

CC ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE. ALSO PRESENT

CC FOR EACH HETEROGENEOUS REGION

CL (TJ (T), I=1, NRES)

CW NRES

CD TJ TOTAL RESONANCE INTEGRALS
APPENDIX D. MC²-2 Binary Files. RESINT (Contd.)

<table>
<thead>
<tr>
<th>CR</th>
<th>UNRESOLVED OVERLAP CORRECTED CAPTURE INTEGRALS (TYPE 9)</th>
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<tbody>
<tr>
<td>CC</td>
<td>PRESENT ONLY IF PROBLEM CONTAINS UNRESOLVED DATA</td>
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<tr>
<td>CL</td>
<td>(CJFL(I), I=1, NRES)</td>
</tr>
<tr>
<td>CW</td>
<td>NRES</td>
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<tr>
<td>CD</td>
<td>CJFL</td>
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<td>CC</td>
<td>PRESENT ONLY IF PROBLEM CONTAINS UNRESOLVED DATA</td>
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<td>CL</td>
<td>(FJFL(I), I=1, NRES)</td>
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<tr>
<td>CW</td>
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<td>FJFL</td>
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<th>UNRESOLVED OVERLAP CORRECTED TOTAL INTEGRALS (TYPE 10)</th>
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<tr>
<td>CC</td>
<td>PRESENT ONLY IF PROBLEM CONTAINS UNRESOLVED DATA</td>
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<tr>
<td>CL</td>
<td>(TJFL(I), I=1, NRES)</td>
</tr>
<tr>
<td>CW</td>
<td>NRES</td>
</tr>
<tr>
<td>CD</td>
<td>TJFL</td>
</tr>
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</table>

CEOF
APPENDIX D. MC²-2 Binary Files. SCR001

C***************************************************************************************
CP               PREPARED 3/05/75 AT ANL
CP               SCRO01 SCRATCH DATA SET SCRO01
CM               THIS SCRATCH DATA SET IS WRITTEN BY
CM               MC**2-II AREA 6 (CSC005)
C***************************************************************************************
CD               NOLINT NUMBER OF ULTRA FINE GROUPS HAVING
CD               LORENTZIAN SHAPE RESONANCE INTEGRALS FOR
CD               EACH RESONANCE SO TREATED
CD               NOLRES NUMBER OF RESONANCES GIVEN A LORENTZIAN SHAPE
CD               TREATMENT FOR EACH REGION. NOLRES IS WRITTEN
CD               IN DATA SET SCRO02
C

CS               FILE STRUCTURE
CS               RECORD TYPE                     PRESENT IF
CS               =========                        =============
CS               ***** (REPEAT NOLRES TIMES)     
CS               * ULTRA FINE GROUP NUMBERS    ALWAYS
CS               * LORENTZIAN RESONANCE INTEGRALS ALWAYS
CS               *****
C

CR               ULTRA FINE GROUP NUMBERS (TYPE 1)
C   CC ALWAYS PRESENT
C   CL NOLINT,N1,N2
C   CW 3
C   CD N1 HIGHEST ENERGY ULTRA FINE GROUP HAVING
C   CD N1 LORENTZIAN SHAPE RESONANCE INTEGRALS
C   CD N2 LOWEST ENERGY ULTRA FINE GROUP HAVING
C   CD N2 LORENTZIAN SHAPE RESONANCE INTEGRALS
C
APPENDIX D. MC²-2 Binary Files. SCOOL (Contd.)

CF  LOREXTZIAN RESONANCE INTEGRALS (TYPE 2)

CC  ALWAYS PRESENT

CL  CJINTL(I), I=1, NOLINT

CM  NOLINT

CD  CJINTL  LORENTZIAN SHAPE RESONANCE INTEGRALS

CEOF
APPENDIX D. MC^2-2 Binary Files. SCR001 (Contd.)

C*******************************************************************************************
C
C PREPARED 3/07/75 AT ANL
C
C SCP001
C ULTRA FINE GROUP SCATTERING CROSS SECTIONS
C
C BOTH CONFIGURATIONS OF THIS SCRATCH DATA SET SCR001 ARE WRITTEN BY MC**2-II AREA 10
C
C (CSCO11)
C
C*******************************************************************************************

CD   I1 FIRST ULTRA FINE GROUP READ FOR CURRENT PASS
CD   I2 LAST ULTRA FINE GROUP READ FOR CURRENT PASS
CD   NPASS NUMBER OF TYPE 1 RECORDS PRESENT IN THE FILE.
CD   IF NULTRA.GT.NUFGRD*NPASS, THERE WILL BE ONE
CD   ADDITIONAL RECORD READ FOR THE REMAINING
CD   NULTRA-NPASS*NUFGRD ULTRA FINE GROUPS
CD   NPRMSC NUMBER OF MATERIALS IN THE PROBLEM MIXTURE
CD   WHICH HAVE TABULATED SCATTERING CROSS SECTIONS
CD   IN THE AREA 10 (CSCO11) ENERGY RANGE
CD   NUFGRD NUMBER OF ULTRA FINE GROUPS READ PER PASS.
CD   NUFGRD=I2-I1+1

C*******************************************************************************************
C
C FIRST CONFIGURATION
C*******************************************************************************************

CS --- FILE STRUCTURE ---
CS
CS RECORD TYPE
CS ******************************** Present if
CS "********" (REPEAT NPRMSC TIMES)
CS * THE CURRENT MATERIAL
CS * HAS SCATTERING CROSS
CS * SECTIONS IN THE AREA
CS * 10 (CSCO11) ENERGY
CS * RANGE
CS ********
C
APPENDIX D. MC²-2 Binary Files. SCRG01 (Contd.)

---

.ultra fine group scattering cross sections (type 1)
always present

(sigsct(i), i=nitupg, ngroup)

ngroup-nitupg+1

sigsct(i)    ultra fine group microscopic scattering cross section for ultra fine group i
nitupg    highest energy ultra fine group on the area 10
 Nguy    lowest energy ultra fine group in the problem

---

file structure

---

record type

---

********** (repeat npass times)
ultra fine group scattering cross always present
sections

ultra fine group scattering cross nultra.gt.
sections nufgrd*npass

---

ultra fine group scattering cross sections (type 1)
always present

((sigsct(m,i), m=1, nprmats), i=1,12)
nprmats*nufgrd
APPENDIX D. $\text{Mc}^2-2$ Binary Files. SCRO01 (Contd.)

<table>
<thead>
<tr>
<th>C</th>
<th>CD</th>
<th>SIGSCT $(m, i)$</th>
<th>ULTRA FINE GROUP SCATTERING CROSS SECTION FOR MATERIAL M AND ULTRA FINE GROUP I</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>CD</td>
<td>NUMMAT</td>
<td>NUMBER OF MATERIALS IN THE PROBLEM</td>
</tr>
<tr>
<td>C</td>
<td>CN</td>
<td>NUFGRD</td>
<td>NUFGRD ULTRA FINE GROUPS ARE READ FOR EACH PASS WHERE NUFGRD=$2^{i+1}$</td>
</tr>
<tr>
<td>C</td>
<td>CN</td>
<td></td>
<td>THERE WILL BE ONE ADDITIONAL RECORD AFTER THE NPASS RECORDS</td>
</tr>
<tr>
<td>C</td>
<td>CN</td>
<td></td>
<td>WHICH CONTAINS $\text{NULTRA}\cdot\text{NPFGRD}$ ULTRA FINE GROUPS</td>
</tr>
<tr>
<td>C</td>
<td>CN</td>
<td></td>
<td>IF $\text{NULTRA}$ IS NOT AN INTEGRAL MULTIPLE OF $\text{NUFGRD}$. $\text{NULTRA}$ IS THE NUMBER OF ULTRA FINE GROUPS IN THE AREA 10 ($\text{CSCO11}$) ENERGY RANGE</td>
</tr>
<tr>
<td>C</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

EOF
APPENDIX D. MC^2-2 Binary Files. SCR002

C******************************************************************************
C
C PREPARED 3/05/75 AT ANL
C
CF SCR002
CE CSC005 SCRATCH DATA SET SCR002
C
CN THIS SCRATCH DATA SET IS WRITTEN BY
CN MC^2-II AREA 6 (CSC005)
C
C******************************************************************************

CD NOLRES NUMBER OF RESONANCES GIVEN A LORENTZIAN SHAPE
CD NREG1 1 FOR HOMOGENEOUS PROBLEMS, 2 FOR CYLINDRICAL
CD PROBLEMS, 1+THE NUMBER OF SLAB REGIONS FOR
CD SLAB GEOMETRY PROBLEMS

C---------------------------------------------------------------
CS
CS RECORD TYPE
CS ======================================================= PRESENT IF
CS
CS ******* (REPEAT NREG1 TIMES)
CS * RESONANCE SPECIFICATIONS
CS * RESONANCE NUMBERS
CS ******
C
C---------------------------------------------------------------

C---------------------------
CR
CR RESONANCE SPECIFICATIONS (TYPE 1)
C
CC ALWAYS PRESENT
C
CL NOLRES,N1MIN,N2MAX
C
C 3
C
CD N1MIN HIGHEST ENERGY ULTRA FINE GROUP HAVING
CD LORENTZIAN SHAPE RESONANCE INTEGRAALS
CD N2MAX LOWEST ENERGY ULTRA FINE GROUP HAVING
CD LORENTZIAN SHAPE RESONANCE INTEGRAALS
C
C---------------------------------------------------------------
APPENDIX D. MC²-2 Binary Files. SCR002 (Contd.)

<table>
<thead>
<tr>
<th>CR</th>
<th>RESONANCE NUMBERS (TYPE 2)</th>
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<tbody>
<tr>
<td>C</td>
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</tr>
<tr>
<td>CC</td>
<td>ALWAYS PRESENT</td>
</tr>
<tr>
<td>CL</td>
<td>LRESNO(I),I=1,NOLRES</td>
</tr>
<tr>
<td>CW</td>
<td>NOLRES</td>
</tr>
<tr>
<td>CD</td>
<td>LRESNO</td>
</tr>
<tr>
<td></td>
<td>RESOLVED RESONANCE NUMBERS FOR RESONANCES HAVING A LORENTZIAN SHAPE TREATMENT</td>
</tr>
<tr>
<td>C</td>
<td></td>
</tr>
</tbody>
</table>

CEOFT
APPENDIX D. \( \text{MC}^2 \)-2 Binary Files. SCRQ02 (Contd.)

C******************************************************************************
C
C PREPARED 3/10/75 AT ANL
C
CF
SCR002
CE ULTRA FINE GROUP FISSION CROSS SECTIONS
C
CN BOTH CONFIGURATIONS OF THIS SCRATCH DATA SET
CN SCR002 ARE WRITTEN BY MC**2-II AREA 10
CN (CSC011)
C
C******************************************************************************

CD I1 FIRST ULTRA FINE GROUP READ FOR CURRENT PASS
CD I2 LAST ULTRA FINE GROUP READ FOR CURRENT PASS
CD NPASS NUMBER OF TYPE 1 RECORDS PRESENT IN THE FILE.
CD IF NULTRA.GT.NUFGRD*NPASS, THERE WILL BE ONE
CD ADDITIONAL RECORD READ FOR THE REMAINING
CD NULTRA-NPASS*NUFGRD ULTRA FINE GROUPS
CD NPRMFS NUMBER OF MATERIALS IN THE PROBLEM MIXTURE
CD WHICH HAVE TABULATED FISSION CROSS SECTIONS
CD IN THE AREA 10 (CSC011) ENERGY RANGE
CD NUFGRD NUMBER OF ULTRA FINE GROUPS READ PER PASS.
CD NUFGRD=I2-I1+1

C******************************************************************************
C
C
C******************************************************************************

CS FILE STRUCTURE
CS
CS RECORD TYPE
CS ************************************************************
CS PRESENT IF
CS ************************************************************
CS ****** (REPEAT NPRMFS TIMES)
CS THE CURRENT MATERIAL
CS * ULTRA FINE GROUP FISSION
CS * HAS FISSION CROSS
CS * SECTIONS IN THE AREA
CS * 10 (CSC011) ENERGY
CS * RANGE
CS
CS
C
APPENDIX D. MC\textsuperscript{2}-2 Binary Files. SCRO02 (Contd.)

**ULTRA FINE GROUP FISSION CROSS SECTIONS (TYPE 1)**

**ALWAYS PRESENT**

((SIGFIS(I), I=NITUPG, NGROUP)

NGROUP-NITUPG+1

SIGFIS(I) ULTRA FINE GROUP MICROSCOPIC FISSION CROSS SECTION FOR ULTRA FINE GROUP I

NITUPG HIGHEST ENERGY ULTRA FINE GROUP ON THE AREA 10

(CSC011) ENERGY RANGE

NGROUP LOWEST ENERGY ULTRA FINE GROUP IN THE PROBLEM

**FILE STRUCTURE**

**RECORD TYPE**

**PRESENT IF**

**RECORD TYPE**

**PRESENT IF**

**ALWAYS PRESENT**

**ULTRA FINE GROUP FISSION CROSS SECTIONS**

**ULTRA FINE GROUP FISSION CROSS SECTIONS**

**NULTRA.GT.**

**NUFGRD*NPASS**

**ULTRA FINE GROUP FISSION CROSS SECTIONS (TYPE 1)**

**ALWAYS PRESENT**

**((SIGFIS(M,I), M=1,NPRMAT), I=I1,I2)**

**NPRMAT*NUFGRD**
APPENDIX D. MC²-2 Binary Files. SCRQ02 (Contd.)

<table>
<thead>
<tr>
<th>C</th>
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<tbody>
<tr>
<td>C</td>
<td>SIGFIS(M,I)</td>
<td>ULTRA FINE GROUP FISSION CROSS SECTION FOR MATERIAL M AND ULTRA FINE GROUP I</td>
</tr>
<tr>
<td>C</td>
<td>NPRMAT</td>
<td>NUMBER OF MATERIALS IN THE PROBLEM</td>
</tr>
<tr>
<td>C</td>
<td>NPRGRD*</td>
<td>NUFGRD ULTRA FINE GROUPS ARE READ FOR EACH PASS WHERE NUFGRD=I2-I1+1. THERE WILL BE ONE ADDITIONAL RECORD AFTER THE NPASS RECORDS WHICH CONTAINS NULTRA-NPASS*NUFGRD ULTRA FINE GROUPS IF NULTRA IS NOT AN INTEGRAL MULTIPLE OF NUFGRD. NULTRA IS THE NUMBER OF ULTRA FINE GROUPS IN THE AREA 10 (CSCU11) ENERGY RANGE</td>
</tr>
</tbody>
</table>

CEOF
APPENDIX D. MC²-2 Binary Files. SCR003

C*****************************************************************************
C PREPARED 3/05/75 AT ANL
C
CP SCR003
CE CSC004 SCRATCH DATA SET SCR003
C
CN THIS SCRATCH DATA SET IS WRITTEN BY
CN MC**2-II AREA 5 (CSC004) IF UNRESOLVED
CN MATERIALS ARE PRESENT
C
C*****************************************************************************

CD IFT
FISSILE MATERIAL INDEX
CD IFI=0 FOR NON-FISSILE MATERIAL
CD IFI=1 FOR FISSILE MATERIAL
CD
CD JL NUMBER OF SPIN STATES FOR CURRENT ISOTOPE
CD
CD NESP NUMBER OF FIXED ENERGY MESH POINTS
CD
CD NISO NUMBER OF ISOTOPES
CD
CD NREG NUMBER OF REGIONS
CD
CD NREG=1 FOR HOMOGENEOUS PROBLEMS
CD
CD NREG=2 FOR CYLINDRICAL GEOMETRY
CD
CD NREG=1 + THE NUMBER OF SLAB REGIONS FOR
CD SLAB GEOMETRY
CD

C FILE STRUCTURE
C
CS RECORD TYPE
CS ******************************* PRESENT IF
CS *******************************
CS ********************** (REPEAT FOR NFRMAT MATERIALS)
CS *
CS MATERIAL SPECIFICATIONS
CS *
CS ************** (REPEAT FOR NISO ISOTOPES)
CS *
CS SPIN STATE DATA
CS *
CS LEVEL SPACING
CS *
CS ************** (REPEAT FOR 1+NO. OF REGIONS)
CS *
CS ** IN WHICH MATERIAL IS TREATED
CS *
CS *** HETEROGENEOUSLY)
CS *
CS ** CAPTURE J INTEGRAL
CS *
CS ** TOTAL J INTEGRAL
CS *
CS ** FISSION J INTEGRAL
CS *
CS *************
C
C*****************************************************************************

CR MATERIAL SPECIFICATIONS (TYPE 1)
C
APPENDIX D. MC\textsuperscript{2}-2 Binary Files. SCRQ03 (Contd.)

CC
PRESENT IF \text{NUNRES.EQ.1}

CL
\text{NISO,IFI}

CW
2

CR
SPIN STATES (TYPE 2)

CC
PRESENT IF \text{NUNRES.EQ.1}

CL
JL

CW
1

CR
LEVEL SPACING (TYPE 3).

CC
PRESENT IF \text{NUNRES.EQ.1}

\text{((D(I,J),I=1,NESF),J=1,JL)}

CW
NESP*JL

CD
D
\text{AVERAGE LEVEL SPACING}

CR
CAPTURE J INTEGRAL (TYPE 4)

CC
\text{ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE. ALSO PRESENT FOR EACH HETEROGENEOUS REGION IN WHICH CURRENT MATERIAL IS TREATED HETEROGENEously}

\text{((CJESF(I,J),I=1,NESF),J=1,JL)}

CW
NESP*JL

CD
CJESF
UNRESOLVED RESONANCE CAPTURE INTEGRAL
APPENDIX D. MC²-2 Binary Files. SCR003 (Contd.)

C-----------------------------------------------------------------------
CR TOTAL J INTEGRAL (TYPE 5)
C CC ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE.
CC ALSO PRESENT FOR EACH HETEROGENEOUS REGION IN WHICH
CC CURRENT MATERIAL IS TREATED HETEROGENEOUSLY
C CL ((TJESF(I,J),I=1,NESF),J=1, JL)
C CW NESF*JL
C CD TJESF UNRESOLVED RESONANCE TOTAL INTEGRAL
C C-----------------------------------------------------------------------
C-----------------------------------------------------------------------
C FISSION J INTEGRAL (TYPE 6)
C CC IF IF1.EQ.1, ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE.
CC ALSO PRESENT FOR EACH HETEROGENEOUS REGION IN WHICH
CC CURRENT MATERIAL IS TREATED HETEROGENEOUSLY
C CL ((FJESF(I,J),I=1,NESF),J=1, JL)
C CW NESF*JL
C CD FJESF UNRESOLVED RESONANCE FISSION INTEGRAL
C C-----------------------------------------------------------------------
CEOF
APPENDIX D. MC²-2 Binary Files. SCR003 (Contd.)

C**************************************************************************************************
C PREPARED 3/05/75 AT ANL
C
CF SCP003
CF CSC005 SCRATCH DATA SET SCR003
C
CN THIS SCRATCH DATA SET IS WRITTEN
CN BY MC²-2-II AREA 6 (CSC005)
C
C**************************************************************************************************

CD NREG
CD NUMBER OF REGIONS
CD NREG=1 FOR HOMOGENEOUS PROBLEMS
CD NREG=2 FOR CYLINDRICAL GEOMETRY
CD NREG=1 * THE NUMBER OF SLAB REGIONS
CD FOR SLAB GEOMETRY

CS---------------------------------------------
CS FILE STRUCTURE
CS---------------------------------------------
CS RECORD TYPE
CS =------------------------------------------ PRESENT IF
CS ********* (REPEAT NREG TIMES)
CS * PEAK CROSS SECTION ALWAYS PRESENT
CS *********

CS---------------------------------------------
CS PEAK CROSS SECTION (TYPE 1)
CS---------------------------------------------
CS ALWAYS PRESENT
CS---------------------------------------------
CL (NSIGO (I), I=1, MAXRES)
CS---------------------------------------------
CW MAXRES
CS---------------------------------------------
CD MAXRES MAXIMUM NUMBER OF RESOLVED RESONANCES
CD NSIGO HOMOGENIZED MACROSCOPIC SIGMA ZERO,
CD PEAK RESONANCE CROSS SECTIONS
C
CN NSIGO IS FILLED WITH ZEROS AS NECESSARY
C
CEOF
APPENDIX D. MC²-2 Binary Files. SCR003 (Contd.)

PREPARED 3/10/75 AT ANL

SCR003

ULTRA FINE GROUP CAPTURE CROSS SECTIONS

Both configurations of this scratch data set

SCR003 are written by MC²-II area 10

(CSC011)

FIRST ULTRA FINE GROUP READ FOR CURRENT PASS

LAST ULTRA FINE GROUP READ FOR CURRENT PASS

NUMBER OF TYPE 1 RECORDS PRESENT IN THE FILE.

IF NULTRA.GT.NUFGRD*NPASS, THERE WILL BE ONE

ADDITIONAL RECORD READ FOR THE REMAINING

NUTRA-NPASS*NUFGRD ULTRA FINE GROUPS

NUMBER OF MATERIALS IN THE PROBLEM MIXTURE

IN THE AREA 10 (CSC011) ENERGY RANGE

NUMBER OF ULTRA FINE GROUPS READ PER PASS.

NUFGRD=I2-I1+1

FILE STRUCTURE

RECORD TYPE

PRESENT IF

(REPEAT NPRMCP TIMES)

THE CURRENT MATERIAL

ULTRA FINE GROUP CAPTURE

HAS CAPTURE CROSS

SECTIONS IN THE AREA

(10 CSC011) ENERGY

RANGE

********

**********

**********
APPENDIX D. MC²-2 Binary Files. SCROQ3 (Contd.)

C------------------------
CR ULTRA FINE GROUP CAPTURE CROSS SECTIONS (TYPE 1)
CC ALWAYS PRESENT
CL (SIGCAP(I), I=NITUFG,NGROUP)
CN NGROUP-NITUFG+1
CD SIGCAP(I) ULTRA FINE GROUP MICROSCOPIC CAPTURE CROSS
CD SECTION FOR ULTRA FINE GROUP I
CD NITUFG HIGHEST ENERGY ULTRA FINE GROUP ON THE AREA 10
CD NGROUP LOWEST ENERGY ULTRA FINE GROUP IN THE PROBLEM

CEOF

C******************************
C* SECOND CONFIGURATION *
C******************************

C------------------------
CS FILE STRUCTURE
CS RECORD TYPE
CS ===================================================
CS (REPEAT NPASS TIMES)
CS * ULTRA FINE GROUP CAPTURE CROSS
CS * SECTIONS
CS ULTRA FINE GROUP CAPTURE CROSS
CS SECTIONS

C------------------------
CR ULTRA FINE GROUP CAPTURE CROSS SECTIONS (TYPE 1)
CC ALWAYS PRESENT
CL ((SIGCAP(M,I), M=1,NPRMAT), I=I1,I2)
CW NPRMAT*NUFGRD
<table>
<thead>
<tr>
<th>CN</th>
<th>CN</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD</td>
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<td>CN</td>
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</tr>
<tr>
<td>CN</td>
<td>CN</td>
</tr>
</tbody>
</table>

APPENDIX D. MC²-2 Binary Files. SCRQQ3 (Contd.)

**SIGCAP(M,I)**
- Ultra fine group capture cross section for material M and ultra fine group I.

**NPRMAT**
- Number of materials in the problem.

**NUFGRD**
- Ultra fine groups are read for each pass where NUFGRD = I2 - I1 + 1. There will be one additional record after the NPASS records which contains NULTRA * NPASS * NUFGRD ultra fine groups if NULTRA is not an integral multiple of NUFGRD. NULTRA is the number of ultra fine groups in the area 10 (CSCO11) energy range.

CEOF
APPENDIX D. MC²-2 Binary Files. SCR003 (Contd.)

C***************************************************************************************
C
C PREPARED 10/29/75 AT ANL
C
CF SCR003
CE CSC006 SCRATCH DATA SET
C
CN THIS SCRATCH DATA SET IS WRITTEN BY MC**2-II.
CN BOTH CONFIGURATIONS OF THIS SCRATCH DATA SET
CN SCR003 ARE WRITTEN BY MC**2-II AREA 6.5
(CSC006)
C
C***************************************************************************************

CD IFT FISSILE MATERIAL INDEX
CD IFI=0 FOR NON-FISSILE MATERIAL
CD IFI=1 FOR FISSILE MATERIAL
CD JL NUMBER OF SPIN STATES FOR CURRENT ISOTOPE
CD NESP NUMBER OF FIXED ENERGY MESH POINTS
CD NREG NUMBER OF REGIONS
CD NREG=1 FOR HOMOGENEOUS PROBLEMS
CD NREG=2 FOR CYLINDRICAL GEOMETRY
CD NREG=1 + THE NUMBER OF SLAB REGIONS FOR
CD SLAB GEOMETRY
CD NRMS NUMBER OF RESOLVED RESONANCES
CD NUMRES NUMBER OF UNRESOLVED RESONANCE MATERIALS

C***************************************************************************************
C
C=          FIRST CONFIGURATION          ===========================================
C
C***************************************************************************************

C FILE STRUCTURE

CS RECORD TYPE
CS =============== PRESENT IF
CS ===============
CS ********** (REPEAT FOR NUMRES MATERIALS)
CS * MATERIAL SPECIFICATIONS
CS * ********** (REPEAT FOR NISO ISOTOPES)
CS * * SPIN STATE DATA
CS * * LEVEL SPACING
CS * * * ***** (REPEAT FOR 1+NO. OF REGIONS
CS * * * IN WHICH MATERIAL IS TREATED
CS * * * HETEROGENEOUSLY)
CS * * * CAPTURE J INTEGRAL
CS * * * TOTAL J INTEGRAL
APPENDIX D. MC²-2 Binary Files. SCR003 (Contd.)

CS * * * FISSION J INTEGRAL
CS **********

---

CR MATERIAL SPECIFICATIONS (TYPE 1)
C
CC ALWAYS PRESENT
C
CL NISO, IFI
C
CW 2
C
CD NISO NUMBER OF ISOTOPES
C

---

CR SPIN STATE DATA (TYPE 2)
C
CC ALWAYS PRESENT
C
CL JL
C
CW 1
C

---

CR LEVEL SPACING (TYPE 3)
C
CC ALWAYS PRESENT
C
CL ((D(I,J), I=1, NESP), J=1, JL)
C
CW NESP*JL
C
CD D AVERAGE LEVEL SPACING
C

---

CR CAPTURE J INTEGRAL (TYPE 4)
C
CC ALWAYS PRESENT FOR THE HOMOGENEOUS MIXTURE.
APPENDIX D. MC²-2 Binary Files. SCRO03 (Contd.)

ALSO PRESENT FOR EACH HETEROGENEOUS REGION IN WHICH CURRENT MATERIAL IS TREATED HETEROGENEously

\[ \psi_{UJ}(I,J) = \psi_{NESP}(J) \psi_{JL}(J) \]

UNRESOLVED RESONANCE CAPTURE INTEGRAL TIMES THE TOTAL RESOLVED OVERLAP FACTOR

TOTAL J INTEGRAL (TYPE 5)

ALWAYS PRESENT FOR THE HOMOGENEOUS MIXTURE.

\[ \psi_{UJ}(I,J) = \psi_{NESP}(J) \psi_{JL}(J) \]

UNRESOLVED RESONANCE TOTAL INTEGRAL TIMES THE TOTAL RESOLVED OVERLAP FACTOR

FISSION J INTEGRAL (TYPE 6)

IF IFJ EQ 1, ALWAYS PRESENT FOR THE HOMOGENEOUS MIXTURE.

\[ \psi_{UJ}(I,J) = \psi_{NESP}(J) \psi_{JL}(J) \]

UNRESOLVED RESONANCE FISSION INTEGRAL TIMES THE TOTAL RESOLVED OVERLAP FACTOR

CEOF

************************************************************************
APPENDIX D. MC²-2 Binary Files. SCRQ03 (Contd.)

C * SECOND CONFIGURATION *
C
C ***********************************************

C-----------------------------------------------
CS
CS FILE STRUCTURE
CS
CS RECORD TYPE --------------------------------- PRESENT IF
CS
CS ********** (REPEAT NREG TIMES)
CS *
CS * RESOLVED CAPTURE INTEGRALS ALWAYS
CS *
CS * RESOLVED FISSION INTEGRALS ALWAYS
CS *
CS * TOTAL RESONANCE INTEGRALS ALWAYS
CS
CS ********

C-----------------------------------------------
CR
CR RESOLVED CAPTURE INTEGRAL (TYPE 1)
CR
CC ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE. ALSO PRESENT
CC FOR EACH HETEROGENEOUS REGION
C
CL (CJ(I), I=1,NRES)
C
CW NRES
C
CD CJ RESOLVED CAPTURE INTEGRALS TIMES THE
CD APPROPRIATE UNRESOLVED OVERLAP FACTORS
C
C-----------------------------------------------
CR
CR RESOLVED FISSION INTEGRAL (TYPE 2)
CR
CC ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE. ALSO PRESENT
CC FOR EACH HETEROGENEOUS REGION
C
CL (FJ(I), I=1,NRES)
C
CW NRES
C
CD FJ RESOLVED FISSION INTEGRALS TIMES THE
CD APPROPRIATE UNRESOLVED OVERLAP FACTORS
C
C-----------------------------------------------
APPENDIX D. MC$^2$-2 Binary Files. SCR003 (Contd.)

<table>
<thead>
<tr>
<th>CR</th>
<th>TOTAL RESONANCE INTEGRAL (TYPE 3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CC</td>
<td>ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE. ALSO PRESENT</td>
</tr>
<tr>
<td></td>
<td>FOR EACH HETEROGENEOUS REGION</td>
</tr>
<tr>
<td>CL</td>
<td>(TJ(I), I=1, NRES)</td>
</tr>
<tr>
<td>CW</td>
<td>NRES</td>
</tr>
<tr>
<td>CD</td>
<td>TJ</td>
</tr>
<tr>
<td></td>
<td>TOTAL RESONANCE INTEGRAL TIMES THE</td>
</tr>
<tr>
<td></td>
<td>APPROPRIATE OVERLAP FACTORS</td>
</tr>
</tbody>
</table>

CEOФ
APPENDIX D. MC²-2 Binary Files. SCR004

************************************************************************************
C
C PREPARED 3/10/75 AT ANL
C
CF SCR004
C ULTRA FINE GROUP FIXED SOURCES
C
CN SCRATCH DATA SET WRITTEN BY MC**2-II AREA 10
(CSC011)
C
C************************************************************************************

CD I1 FIRST ULTRA FINE GROUP READ FOR CURRENT PASS
CD I2 LAST ULTRA FINE GROUP READ FOR CURRENT PASS
CD NPASS NUMBER OF TYPE 1 RECORDS PRESENT IN THE FILE.
CD IF NULTRA.GT.NUFGRD*NPASS, THERE WILL BE ONE
CD ADDITIONAL RECORD READ FOR THE REMAINING
CD NULTRA-NPASS*NUFGRD ULTRA FINE GROUPS
CD NUFGRD NUMBER OF ULTRA FINE GROUPS READ PER PASS.
CD NUFGRD=I2-I1+1

C------------------------------------------------------------
CS FILE STRUCTURE
CS RECORD TYPE
CS ==----------------== PRESENT IF
CS """" (REPEAT NPASS TIMES)
CS * ULTRA FINE GROUP FIXED SOURCES ALWAYS PRESENT
CS """" ULTRA FINE GROUP FIXED SOURCES NULTRA.GT.
CS NUFGRD*NPASS
C
C------------------------------------------------------------

C ULTRA FINE GROUP FIXED SOURCES (TYPE 1)
C
C CC ALWAYS PRESENT
C
C CL ((SFIX(M,I),M=1,NPRMAT),I=I1,I2)
C CW NPRMAT*NUFGRD
C CD SFIX(M,I) ULTRA FINE GROUP FIXED SOURCES FOR
CD MATERIAL M AND ULTRA FINE GROUP I
C
CN NUFGRD ULTRA FINE GROUPS ARE READ FOR EACH PASS-
WHERE NUFGRD = I2-I1+1. THERE WILL BE
ONE ADDITIONAL RECORD AFTER THE NPASS RECORDS
WHICH CONTAINS NULTRA*NPASS*NUFGRD ULTRA FINE
GROUPS IF NULTRA IS NOT AN INTEGRAL MULTIPLE OF
NUFGRD. NULTRA IS THE NUMBER OF ULTRA FINE
GROUPS IN THE AREA 10 (CSC011) ENERGY RANGE
APPENDIX D. MC²-2 Binary Files. SCR005

C*******************************************************************************
C
C PREPARED 3/10/75 AT ANL
C
C CP SCR005
CE RESONANCE FOIL CROSS SECTIONS
C
C*******************************************************************************

CD NBROAD NUMBER OF BROAD GROUPS IN THE AREA 10 (CSC011)
CD NCNTF NUMBER OF RESONANCE FOIL MATERIALS
CD NFOILS NUMBER OF FOILS
CD NINTI NUMBER OF MESH INTERVALS IN THE CELL. NINTI=1
CD

C--------------------------------------------------------
CS FILE STRUCTURE
CS
CS RECOD TYPE PRESENT IF
CS -=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-=-
CS ******* (REPEAT NBROAD TIMES)
CS * FOIL CAPTURE CROSS SECTIONS ALWAYS
CS * FOIL FISSION CROSS SECTIONS ALWAYS
CS * FOIL SCATTERING CROSS SECTIONS ALWAYS
CS *******
C

C--------------------------------------------------------
CR FOIL CAPTURE CROSS SECTIONS (TYPE 1)
C
C CL (((FOLCAP(M,K,L), M=1, NCNTF), K=1, NINTI), L=1, NFOILS)
C CW NCNTF*NINTI*NFOILS
C CD FOLCAP(M,K,L) RESONANCE CAPTURE CROSS SECTION FOR MATERIAL M IN FOIL L AT THE RIGHT EDGE OF MESH INTERVAL I

C--------------------------------------------------------
CR FOIL FISSION CROSS SECTIONS (TYPE 2)
APPENDIX D. MC\textsuperscript{2}-2 Binary Files. SCRO05 (Contd.)

C
CC
  ALWAYS PRESENT
C
CL  (((FOLPIS (M,K,L), M=1, NCNTF), K=1, NINTI), L=1, NFOILS)
C
CW  NCNTF*NINTI*NFOILS
C
CD  FOLPIS (M,K,L)  RESONANCE FISSION CROSS SECTION FOR MATERIAL
CD  M IN FOIL L AT THE RIGHT EDGE OF MESH
CD  INTERVAL I
C

CR  FOIL SCATTERING CROSS SECTIONS (TYPE 3)
C
CC
  ALWAYS PRESENT
C
CL  (((FOLSCT (M,K,L), M=1, NCNTF), K=1, NINTI), L=1, NFOILS)
C
CW  NCNTF*NINTI*NFOILS
C
CD  FOLSCT (M,K,L)  RESONANCE SCATTERING CROSS SECTION FOR MATERIAL
CD  M IN FOIL L AT THE RIGHT EDGE OF MESH
CD  INTERVAL I
C

CEO
APPENDIX D. MC2-2 Binary Files. SIGMAP.

C*******************************************************************************
C PREPARED 3/06/75 AT ANL
C
CF SIGMAP
CE BACKGROUND SMOOTH SCATTERING CROSS SECTIONS
C
CN THIS DATA SET IS WRITTEN BY MC**2-II
CN AREA 6.5 (CSC006) AND PRESENT IF DATA SET
CN ATNUAT HAS BEEN WRITTEN, OR IF DATA SET
C
C*******************************************************************************

CD MAXHTM MAXIMUM NUMBER OF MATERIALS IN ANY
CD HETEROGENEOUS REGION
CD MGCUT UPG ABOVE THE HIGHEST RESONANCE ENERGY IN THE
CD PROBLEM (RESOLVED OR UNRESOLVED)
CD NGROUP MULTIGROUP TO CONTINUOUS SLOWING DOWN
CD NPRMAT NUMBER OF ENERGY GROUPS
CD NREG1 NUMBER OF PROBLEM MATERIALS
CD NREG1 REGION INDEX
CD NREG1=1 FOR CYLINDERS
CD NREG1=NUMBER OF SLAB REGIONS FOR SLABS

C---------------------------- FILE STRUCTURE ----------------------------
CS RECORD TYPE Present if
CS SPECIFICATIONS Always
CS HOMOGENEOUS SMOOTH SCATTERING Always
CS CROSS SECTIONS
CS ****** (Repeat for NREG1 HETEROGENEOUS
CS * REGIONS)
CS ****** (Repeat for NPRMAT MATERIALS
CS * * OMITTING THOSE WHICH ARE NOT
CS * * TREATED HETEROGENEOUSLY IN THE
CS * * CURRENT REGION. FOR CYLINDERS,
CS * * ONLY 1 RECORD IS PRESENT SINCE
CS * * ALL MATERIALS HAVE THE SAME
CS * * ESCAPE CROSS SECTION)
CS * * HETEROGENEOUS SMOOTH SCATTERING MAXHTM.GT.0
CS * * CROSS SECTIONS
CS ******
C
C----------------------------
APPENDIX D. MC²-2 Binary Files: SIGMAP

-------------------------------
CR SPECIFICATIONS (TYPE 1)

CC ALWAYS PRESENT

CL NGROUP, MGCUT, NPRMAT, NGEOM, NREG1, MAXHTM

CW 6

CD NGEOM GEOMETRY TYPE
   NGEOM=0 FOR HOMOGENEOUS PROBLEMS
   NGEOM=1 FOR SLAB GEOMETRY
   NGEOM=2 FOR CYLINDRICAL GEOMETRY

-------------------------------
CR HOMOGENEOUS SMOOTH SCATTERING CROSS SECTIONS (TYPE 2)

CC ALWAYS PRESENT

CL (SIGMAP(I), I=MGCUT, NGROUP)

CW NGROUP - MGCUT + 1

CD SIGMAP HOMOGENIZED SMOOTH UFG CROSS SECTIONS FOR
   THE HOMOGENEOUS MIXTURE

-------------------------------
CR HETEROGENEOUS SMOOTH SCATTERING CROSS SECTIONS (TYPE 3)

CC PRESENT IF MAXHTM.GT.0

CL (SIGPP(I), I=MGCUT, NGROUP)

CW NGROUP - MGCUT + 1

CD SIGPP HOMOGENIZED SMOOTH UFG CROSS SECTIONS PLUS
   THE ESCAPE CROSS SECTION FOR THE REGION
   IN QUESTION

-------------------------------
CEOF
APPENDIX D.  MC²-2 Binary Files: SMSIGS

C******************************************************************************
C
C          PREPARED 3/10/75 AT ANL
C
CF          SMSIGS
CE          MICROSCOPIC ELASTIC SCATTERING
C
CN          THIS FILE IS WRITTEN BY MC²-2-II AREA 7
(CSC008)
C
C******************************************************************************

CD       ISPOPT
         SPECTRUM OPTION
CD       ISPOPT=1 FOR P1
CD       ISPOPT=2 FOR B1
CD       ISPOPT=3 FOR CONSISTENT P1
CD       ISPOPT=4 FOR CONSISTENT B1
CD       MULT
         2 FOR IBM MACHINES, 1 OTHERWISE
CD       NGRP
         NUMBER OF GROUPS IN PROBLEM
CD       NORDER
         ORDER OF EXTENDED TRANSPORT APPROXIMATION
CD       NPRMAT
         NUMBER OF PROBLEM MATERIALS

CS-------------------FILE STRUCTURE-------------------
CS
CS    RECORD TYPE
CS    ===================
CS    SPECIFICATIONS
CS    MATERIAL NAMES
CS    ****** (REPEAT FOR NPRMAT MATERIALS)
CS    * ****** (REPEAT FOR NGRP GROUPS)
CS    * * ELASTIC SCATTERING DATA
CS    ******
C

CR-------------------SPECIFICATIONS (TYPE 1)-------------------
C
CC    ALWAYS PRESENT
C
CCL    NPRMAT, NGRP, ISPOPT, NORDER, NGRP, ITRANS
C
COW    6
C
CD    NGRP
         LIBRARY UFG NUMBER CORRESPONDING TO THE
CD    HIGHEST UFG IN THE PROBLEM
APPENDIX D. MC²-2 Binary Files. SMSIGS (Contd.)

<table>
<thead>
<tr>
<th>CD</th>
<th>ITRANS</th>
<th>TRANSPORT APPROXIMATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD</td>
<td></td>
<td>ITRANS=0 USE ALL LEGENDRE COMPONENTS</td>
</tr>
<tr>
<td>CD</td>
<td></td>
<td>ITRANS=1 USE STANDARD TRANSPORT APPROXIMATION</td>
</tr>
<tr>
<td>CD</td>
<td></td>
<td>ITRANS=2 USE IMPROVED TRANSPORT APPROXIMATION</td>
</tr>
</tbody>
</table>

CR MATERIAL NAMES (TYPE 2)

CC ALWAYS PRESENT

CL (PRBNAM(I),I=1,NPRMAT)

CW MULT*NPRMAT

CD PRBNAM PROBLEM MATERIAL NAMES

CR PLASTIC SCATTERING DATA (TYPE 3)

CC ALWAYS PRESENT

CL (SIGS(I),I=1,NORD1),SIGURN,BETA,(SIG0(I),I=1,NDN1),

CL 1(SIG1(I),I=1,NDN1)

CW NORD1+ISP*NDN1+2

CD NORD1=NORDER+1

CD ISP=1 IF ISPOPT.LE.2

CD ISP=2 IF ISPOPT.GT.2

CD NDN1=NUMBER OF GROUPS OF DOWNSCATTER PLUS 1

CD SIGS LEGENDRE MOMENTS OF NONRESONANCE SCATTERING

CD I=1 CORRESPONDS TO THE NORDER COMPONENT

CD I=NORDER CORRESPONDS TO THE P1 COMPONENT

CD I=NORD1 CORRESPONDS TO THE P0 COMPONENT

CD SIGURN UNRESOLVED RESONANCE SCATTERING CROSS SECTION

CD BETA TRANSPORT CORRECTION FACTOR

CD SIG0 P0 SCATTERING MATRIX ORDERED AS

CD J TO J+I-1 SO THAT I=1 IS THE IN-GROUP TERM

CD SIG1 P1 SCATTERING MATRIX ORDERED AS

CD J TO J+I-1 SO THAT I=1 IS THE IN-GROUP TERM

CN THE ARRAY SIG1 IS PRESENT ONLY FOR ISP=2
APPENDIX D. \( MC^2 \)-2 Binary Files. SMSIGS (Contd.)

THE MATRIX ELEMENTS SIG0 AND SIG1 ARE
NORMALIZED TO THE TRANSPORT CORRECTED SMOOTH
PLUS UNRESOLVED SCATTERING CROSS SECTION,
THAT IS \((SIGS(NORD1)+SIGUNR)*(1.-BETA)\)

CEOFS
APPENDIX D. MC²-2 Binary Files. SPECTR

C******************************************************************************
C PREPARED 5/13/76 AT ANL
C
CP SPECTR
CE ULTRA FINE GROUP SPECTRUM
CN THIS FILE IS WRITTEN BY M**2-II AREA 8 (CSC009)
C
C******************************************************************************

CD ISP 1 FOR INCONSISTENT SPECTRUM OPTIONS
CD NGRP 2 FOR CONSISTENT SPECTRUM OPTIONS
CD NGRP NUMBER OF UFG IN PROBLEM

C-----------------------------------------------
CS FILE STRUCTURE
CS
CS RECORD TYPE
CS =========== PRESENT IF
CS SPECIFICATIONS ALWAYS
CS FLUX ALWAYS
CS CURRENT ISP.EQ.2
C
C-----------------------------------------------

C-----------------------------------------------
CR SPECIFICATIONS (TYPE 1)
C
CC ALWAYS PRESENT
C
CL RHO, BSQ, EMQX, DELTAU, NGRP, MGCSID, NCSD
C
CW 7
C
CD RHO ULTRA FINE GROUP EIGENVALUE
CD BSQ B**2 FROM UFG CALCULATION
CD EMX HIGHEST ENERGY IN PROBLEM
CD DELTAU UFG LETHARGY WIDTH
CD MGCSID UFG NUMBER AT WHICH CONTINUOUS SLOWING DOWN
CD CALCULATION BEGINS
CD NCSD NUMBER OF UFG IN CONTINUOUS SLOWING DOWN
C
C-----------------------------------------------
APPENDIX D. MC$^2$-2 Binary Files. SPECTR (Contd.)

CR FLUX (TYPE 2)
CC ALWAYS PRESENT
CL (PHI(I), I=1, NGRP)
CW NGRP
CD PHI ULTRA FINE GROUP FLUX

CR CURRENT (TYPE 3)
CC PRESENT IF ISP.EQ.2
CL (CURNT(I), I=1, NGRP)
CW NGRP
CD CURNT ULTRA FINE GROUP CURRENT

CEOF
APPENDIX D. MC²-2 Binary Files. SPECXS

C******************************************************************************C
C PREPARED 3/12/75 AT ANL

C SPECXS:
C MACROSCOPIC CROSS SECTIONS AND MODERATING PARAMETERS
C
C THIS FILE IS WRITTEN BY MC²-II AREA 7
C
C******************************************************************************C

CD ISP
SPECTRUM OPTION
ISP=1 FOR INCONSISTENT OPTION (ISPOPT.LE.2)
ISP=2 FOR CONSISTENT SPECTRUM OPTION
(ISPOPT.GE.3)

CD NCSD
NUMBER OF ENERGY POINTS IN CONTINUOUS SLOWING
DOWN REGION (=NGRP-MGCS+2)

CD NGRP
NUMBER OF UFG IN PROBLEM

C------------------------------------------------------------------------
C NUSIGMA FISSION (TYPE 1)
C
C ALWAYS PRESENT
C
C (BNSIGF(I),I=1,NGRP)
C
C NW NGRP
MACROSCOPIC UFG FISSION CROSS SECTION*

CD BNSIGF
AVERAGE NUMBER OF NEUTRONS PER FISSION

C------------------------------------------------------------------------
C NU COEFFICIENTS (TYPE 2)
C
C ALWAYS PRESENT
C
C (A0(I),A1(I),A2(I),A3(I),I=1,NPRMAT)
C
C NW 4*NPRMAT

CD NPRMAT
NUMBER OF PROBLEM MATERIALS

CD A0,A1,A2,A3
MATERIAL DEPENDENT COEFFICIENTS USED IN
FIT OF AVERAGE NUMBER OF NEUTRONS PER FISSION
VERSUS ENERGY
APPENDIX D. MC²-2 Binary Files. SPECXS (Contd.)

TOTAL CROSS SECTION (TYPE 3)
ALWAYS PRESENT
(BSIGT(I), I=1, NGRP)
NGRP

MACROSCOPIC UFG TOTAL CROSS SECTION

SCATTERING CROSS SECTION (TYPE 4)
ALWAYS PRESENT
(BSIGS(I), I=1, NGRP)
NGRP

MACROSCOPIC UFG P0 SCATTERING CROSS SECTION

EXTENDED TRANSPORT CROSS SECTION (TYPE 5)
ALWAYS PRESENT
((AL(I,K), I=1, NGRP), K=1, NORDER)
NGRP*NORDER
NORDER
ORDER OF EXTENDED TRANSPORT APPROXIMATION
AL
MACROSCOPIC UFG EXTENDED TRANSPORT CROSS SECTION

P1 SCATTERING (TYPE 6)
APPENDIX D. MC\(^2\)-2 Binary Files. SPECXS (Contd.)

C
ALWAYS PRESENT
C
(SIGTRN(I), I=1,NGRP)
C
NGRP
C
SIGTRN MACROSCOPIC UFG P1 SCATTERING CROSS SECTION
C

-----------------
C
CR MODERATING PARAMETER ZETA (TYPE 7)
C
ALWAYS PRESENT
C
((ZETA(I,J), J=1,NCSD), J=1,ISP)
C
ISP*NCSD
C
ZETA CONTINUOUS SLOWING DOWN MODERATING PARAMETER
C
ZETA AT EACH ENERGY POINT IN CSD REGION FOR
C
P0 AND P1 SCATTERING
C

C-----------------
C
CR MODERATING PARAMETER EPS (TYPE 8)
C
ALWAYS PRESENT
C
((EPS(I,J), I=1,NCSD), J=1,ISP)
C
TSP*NCSD
C
EPS CONTINUOUS SLOWING DOWN MODERATING PARAMETER
C
1./GAMMA AT EACH ENERGY POINT IN CSD REGION FOR
C
P0 AND P1 SCATTERING
C

CEND
APPENDIX D. \( \text{MC}^2 \)-2 Binary Files. SRATES

C******************************************************************************
C
PREPARED 3/06/75 AT ANL
C
C
SRATES
C
SCATTERING RATES AND SOURCES
C
SCATTERING RATES AND SOURCES FOR USE IN
C
AREA 10 (CSCO11) INTEGRAL TRANSPORT THEORY
C
CALCULATIONS
C
******************************************************************************

CD MAXUPG LOWEST ENERGY ULTRA FINE GROUP FOR WHICH
CD SCATTERING RATES ARE PROVIDED. ULTRA FINE
CD GROUP MAXUPG IS THE ULTRA FINE
CD IMMEDIATELY ABOVE THE TOP OF THE HIGHEST
CD ENERGY BROAD GROUP IN THE AREA 10 (CSCO11)
CD ENERGY RANGE
CD MINUPG HIGHEST ENERGY ULTRA FINE GROUP NUMBER FOR
CD WHICH SCATTERING RATES ARE PROVIDED
CD NPRMAT NUMBER OF TYPE 2 RECORDS PRESENT IN THE FILE
CD NUFGRD NUMBER OF ULTRA FINE GROUPS READ FOR EACH PASS
CD NPASS OF RECORD 2. NUFGRD=I2-I1+1 (SEE RECORD 2)

C-----------------------------------------------------------------------
CS FILE STRUCTURE
CS
CS RECORD TYPE
CS "==============================
CS SPECIFICATIONS
CS "* (REPEAT NPASS TIMES)
CS SOURCES
CS "* SCATTERING RATES
CS HYDROGEN SCATTERING RATES
CS
CS
C-----------------------------------------------------------------------

CP SPECIFICATIONS (TYPE 1)
CP
C MINUPG, MAXUPG, NUFGRD, NPASS
APPENDIX D. MC²-2 Binary Files. SRATES (Contd.)

\$
\begin{align*}
\text{CR} & \quad 4 \\
\text{C} & \\
\text{C} & \\
\text{CR} & \quad \text{SOURCES (TYPE 2)} \\
\text{C} & \quad \text{PRESENT IF NPASS.GT.0} \\
\text{C} & \quad ((SPIX(M,I), M=1, NPRMAT), I=I1, I2) \\
\text{C} & \quad \text{NUFGRD*NPRMAT} \\
\text{C} & \quad \text{SPIX(M,I)} \\
\text{CD} & \quad \text{MICROSCOPIC SOURCE INTO ULTRA FINE GROUP I} \\
\text{CD} & \quad \text{DUE TO FISSION, INELASTIC SCATTERING, AND} \\
\text{CD} & \quad \text{N,2N SCATTERING IN MATERIAL M.} \\
\text{CD} & \quad \text{I RANGES OVER THE ULTRA FINE GROUPS IN THE} \\
\text{CD} & \quad \text{AREA 10 (CSC011) ENERGY RANGE, MAXUGF+1} \\
\text{CD} & \quad \text{THROUGH NGROUP, WHERE NGROUP IS THE} \\
\text{CD} & \quad \text{LOWEST ENERGY ULTRA FINE GROUP IN THE PROBLEM.} \\
\text{CD} & \quad \text{NUFGRD ULTRA FINE GROUPS ARE INCLUDED FOR EACH} \\
\text{CD} & \quad \text{PASS.} \\
\text{CD} & \quad \text{I1} \\
\text{CD} & \quad \text{FIRST ULTRA FINE GROUP READ FOR CURRENT PASS} \\
\text{CD} & \quad \text{I2} \\
\text{CD} & \quad \text{LAST ULTRA FINE GROUP READ FOR CURRENT PASS} \\
\text{C} & \\
\text{C} & \\
\text{CR} & \quad \text{SCATTERING RATES (TYPE 3)} \\
\text{C} & \quad \text{ALWAYS PRESENT} \\
\text{C} & \quad ((SS(I,M), I=1, MINMAX), M=1, NPRO) \\
\text{C} & \quad \text{NPRO*MINMAX} \\
\text{C} & \quad \text{SS} \\
\text{CD} & \quad \text{PRODUCT OF MICROSCOPIC SCATTERING CROSS} \\
\text{CD} & \quad \text{SECTION TIMES ULTRA FINE GROUP PLUX DIVIDED BY} \\
\text{CD} & \quad \text{THE ULTRA FINE GROUP LETHARGY WIDTH FOR THE} \\
\text{CD} & \quad \text{FINE GROUPS MINUGF THROUGH MAXUGF FOR EACH} \\
\text{CD} & \quad \text{MATERIAL} \\
\text{CD} & \quad \text{MINMAX} \\
\text{CD} & \quad \text{MAXUGF-MINUGF+1} \\
\text{CD} & \quad \text{NPRMAT IF HYDROGEN IS NOT PRESENT IN THE} \\
\text{CD} & \quad \text{PROBLEM MIXTURE. NPRMAT-1 IF HYDROGEN IS IN} \\
\text{CD} & \quad \text{PROBLEM MIXTURE} \\
\text{C} & \\
\text{C} & \\
\end{align*}
\$
APPENDIX D. MC²-2 Binary Files. SRATES (Contd.)

C-----------------------------
CR HYDROGEN SCATTERING RATES (TYPE 4)
CC PRESENT IF NHYDRO=1 (SEE RECORD 1 OF DATA SET PRBSPC)
CL (SHYDRO(I),I=1,MAXUFG)
CT MAXUFG
CD SHYDRO PRODUCT OF HYDROGEN MICROSCOPIC SCATTERING
CD CROSS SECTION TIMES ULTRA FINE GROUP FLUX
CD DIVIDED BY THE ULTRA FINE GROUP LETHARGY WIDTH
CD FOR ALL ULTRA FINE GROUPS ABOVE THE AREA 10
CD (CSC011) ENERGY RANGE

C-----------------------------
CEO
APPENDIX D. MC$^2$-2 Binary Files. UNREG

PREPARED 3/10/75 AT ANL

UNRESOLVED UPG CROSS SECTIONS

THIS FILE IS WRITTEN BY MC$^2$-II AREA 7 (CSC008)

FISSION FLAG
IFIC=0 MATERIAL IS NOT FISSIONABLE
IFIC=1 MATERIAL IS FISSIONABLE

LOWEST ENERGY UPG FOR WHICH MATERIAL HAS
NON-ZERO UNRESOLVED CROSS SECTION

HIGHEST ENERGY UPG FOR WHICH MATERIAL HAS
NON-ZERO UNRESOLVED CROSS SECTION

2 FOR IBM MACHINES, 1 OTHERWISE

NUMBER OF REGIONS

NREG=1 FOR HOMOGENEOUS PROBLEMS (NGEOM=0)
NREG=2 FOR PIN CELLS (NGEOM=2) AND IF
MAXHTM.GT.0

NREG=1 + NUMBER OF SLAB REGIONS FOR SLAB
PROBLEMS (NGEOM=1) AND IF MAXHTM.GT.0

(MAXHTM IS THE MAXIMUM NUMBER OF MATERIALS IN
ANY HETEROGENEOUS REGION)

NUMBER OF UNRESOLVED RESONANCE MATERIALS

FILE STRUCTURE

PECORD TYPE
SPECIFICATIONS
UNRESOLVED MATERIAL NAMES

(Repeat for NUMRES materials)

MATERIAL SPECIFICATIONS

(Repeat for 1+no. of regions)

In which material is treated heterogeneously

CAPTURE CROSS SECTION
FISSION CROSS SECTION
TOTAL CROSS SECTION

**********
APPENDIX D. MC^2-2 Binary Files. UNREG (Contd.)

CR specifications (Type 1)
CR
CC always present
CL
CW

Unresolved material names (Type 2)
CR
CC always present
CL
CW
CD

Material specifications (Type 3)
CR
CC always present
CL
CW

Capture cross section (Type 4)
CR
CC
CC
CL
CW
APPENDIX D. MC²-2 Binary Files. UNREG (Contd.)

UNRESOLVED RESONANCE CAPTURE CROSS SECTIONS

FISSION CROSS SECTION (TYPE 5)

PRESENT FOR HOMOGENEOUS MIXTURE IF IMIN1.GT.0, IFI.GT.0.
ALSO PRESENT FOR EACH HETEROGENEOUS REGION IN WHICH CURRENT
MATERIAL IS TREATED HETEROGENEously AND IFI.GT.0

(SIGF(I),I=IMIN1,IMAX1)

IMAX1-IMIN1+1

UNRESOLVED RESONANCE FISSION CROSS SECTIONS

TOTAL CROSS SECTION (TYPE 6)

PRESENT FOR HOMOGENEOUS MIXTURE IF IMIN1.GT.0.
ALSO PRESENT FOR EACH HETEROGENEOUS REGION IN WHICH CURRENT
MATERIAL IS TREATED HETEROGENEously

(SIGT(I),I=IMIN1,IMAX1)

IMAX1-IMIN1+1

UNRESOLVED RESONANCE TOTAL CROSS SECTIONS

CECF
APPENDIX D. MC²-2 Binary Files. UNRES

C**********************************************************************************************************
C
C PREPARED 3/05/75 AT ANL
C
CF UNRES
CE UNRESOLVED RESONANCE CROSS SECTIONS
C
CN THIS DATA SET IS WRITTEN BY MC²-2-II AREA 5
CN (CSC004) IF UNRESOLVED MATERIALS ARE PRESENT
C
C**********************************************************************************************************

CD MULT 2 FOR IBM MACHINES, 1 OTHERWISE
CD NISO NUMBER OF ISOTOPES FOR EACH MATERIAL
CD NPTS NUMBER OF ENERGY (ESTAR) POINTS FOR EACH ISOTOPE
CD NREG NUMBER OF REGIONS
CD NREG=1 FOR HOMOGENEOUS PROBLEMS (NGEOM=0)
CD NREG=2 FOR PIN CELLS (NGEOM=2) AND IF MAXHTM.GT.0
CD NREG=1 + NUMBER OF SLAB REGIONS FOR SLAB PROBLEMS (NGEOM=1) AND IF MAXHTM.GT.0
CD ANY HETEROGENEOUS REGION
CD NUMRES NUMBER OF UNRESOLVED RESONANCE MATERIALS

C----------------------------------- FILE STRUCTURE -----------------------------------
C
CS RECORD TYPE
CS ------------------- PRESENT IF
CS SPECIFICATIONS ALWAYS
CS MATERIAL NAMES ALWAYS
CS ********** (REPEAT FOR NUMRES MATERIALS)
CS * MATERIAL SPECIFICATION ALWAYS
CS * ENERGY POINT INDEX ALWAYS
CS * ********** (REPEAT NISO TIMES)
CS * * ENERGY SPECIFICATIONS ALWAYS
CS * * ***** (REPEAT FOR 1+NO. OF REGIONS)
CS * * * IN WHICH MATERIAL IS TREATED
CS * * * HETERogeneously)
CS * * * CAPTURE CROSS SECTIONS ALWAYS
CS * * * FISSION CROSS SECTIONS IF I.EQ. 1
CS * * * TOTAL CROSS SECTIONS ALWAYS
CS **********
C
APPENDIX D. MC²-2 Binary Files. UNRES (Contd.)

CR                ENERGY POINT INDEX (TYPE 4)
C
CC                ALWAYS PRESENT
C
CL                (NPTS(I), I=1,NISO)
C
CW                NISO
C

CR                ENERGY SPECIFICATIONS (TYPE 5)
C
CC                ALWAYS PRESENT
C
CL                (ESTAR(I), I=1,NPTS)
C
CW                NPTS
C
CD                ESTAR ENERGY POINTS
C

CR                CAPTURE CROSS SECTIONS (TYPE 6)
C
CC                ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE, ALSO PRESENT
CC FOR EACH HETEROGENEOUS REGION IN WHICH CURRENT MATERIAL
CC IS TREATED HETEROGENEOUSLY
C
CL                (SIGCAP(I), I=1,NPTS)
C
CW                NPTS
C
CD                SIGCAP UNRESOLVED RESONANCE CAPTURE CROSS SECTIONS
C

CR                FISSION CROSS SECTIONS (TYPE 7)
C
CC                ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE IF IFI.EQ.1
CC ALSO PRESENT FOR EACH HETEROGENEOUS REGIONS IF IFI.EQ.1
CC AND CURRENT MATERIAL IS TREATED HETEROGENEOUSLY IN REGION
C
CL                (SIGFIS(I), I=1,NPTS)
C
APPENDIX D. MC^2-2 Binary Files. UNRES (Contd.)

---

**SPECIFICATIONS (TYPE 1)**

ALWAYS PRESENT

**NUMRES**, **NREG**, **NPTMAX**, **MAXISO**

**NPTMAX**

MAXIMUM NUMBER OF POINTS FOR ANY MATERIAL IN THE LIBRARY

**MAXISO**

MAXIMUM NUMBER OF ISOTOPES IN THE MIXTURE

---

**MATERIAL NAMES (TYPE 2)**

ALWAYS PRESENT

**UNRMAT**

DOUBLE PRECISION (R*8) UNRESOLVED RESONANCE MATERIAL NAMES

---

**MATERIAL SPECIFICATION (TYPE 3)**

ALWAYS PRESENT

**NISO**, **IFI**

**IFI**

FISSILE MATERIAL INDEX

IFI=0 FOR NON-FISSIONAL MATERIAL

IFI=1 FOR FISSILE MATERIAL
APPENDIX D. MC²-2 Binary Files. UNRES (Contd.)

<table>
<thead>
<tr>
<th>CW</th>
<th>NPTS</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD</td>
<td>SIGFIS</td>
</tr>
</tbody>
</table>

UNRESOLVED RESONANCE FISSION CROSS SECTIONS

<table>
<thead>
<tr>
<th>CR</th>
<th>TOTAL CROSS SECTIONS (TYPE 8)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CC</td>
<td>ALWAYS PRESENT FOR HOMOGENEOUS MIXTURE, ALSO PRESENT</td>
</tr>
<tr>
<td>CC</td>
<td>FOR EACH HETEROGENEOUS REGION IN WHICH CURRENT MATERIAL IS TREATED HETEROGENEously</td>
</tr>
<tr>
<td>CL</td>
<td>(SIGTOT(I),I=1,NPTS)</td>
</tr>
</tbody>
</table>

| CD | SIGTOT |

UNRESOLVED RESONANCE TOTAL CROSS SECTIONS

CEOF
APPENDIX E

BPOINTER, A DYNAMIC STORAGE ALLOCATION PROGRAM
BPOINTER, A Dynamic Storage Allocation Program

1. Description of Subprogram Package

BPOINTER is a FORTRAN subprogram package which was developed to alleviate bookkeeping chores associated with the use of dynamic storage allocation techniques.

Programs which use the BPOINTER capability tend to be structured in subroutine form. A control routine is used to define one or two large blocks of storage (called the container arrays), and make the appropriate calls to BPOINTER to control the allocation of storage within these block(s). Calls to calculational subroutines transmit pointers corresponding to appropriate array locations through the calling sequences. All BPOINTER capabilities are accessed through an appropriate call to an entry point, subroutine, or function subprogram. The following capabilities are available in the BPOINTER system:

(a) Storage of data in and retrieval of data from the container array, via user defined variable arrays.

(b) Purge of variable arrays stored in the container array.

(c) Automatic "cleanup" of the container array when more storage is required.

(d) Re-definition of array sizes without loss of data already stored in the array.

(e) Array dump of selected integer, floating point or BCD arrays in a prescribed format.

(f) Trace dumps of BPOINTER activities.

(g) Status reports of the BPOINTER tables.

Detailed program documentation including flow charts, common block information and subprogram descriptions is available in Reference 1. This Appendix is intended to provide a brief description of how the program package operates. The major differences between the IBM and CDC standalone versions of the program package are also noted.

The short example listed in Fig. 27 is intended to illustrate the structure of a program using the BPOINTER package. This example demonstrates the manner in which a container is allocated, pointers defined and used, and the container released.

Brief descriptions of all the BPOINTER entry points, subroutines and functions are given in Table XIV.
All dynamically allocated arrays are addressed relative to the common block /ARRAY/ which contains a single array element, BLK(1). In the IBM version of the code the element must be declared as DOUBLE PRECISION. A second common block /ARRAY2/ is used in the CDC version of BPOINTER to address arrays allocated to a large core memory container. This common block also contains a single array element BLKECS(1) which must be declared a LEVEL 2 variable. The equivalent of the large core memory container on IBM equipment is a second container which may be given a HIARCHY 1 location but is addressed in precisely the same manner as the first (SCM) container. The one word assigned to the container by the source language program provides a reference address. At execution time machine language routines (ALLOC1, ALLOC2 on IBM, MEMGET1, MEMGET2 on CDC) are used to obtain the addresses of core which are available to the program for the allocation of data arrays. These blocks of core are allocated in the following manner.

(a) IBM allocation

The standard IBM macro instructions GETMAIN and FREEMAIN are used to allocate and free consecutive words of core which are available to the program. The designations subpool 1 and 2 are assigned to the bulk (LCM) and fast (SCM) containers respectively. Since allocations are performed in units of 256 (eight byte) words, it is most efficient to request blocks of core in such multiplies;

(b) CDC allocation

The COMPASS routine MEMGET uses the standard CDC macro instruction MEMORY to determine the jobs SCM and LCM field length. The core available as a container for the BPOINTER SCM arrays is determined by subtracting the address of blank common from the SCM field length. Thus a program using the CDC version of BPOINTER should not use blank common. Blank common is used for this purpose because of the CDC loader convention which places blank common after all other program sections in core. Although blank common is used in this manner to determine the available core for a container, arrays in the container are addressed relative to the common block /ARRAY/ as noted above. The BPOINTER program package accounts for the offsets between the address of /ARRAY/ in core and the address of the container. It should also be noted that the conventions used by BPOINTER are such that the first word of the container is not in general set to the first word of blank common. This is important since the loader convention noted above is not adhered to by all CDC Systems. The user is therefore responsible for providing enough SCM memory to accommodate the program, any SCM buffers, and the BPOINTER container as there is currently no effective check to make sure that data stored in the BPOINTER container do not overlap code. It is assumed by the CDC version of BPOINTER that the LEVEL 2 common block /ARRAY2/ is addressed as the first word of LCM and the entire LCM field length is assumed to be available to BPOINTER for its LCM container.
The letters M and B are used as neumonics within BPOINTER to designate routines which operate on the SCM and LCM containers respectively. Thus PUTM allocates an array in the SCM container while PUTB allocates an array which must be referenced on CDC equipment as a LEVEL 2 array. On IBM equipment without HIARCHY support (e.g. 370/195) the two containers are equivalent. The distinctions noted above between the two dynamic containers are important on CDC equipment where the containers are addressed quite differently and on IBM equipment with HIARCHY support where access to the BULK core container (HIARCHY 1, subpool 1) is significantly slower than access to the MAIN core container (HIARCHY 0, subpool 2).
BPOINTER EXAMPLE

DEFINE CONTAINER COMMON BLOCK

REAL*8 BLK, FLUX, POWER
COMMON/ARRAY/BLK(1)
DIMENSION BLK4(1)
EQUIVALENCE (BLK(1), BLK4(1))
DATA FLUX/6HFLUX /, POWER/6HPower /, MAXSIZ/10000/
DATA I4/4/, I8/8/, I0/0/, NG/27/

ALLOCATE CONTAINER WITH MAXSIZ WORDS OF SCM AND NO LCM

CALL BULK(IO)
CALL POINTR(BLK, MAXSIZ, IO)

ALLOCATE SPACE FOR ARRAYS POWER, FLUX AND CURRENT

CALL PUTM(POWER, I8, NG, IPOWR)
CALL PUTM(FLUX, I4, 2*NG, IFLUX)

DETERMINE POINTER FOR SUB-ARRAY CURRENT WHICH FOLLOWS THE
NG SINGLE PRECISION WORDS FOR THE ARRAY FLUX

ICURNT=IPT2(IFLUX, NG, IO)

CHECK ON BPOINTER ERROR

IF ( IPTERR(DUM).GT.0 ) PRINT 500
500 FORMAT(1H0, 14HBPOINTER ERROR)

CALL SUBROUTINE INIT TO USE THESE ARRAYS

CALL INIT(BLK(IFLUX), BLK(IPOWR), BLK4(ICURNT), NG)

FREE CONTAINER AND RETURN

CALL FREE
RETURN
END
SUBROUTINE INIT(PHI, POWER, CURRENT, NG)

USE BPOINTER ARRAYS JUST AS ANY OTHER VARIABLES

REAL*8 POWER
DIMENSION PHI(1), POWER(1), CURRENT(1)
DO 10 I=1, NG
PHI(I) = 1.0
POWER(I) = 3.1E+06
CURRENT(I) = .333
10 CONTINUE
RETURN
END

Fig. 27. BPOINTER Example
<table>
<thead>
<tr>
<th>Subprogram</th>
<th>Card Sequence Numbers</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>POINTR</td>
<td>(008710 - 010270)*</td>
<td>Initializes tables of dynamic allocation program package and calls ALLOC1 and ALLOC2 to allocate container(s) for variably dimensioned arrays.</td>
</tr>
<tr>
<td>PUTPNT/PUTBLK</td>
<td>(010280 - 010590)</td>
<td>Dummy routine calls PUTM to allocate array storage.</td>
</tr>
<tr>
<td>BULK</td>
<td>(010600 - 010720)</td>
<td>Sets number of words of BULK(LCM) core to be allocated.</td>
</tr>
<tr>
<td>FREE</td>
<td>(010730 - 011020)</td>
<td>Calls FREE1 and FREE2 to release containers allocated by calls from subroutine POINTR.</td>
</tr>
<tr>
<td>WIPOUT/CLEAR</td>
<td>(011030 - 011780)</td>
<td>Deletes a named array from BPOINTER tables; zeroes all locations assigned to a named array.</td>
</tr>
<tr>
<td>GETPNT/GETN/DUMP</td>
<td>(011790 - 013310)</td>
<td>Returns pointer for a named array; return index in BPOINTER tables of a named array; controls printing of a named array.</td>
</tr>
<tr>
<td>IGET</td>
<td>(013320 - 013730)</td>
<td>Returns pointer for a named array.</td>
</tr>
<tr>
<td>IPT2</td>
<td>(013740 - 013870)</td>
<td>Returns pointer to a sub-array relative to a single precision word length container.</td>
</tr>
<tr>
<td>PUTM/PUTB</td>
<td>(013880 - 015460)</td>
<td>Enters named arrays into fast and bulk(LCM) containers respectively.</td>
</tr>
<tr>
<td>IPTERR/NNAMSF</td>
<td>(015470 - 015740)</td>
<td>Returns number of BPOINTER errors; returns number of named arrays in BPOINTER tables.</td>
</tr>
<tr>
<td>ILAST/ILASTB</td>
<td>(015750 - 015940)</td>
<td>Returns word number of first available word in SCM/LCM container.</td>
</tr>
<tr>
<td>REDEF</td>
<td>(015950 - 016130)</td>
<td>Dummy routine calls REDEFM to redefine size and/or location of named array.</td>
</tr>
<tr>
<td>REDEFM/REDEFB</td>
<td>(016140 - 017990)</td>
<td>Redefine the size and/or location of named array within BPOINTER tables and containers.</td>
</tr>
</tbody>
</table>

*Numbers in brackets are card sequence numbers of routine on MC²-2 program tape.
<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PURGE/PURGEB</td>
<td>Sift storage in SCM/LCM containers to eliminate unused blocks created by WIPOUT calls.</td>
</tr>
<tr>
<td>STATUS</td>
<td>Edits status of BPOINTER tables.</td>
</tr>
<tr>
<td>PRTI1 (019670 - 019790)</td>
<td>Prints half word integer array from SCM container.</td>
</tr>
<tr>
<td>PRTI1E (019800 - 020000)</td>
<td>Prints half word integer array from LCM container.</td>
</tr>
<tr>
<td>PRTI2 (020010 - 020090)</td>
<td>Prints full word integer array from SCM container.</td>
</tr>
<tr>
<td>PRTI2E (020100 - 020270)</td>
<td>Prints full word integer array from LCM container.</td>
</tr>
<tr>
<td>PRTR1/PRTA1</td>
<td>Prints full word real array from SCM container.</td>
</tr>
<tr>
<td>PRTR1E/PRTA1E</td>
<td>Prints full word real array from LCM container.</td>
</tr>
<tr>
<td>PRTR2/PRTA2</td>
<td>Prints double word read array from SCM container.</td>
</tr>
<tr>
<td>PRTR2E/PRTA2E</td>
<td>Prints double word real array from LCM container.</td>
</tr>
</tbody>
</table>
APPENDIX F

MC²-2 LIBRARY GENERATION
APPENDIX F

MC²-2 Library Generation

The MC²-2 library contains eight files, MCC2F1-MCC2F8, that were processed from the ENDF/B-IV data files by the code ETOX-II. Appendix C contains a description of these files. The user has the option of obtaining the binary MC²-2 library or generating the MC²-2 library from BCD card images on magnetic tapes. The library data are briefly summarized in Table IX.

The binary library for IBM users is contained on one 9 track, non-labeled, LRECL=X, RECFM=VBS, and BLKSIZE=6447 magnetic tape with a recording density of 1600 BPI. The eight files are written in sequential order MCC2F1-MCC2F8. A sample of the job control cards required to copy these files from tape to a direct access device (e.g. disk pack) is given in Fig. 22. The binary library for CDC users is contained on two 7 track, non-labeled, and x-mode binary tapes written with a recording density of 800 BPI. The first binary tape contains the files MCC2F1-MCC2F4, MCC2F7, and MCC2F8. The second tape contains the files MCC2F5 and MCC2F6. These two binary tapes were generated at BERKELEY. Figure 28 displays the control cards necessary to read the two 7 track x-mode binary tapes and write a 9 track 1600 BPI tape. The BERKELEY example displays the generation of a non-labeled, phase encoded, and x-mode binary-odd parity tape. The BROOKHAVEN example displays the generation of a labeled, SCOPE standard format tape. The 9 track tape which is generated in each case is used directly in the execution of the MC²-2 problem as displayed in Fig. 25.

The user may generate the MC²-2 library from three BCD data tapes which contain the same eight file library data in BCD format along with a BCD tape which contains a Fortran program, MC²-2 LIBGEN, which reads the three BCD data tapes and writes the eight binary files. All four tapes are 7 track, unlabeled, 40 card images per physical block, and written at 800 BPI. Figure 29 displays the CDC control cards used to read the three BCD data tapes as well as the BCD program tape, MC²-2 LIBGEN. The control cards also show the compilation and execution of this program which generates the eight binary MC²-2 library files. The data tapes which are physically labeled MC2BCDLIB1, MC2BCDLIB2, and MC2BCDLIB3 are assigned the data set names TAPE11, TAPE12, and TAPE13 respectively in the program execution. The eight binary library files are written on one data set named TAPE21, and these data are written onto a 9 track 1600 BPI tape. This binary library tape is used directly in the execution of the MC²-2 problem as shown in Fig. 25.
Fig. 28. Generation of $M^2-2$ Library from Two X-Mode Binary Library Tapes that were Generated at Berkeley
Fig. 29. Generation of MC²-2 Library from Three BCD Data Tapes Using the Fortran Program MC²-2 LIBGEN
ACKNOWLEDGMENTS

Many people made significant contributions to the development of the program system MC$^2$-2 so that it would be impossible to acknowledge them all. However, the work of W. M. Stacey, Jr., in neutron slowing down theory and R. N. Hwang in resonance theory were instrumental in the theoretical modelling for the program. The assistance provided by A. Olson in the development of the RABANL module and of E. Pennington in leading the authors through the vagaries of ENDF/B were most appreciated. Special thanks are also due to the users of MC$^2$-2. R. Prael, D. Wade, M. Lineberry, and C. Beck are among those users whose special efforts in specification and verification of the code are largely responsible for any of its good features. The work of Pat Jones, Linda Juergens, and Lyn Young in wading through the many drafts of this report and making sense of it all is most appreciated.
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36. N. M. Steen, G. D. Byrne and E. M. Gelbard, *Gaussian Quadratures for the Integrals*
\[ \int_{0}^{\infty} \exp(-x^{2})f(x)dx \quad \text{and} \quad \int_{0}^{b} \exp(-x^{2})f(x)dx \]

37. A. P. Olson, *Gaussian Quadratures for* \[ \int_{1}^{\infty} \exp(-x)f(x)dx/x^{m} \quad \text{and} \quad \int_{1}^{\infty} g(x)dx/x^{m} \]


