H-2 & UO2 Data Testing at AECL



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Nuclear-theory calculations for ²H (L. Canton - Universita di Padova; J. Svenne - University of Manitoba & Winnipeg Institute for Theoretical Phyiscs)

- Earlier work showed significant differences between ENDF/B-VI.5 to VII.0 & theory, especially at backward scattering angles at ~1 MeV
- Discontinuities in ENDF data in the 3 to 6 MeV range
- Noticeable impact of different ENDF ²H data files on HEU critical measurements (~10 mk) & ZED-2 Coolant Void Reactivity (CVR) bias (~0.6 mk)



²H sensitivity coefficient

- For ACR-700 CVR, ²H elastic cross section has the largest sensitivity (~34.2) based on TSUNAMI (but can't address angular dependence): Sensitivity Analysis of Reactivity Responses Using One-Dimensional Discrete Ordinates and Three-Dimensional Monte Carlo Methods, M.L. Williams, J.C. Gehin & K.T. Clarno, PHYSOR-2006
- Similar results for ZED-2 CVR TSUNAMI analyses
- Confirms ZED-2 CVR experiments as a useful test of ²H data



New nuclear-theory calculations

- Based on solving the Faddeev equation using the formulation by Alt-Grassberger-Sandhas (AGS)
- Various potentials: BonnB, CDBonn, AV18, BEST2000, CDBest2000: little impact on σ_{elastic}(E,μ)
 - Additional BonnB σ_{elastic}(E,μ) data from 3 to 10 MeV
 - New CDBonn $\sigma_{\text{elastic}}(\text{E},\mu)$ data from 50 keV to 29 MeV
- 3-nucleon forces (3NF): little impact on $\sigma_{elastic}(E,\mu)$
- See:
 - Analysis of neutron deuteron scattering for science and atomic applications, L. Canton, K.S. Kozier & J.P. Svenne, The 2nd International Conference Current Problems in Nuclear Physics and Atomic Energy, June 9 - 15, 2008, Kyiv, UKRAINE
 - Nuclear Theory Nuclear Power, J.P. Svenne, L.
 Canton, and K.S. Kozier, Latvian Journal of Physics
 & Technical Sciences, Vol. 45, No. 4, 2008
- To come: magnetic interaction, extension to lower energies



²H elastic scattering cross section comparison (unprocessed ENDF data)

- Small noticeable differences between Bonn-B & CD-Bonn data at low energies (~1%); good agreement between Bonn-B & ENDF/B-VII.0
- Linear extrapolation of Ln(σ_{elastic}) vs E at low energies (?)
- Drop in JENDL-3.3 σ_{elastic} at low E due to being based on $\sigma_{\text{total}} \sigma_{\text{capture}}$ (?)





²H (n,2n) cross section comparison

- Notable differences between theory & ENDF/B-VII.0 between 5 & 15 MeV
- Fair agreement between Bonn-B & CD-Bonn in this energy range





H₂O/air-cooled Low Enriched Uranium experiments

- 52 fuel channels arranged in a square lattice with a spacing of 20 cm or 24 cm.
- Channel consists of five 43-pin fuel assemblies surrounded by CANDU-sized aluminum PT/CT:
 - 48 channels use 0.95% SEU
 - 4 channels use 0.96% RU (recovered uranium)
- H₂O or air (void) coolant.
- D₂O moderator height adjusted to achieve criticality.
- Cu and In-Al foil activation measurements performed axially and radially.



<u>**Results</u>: Dependence of k_{eff} bias on calculated leakage**</u>

- Systematic trend (r²=0.99) with leakage despite different: enrichment, fuel bundle design, coolant, lattice pitch & arrangement, booster fuel
- Suggests a common cause or nuclear data issue



Preliminary ZED-2 CVR bias results for new ²H data

- Lowest MCNP ZED-2 CVR simulation bias with ENDF/B-VII.0; strong correlation with leakage (r²=0.98) despite differences in enrichment, coolant, fuel bundle geometry, lattice pitch & arrangement; but larger spread (-4.1 to +1.3 mk)
- Substituting CD-Bonn P(E,µ) only into ENDF/B-VII.0 makes worse
- Substituting CD-Bonn or Bonn-B $\sigma_{elastic}(E)$ data to 50 keV & $\sigma_{(n,2n)}(E)$ makes worse again; similar if extrapolate CD-Bonn or Bonn-B data to 0 MeV



ZED-2 CVR bias ²H comparison (mk)

Case	ENDF/B-VII.0	ENDF/B-VII.0 + CD-Bonn P(E,m)	JENDL-3.3	Bonn-B + ENDF/B-VII.0 (<50 keV)	Bonn-B extrapolated	CD-Bonn extrapolated
SEU/RU UO ₂ : 20-cm air/H ₂ O	1.59	1.96	1.68	1.96	1.96	2.26
SEU/RU UO ₂ : 24-cm air/H ₂ O	3.73	3.92	4.25	4.24	4.34	4.50
NU-UO ₂ /ZEEP: air/D ₂ O	0.68	1.02	1.20	1.10	1.15	0.96
NU-UO ₂ /U-19: air/D ₂ O	1.19	1.47	1.70	1.55	1.65	1.53
Average	1.80	2.09	2.21	2.21	2.27	2.31

- Good News: ZED-2 CVR bias results are sensitive to the ²H data
- Not so good: new ²H data from nuclear theory makes the bias worse
 - Magnetic interaction important(?)
 - A problem with ZED-2 measurements: Al tube impurities(?): extend comparisons to DCA data in ICSBEP
 - A problem with other data or processing: ²³⁵U, ²³⁸U, TSL ...(?)
- Confirms the need for new (n,d) cross section measurements



Impact of ENDF/B-VII.0 & UO2 TSL on ZED-2 results

- Substantial (~6 mk) reduction of k_{eff} bias with ENDF/B-VII.0; small reduction in CVR bias (~1.1 mk)
- Significant additional k_{eff} & CVR bias reduction using preliminary UO₂ TSL ACE files



- <u>But</u>, little reactivity sensitivity to UO₂ TSL data with ACE files that include coherent elastic scattering (I. Hill – AECL & J.V. Donnelly – NSS)
- Confirmed results using MCNPX & LANL TSL ACE files with improved thermal scattering treatment



Energy dependence of ZED-2 CVR bias: SEU/RU 24-cm pitch

Track-length MCNP5 k_{eff} – based on

fission-yield tallies

CVR (Δk_{eff}) simulation bias – negligible reactivity sensitivity to UO₂ TSL data



Energy dependence of reactivity impact of UO₂ TSL data

Energy (MeV)

10

Cross

<u>But</u>, low impact of UO₂ TSL data on SEU/RU CVR bias is due to cancellation of positive & negative reactivity impacts of ~2.8 mk each at thermal energies above & below ~3x10⁻⁸ MeV



Conclusion

- New ²H data from modern nuclear theory calculations
 - Extended to include various potentials; 3NF; $\sigma_{elastic}(E,\mu)$; $\sigma_{(n,2n)}(E)$; 50 keV to ~20 MeV
 - But do not reduce/resolve simulation biases for ZED-2 integral measurements
 - Magnetic interaction important(?), or something else ...
- UO₂ TSL data appear to have little net reactivity impact (<0.1 mk), when elastic component included, due to cancellation of larger positive & negative reactivity contributions at low energies
- Need to be able to process TSL data in NJOY at arbitrary temperatures & replicate the LANL TSL ACE files (see also "Thermal Scattering Data and Criticality Safety", W. Haeck and N. Leclaire, PHYSOR'08)



