



# The Problem with the Nuclear Data for **Deuterium**-Uranium Systems



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# Outline

- International Criticality Safety Benchmark Evaluation Project (ICSBEP) HEU D<sub>2</sub>O Solution Thermal critical experiments (HST-004 & -020)
- AECL Chalk River Laboratories (CRL) ZED-2 (Zero Energy Deuterium) critical experiments
  - Existing: NU (Natural Uranium) in hexagonal lattices; D<sub>2</sub>O & air 'cooled' fuel channels
  - Recent: SEU (Slightly Enriched Uranium) CANFLEX bundles in square lattices; H<sub>2</sub>O & air cooled
- Numerical benchmark studies
  - CANDU-SCWR (CANada Deuterium Uranium - Supercritical Water Reactor) lattice
  - <sup>2</sup>H-reflected U-metal sphere
- Summary/Conclusions



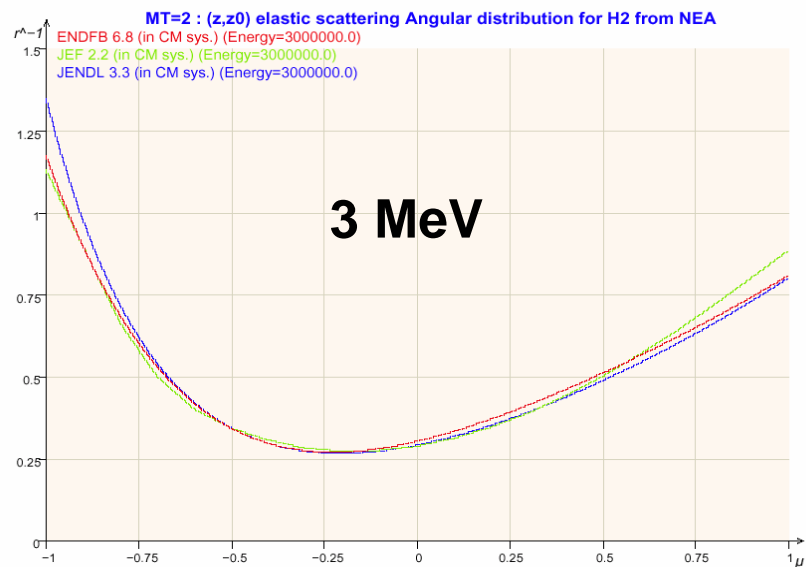
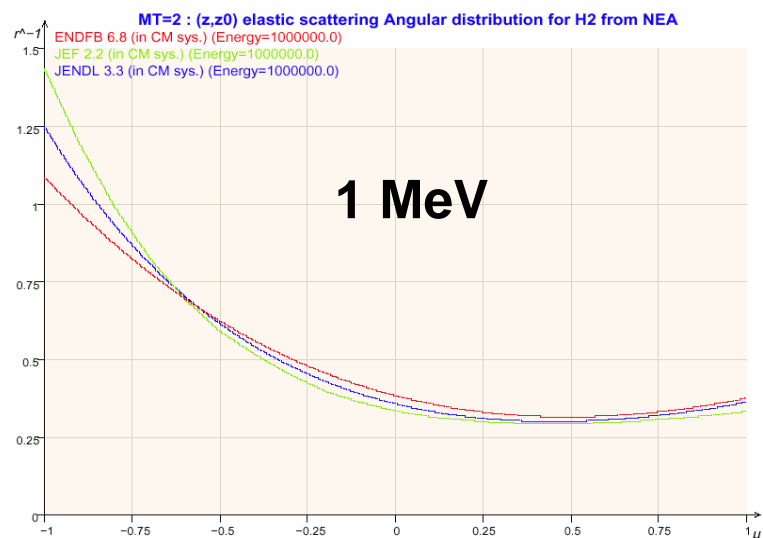
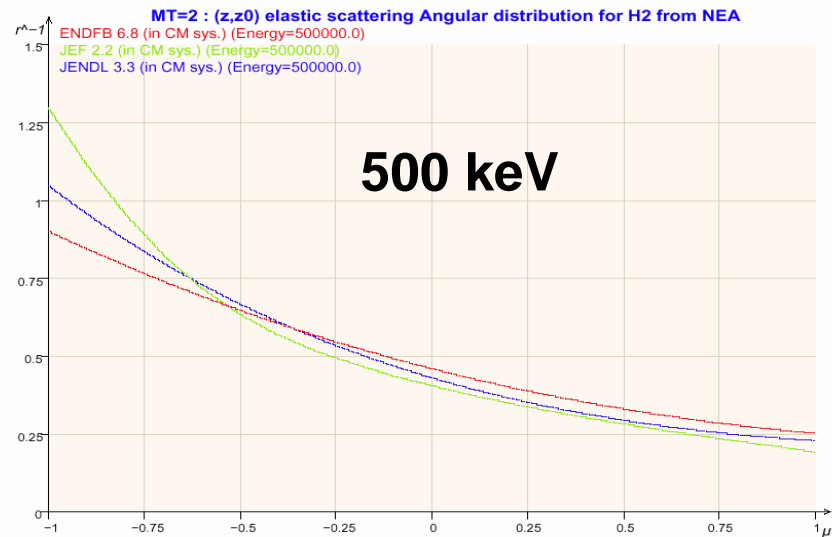
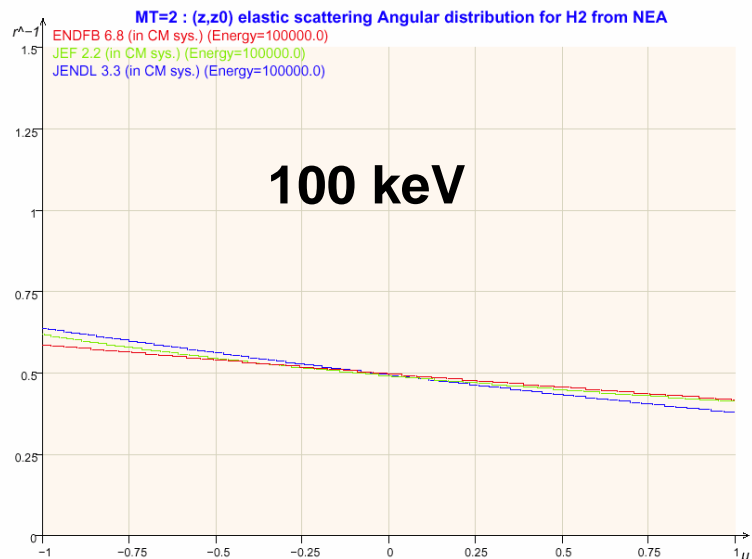
## Background:

# Changes to ENDF/B-VI $^2\text{H}$ cross-section data

- ENDF/B-VI.4 [MCNP ZAID=1002.60c & .64c processed by LANL]
- ENDF/B-VI.5 (through ENDF/B-VI.8) [ZAID=1002.66c]
  - data range extended from 100 to 150 MeV
  - (n,2n), elastic & inelastic cross sections revised slightly above 10 MeV to match experimental data better
  - **angular distributions for elastic scattering** revised slightly >20 MeV & <3.2 MeV to improve agreement with measurement
  - Surprisingly large reactivity change (~9.7 mk) observed by LANL & KAPL for HEU D<sub>2</sub>O solution benchmarks HEU-SOL-THERM (HST-004 & 020)
- Questions raised:
  - What is the impact for other D<sub>2</sub>O critical systems?
  - Which is better: ENDF/B-VI.4 [1002.60c,.64c] or -VI.5 [1002.66c]?
  - Are there indications of additional problems with  $^2\text{H}$  data?



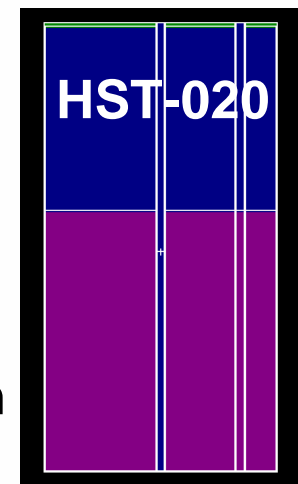
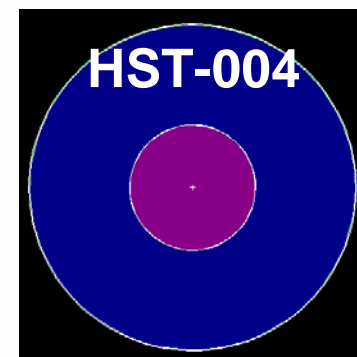
# Comparison of $^2\text{H}$ angular scattering distributions





## Limited $^2\text{H}$ data: HST-004 & -020 ICSBEP benchmarks

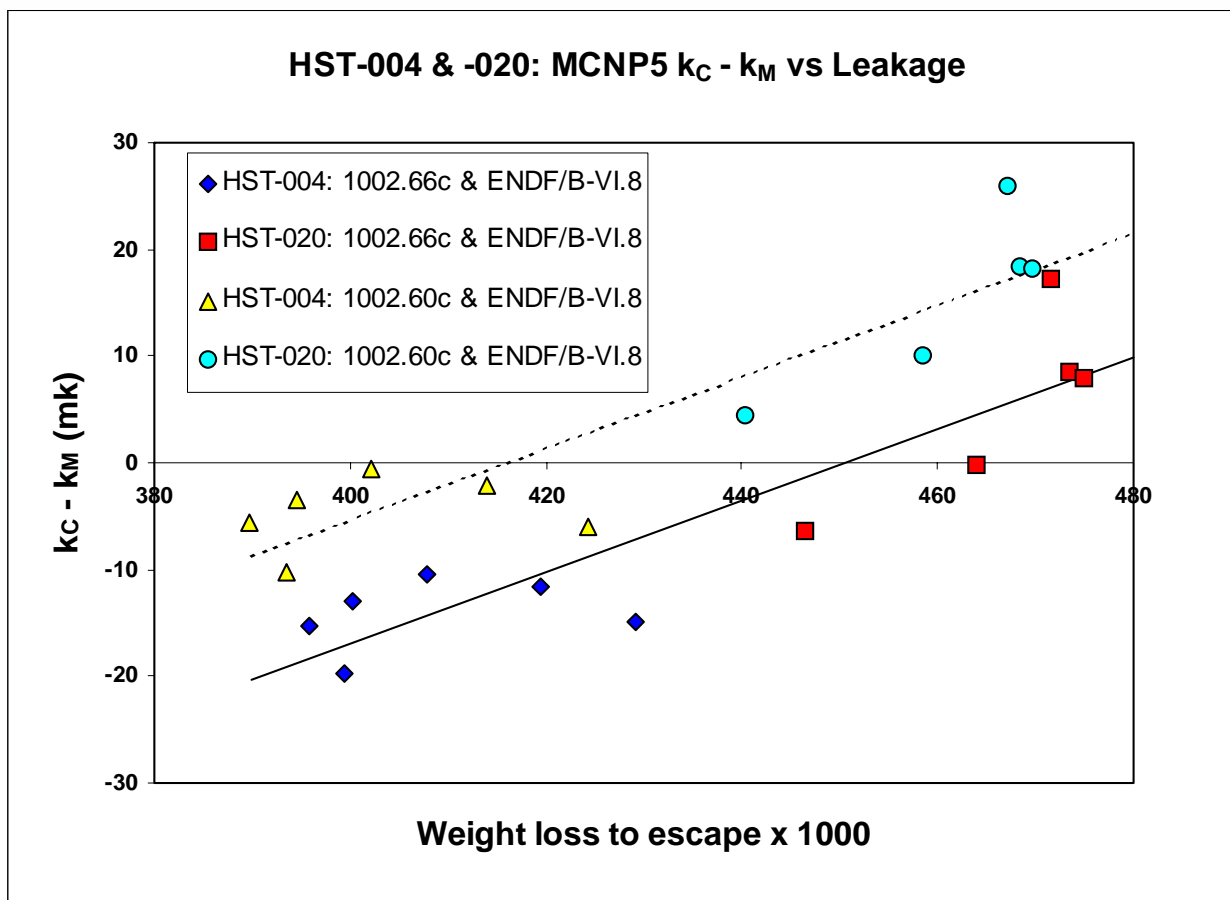
- **High leakage (~40%); HEU; homogeneous uranyl fluoride solutions in  $\text{D}_2\text{O}$ ; large experimental uncertainties for  $k$ ; thermal fission fraction 38-97%**
- **HST-004**
  - 6 expts. with inner **sphere of HEU** uranyl fluoride in  $\text{D}_2\text{O}$  **reflected** by outer annulus of  $\text{D}_2\text{O}$
  - LANL believes HST-004 results are more reliable than HST-020
- **HST-020**
  - 5 expts. with **unreflected cylinders** of HEU uranyl fluoride in  $\text{D}_2\text{O}$
  - have reactivity biases of approximately -4 mk, due to the calculated omission of room return





## CRL HST MCNP5 results

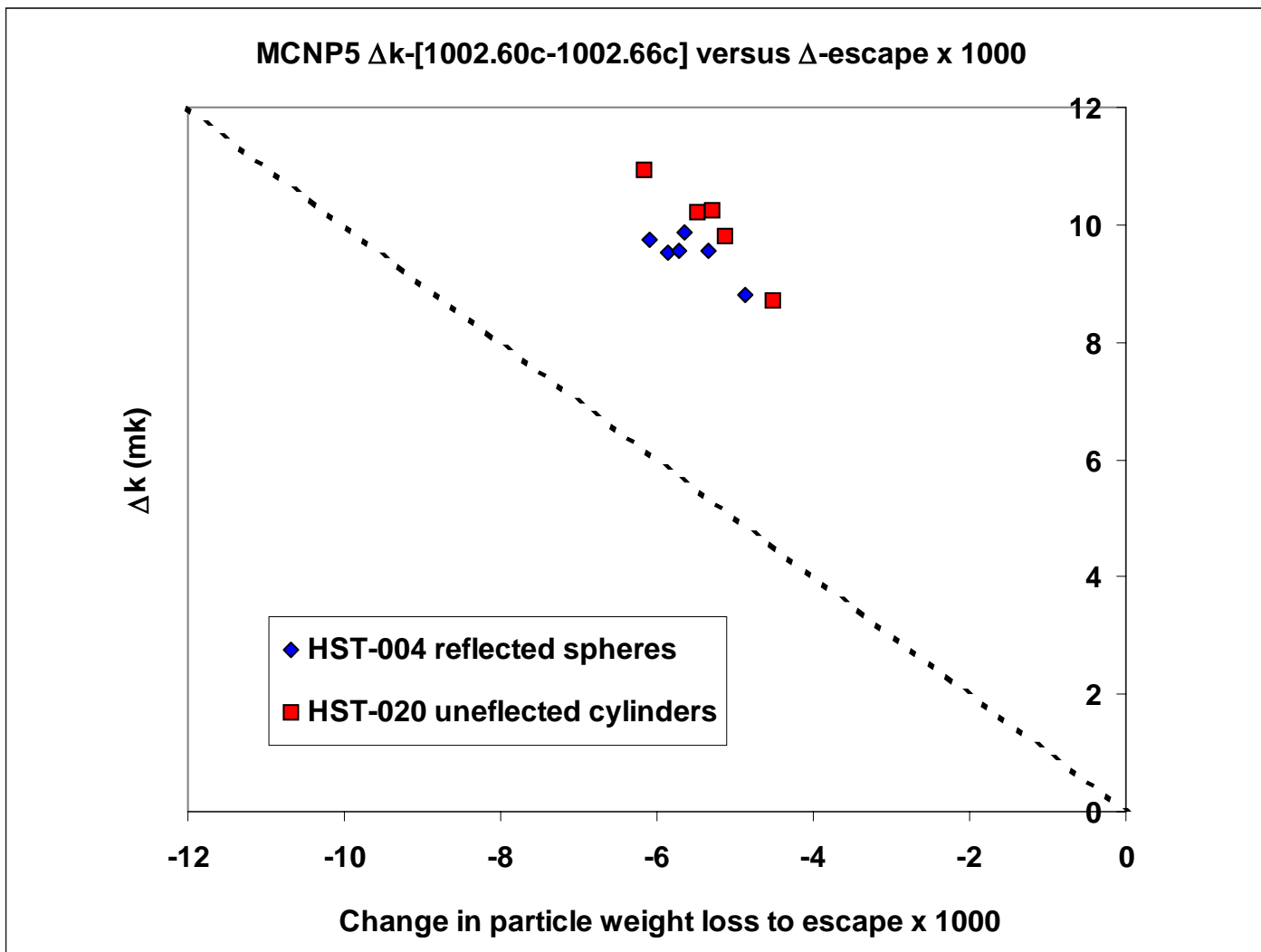
- $k_{\text{Calc.}} - k_{\text{Meas.}}$  shows a large spread of  $\sim 37$  mk & rising trend with calculated leakage
- Using ENDF/B-IV [1002.60c] increases  $k$  by  $\sim 9.7$  mk





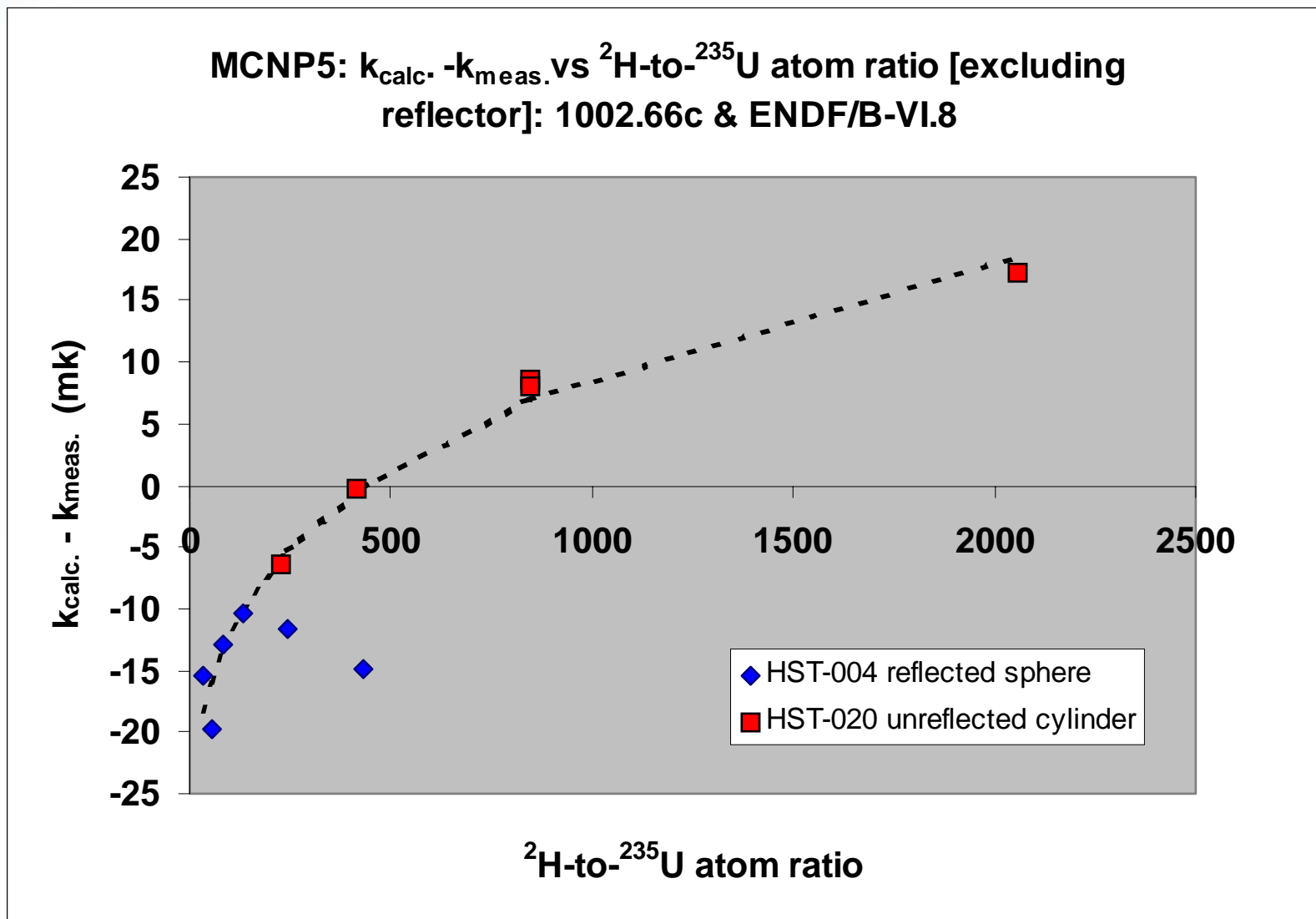
# CRL HST MCNP5 results

- $\Delta k$  [1002.60c – 1002.66c] depends on change in calculated leakage





# CRL HST results: dependence on $^2\text{H}$ -to- $^{235}\text{U}$ atom ratio









## Comparison of HST & ZED-2 critical experiments

- HST & ZED-2 experiments are complementary

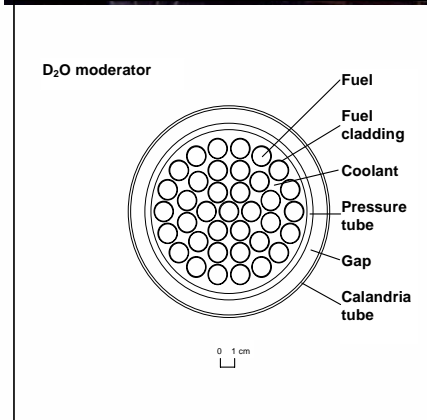
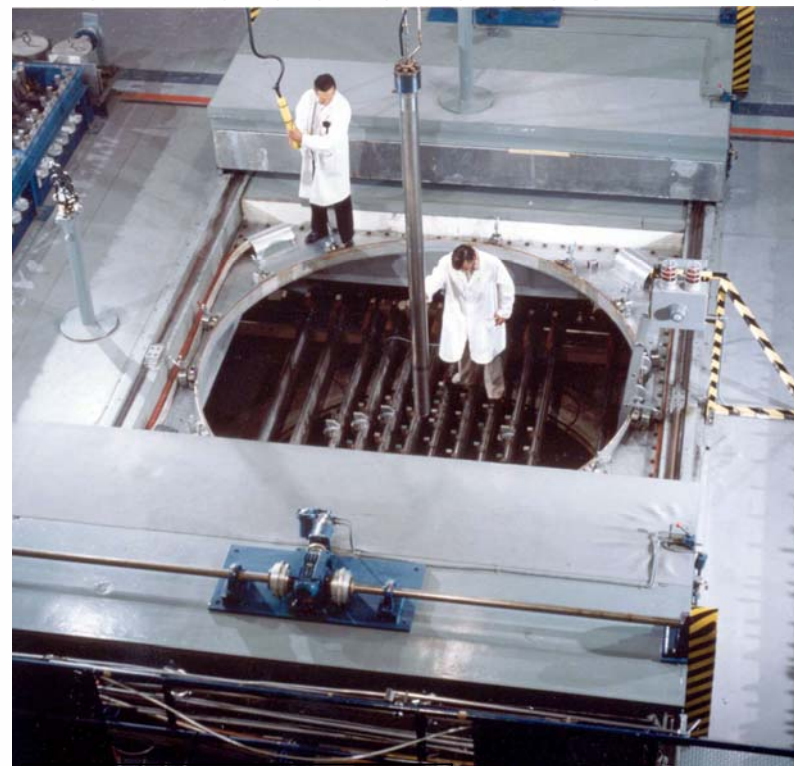
<b>Characteristic</b>		
<b>Neutron leakage</b>	<b>Low</b> (~11% from D <sub>2</sub> O moderator surface)	<b>High</b> (~40%)
<b>Enrichment</b>	<b>Natural Uranium (NU;</b> <b>0.7% <sup>235</sup>U)</b>	<b>HEU (&gt; 90%</b> <b><sup>235</sup>U)</b>
<b>Physical form</b>	<b>Heterogeneous rod lattices</b>	<b>Homogeneous solutions</b>

- HST experiments feature simple geometry & materials
- ZED-2 results potentially more directly relevant to existing reactor applications



# ZED-2 Reactor at Chalk River Laboratories

- Tank-type critical facility, 3.3 m in diameter & depth
  - D<sub>2</sub>O moderator height increased to bring critical; some fuel protrudes above
  - runs at a few Watts; first criticality 1960
- Flexible facility that allows testing of a variety of fuels, different pitches (hex. or square), different coolants: D<sub>2</sub>O, H<sub>2</sub>O, air (voided)
- D<sub>2</sub>O moderated; graphite radial & bottom reflector
- Typical lattice arrangement is 31-cm hexagonal pitch, with 55 channels, each containing 5 fuel bundles
- Mainly used for CANDU reactor physics validation experiments, e.g., coolant void reactivity (CVR)
- **Hope to include some results in IRPhEP (AECL/Canada now involved)**



**CANDU fuel lattice cell**

Figure 1. Cross section of a 37-element CANDU fuel lattice cell

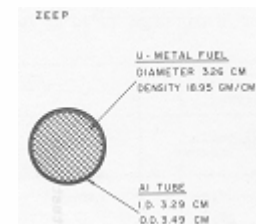


# ZED-2 MCNP5 hex. reference-lattice simulations

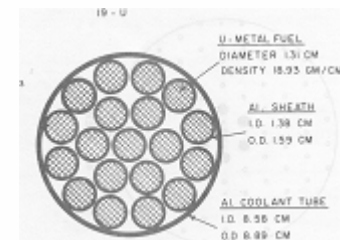
In order of increasing  $^{238}\text{U}$  capture:

1. 91 ZEEP **U-metal** rods; lattice pitch = 22.86 cm
2. 91 ZEEP U-metal rods; lattice pitch = 21.59 cm
3. 91 ZEEP U-metal rods; lattice pitch = 20.00 cm
4. **55 air-cooled (i.e., voided) 28-element  $\text{UO}_2$  assemblies (i.e., 5 Pickering-type bundles each) plus 30 ZEEP U-metal rods; lattice pitch = 31.00 cm**
5. **55 air-cooled 28-element  $\text{UO}_2$  assemblies plus 30 19-element U-metal assemblies; lattice pitch = 31.00 cm**
6. **55 heavy-water-cooled 28-element  $\text{UO}_2$  assemblies plus 30 ZEEP U-metal rods; lattice pitch = 31.00 cm**
7. **55 heavy-water-cooled 28-element  $\text{UO}_2$  assemblies plus 30 19-element U-metal assemblies; lattice pitch = 31.00 cm**

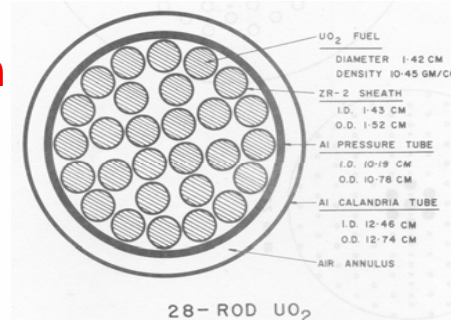
Critical heights ranged from 155.8 to 213.3 cm (14% to 9% calculated leakage from  $\text{D}_2\text{O}$  surfaces)



ZEEP (1945)



19-el. U-metal

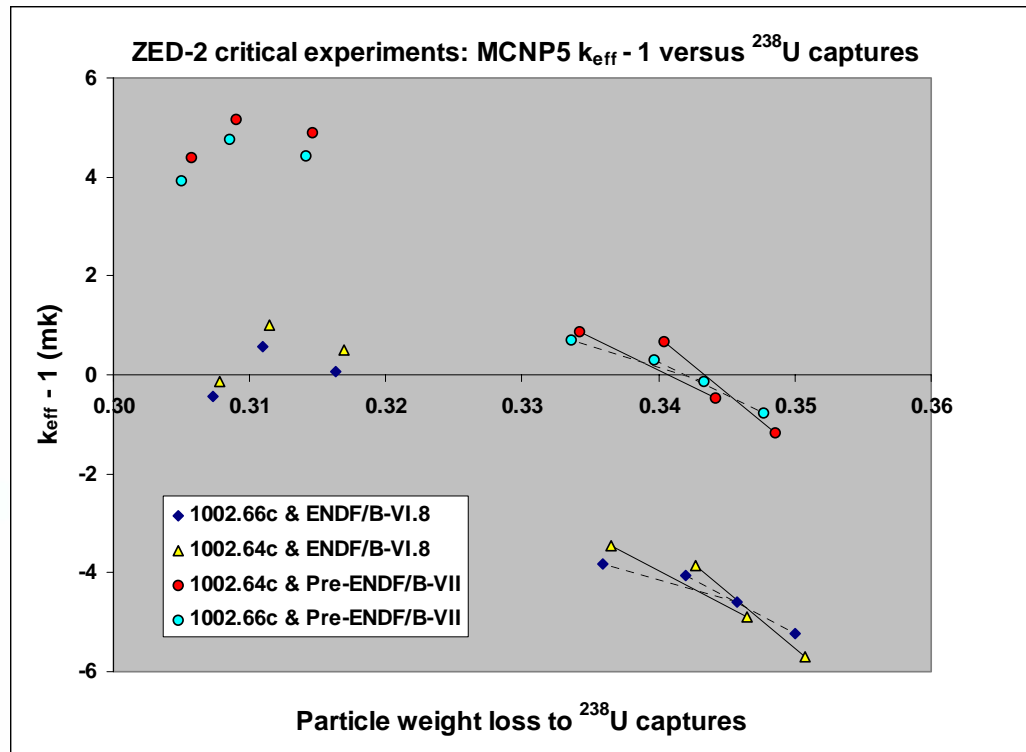


28-el.  $\text{UO}_2$



# Dependence of MCNP5 ZED-2 $k_{eff}$ on nuclear data

- 4 data sets:
  - Deuterium from ENDF/B-VI.8 (1002.66c) & ENDF/B-VI.4 (1002.64c)
  - Uranium from ENDF/B-VI.8 & Pre-ENDF/B-VII

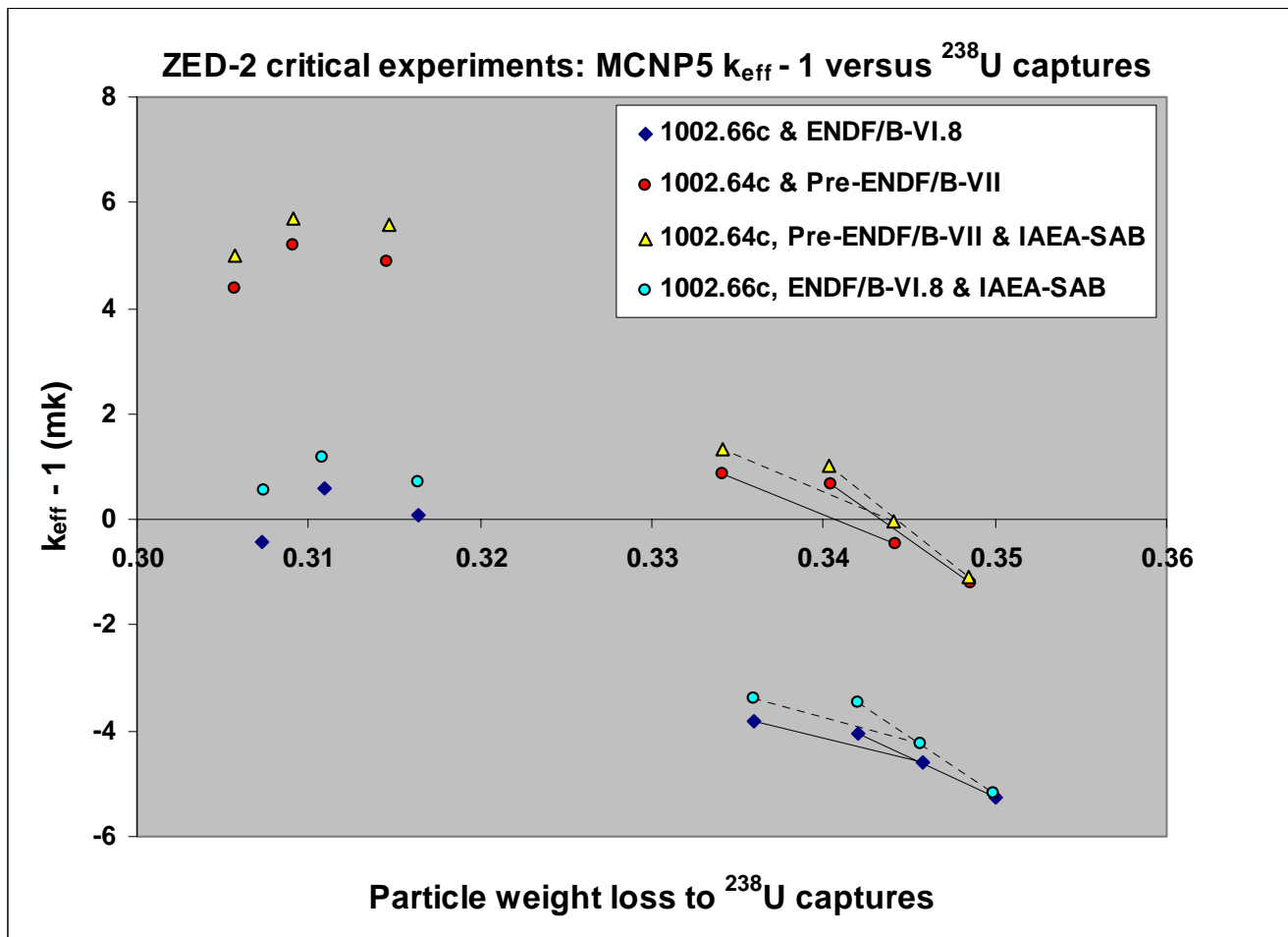


- Decreasing trend with increasing  $^{238}\text{U}$  captures
- Small reactivity impact (<1 mk) due to different  $^2\text{H}$  data; CVR bias worse with 1002.64c
- Behaviour of  $\text{D}_2\text{O}$ -cooled cases differs from air-cooled cases
- Main impact is a gain of ~4 mk due to pre-ENDF/B-VII  $^{238}\text{U}$ ,  $^{235}\text{U}$



## ZED-2 MCNP5 simulations: IAEA-S( $\alpha,\beta$ ) for D<sub>2</sub>O

- Small increase in k (<1 mk)
- CVR bias slightly worse (~0.2mk)

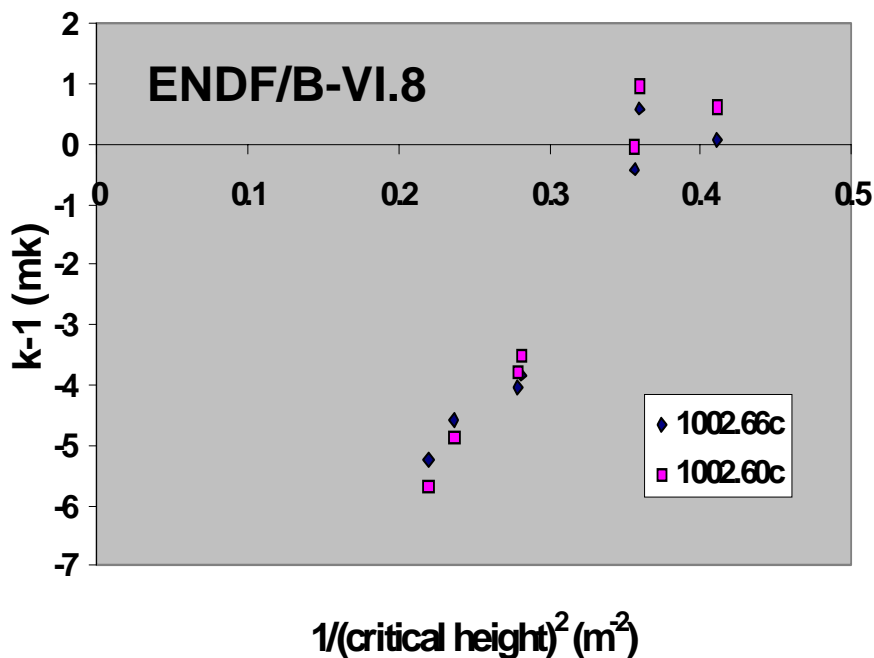




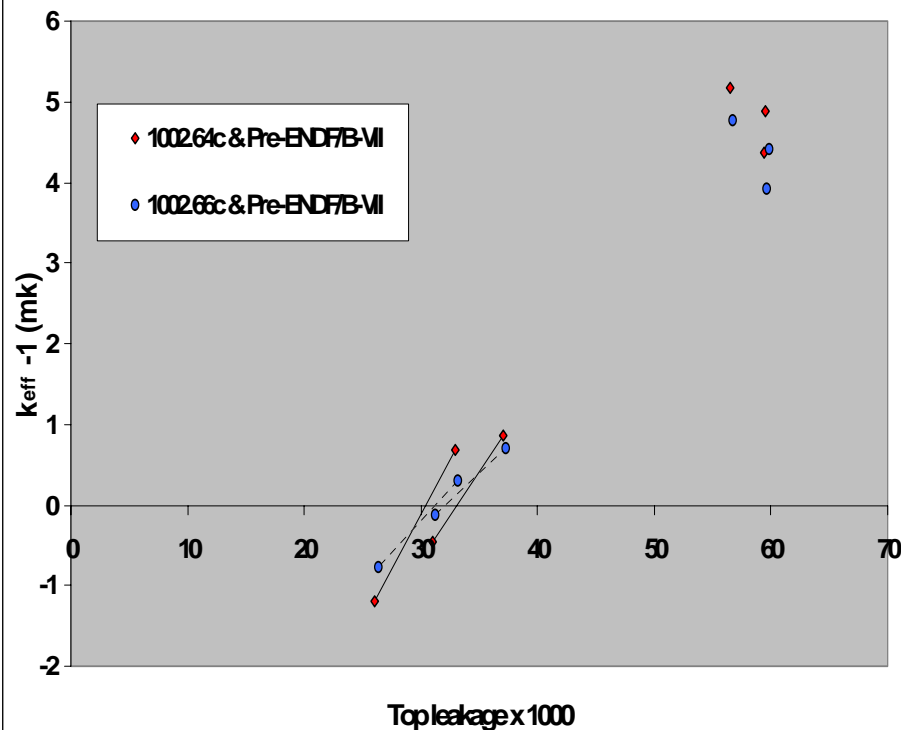
## ZED-2 MCNP5 $k_{eff}$ **also** increases with neutron leakage

- Neutron leakage from D<sub>2</sub>O moderator is predominantly thermal (~87% <0.625 eV)
- Small net in-leakage of fast neutrons (>0.1 MeV) at top moderator surface due to fissions in exposed fuel above
- Axial leakage  $\sim 1/(\text{critical height})^2$

MCNP5  $k-1$  vs  $1/(\text{critical height})^2$



ZED-2 critical experiments: MCNP5  $k_{eff} - 1$  versus calculated top leakage





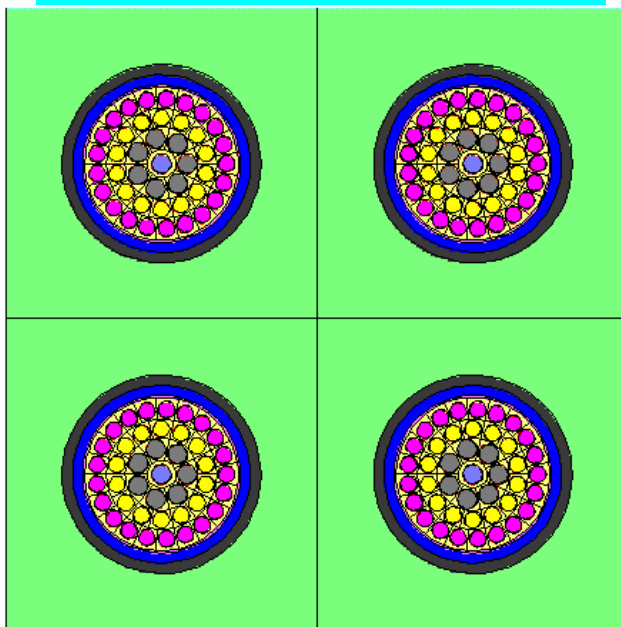


# MCNP5 CANDU-SCWR (Supercritical Water Reactor) benchmark

(Proc. Int. Workshop on Nucl. Data Needs for Generation-IV Nucl. Energy Systems, Antwerp, 2005)

- 21-cm square lattice pitch; 4.25 wt%  $^{235}\text{U}$
- Uniform lattice of mid-life (22.3 MWd/kgU) fuel [composition from WIMS-AECL] & “mixed” lattice (0.2 & 44.2 MWd/kgU)
- $\text{H}_2\text{O}$  cooled [inlet density = 0.44 g/cm $^3$ ] & voided configurations
- Nuclear data at 294 or 300 K
- **Reactivity sensitivity to  $^2\text{H}$  data calculated as a function of axial-neutron-leakage (i.e., finite core length with a vacuum boundary)**

## 2-by-2 MCNP5 model

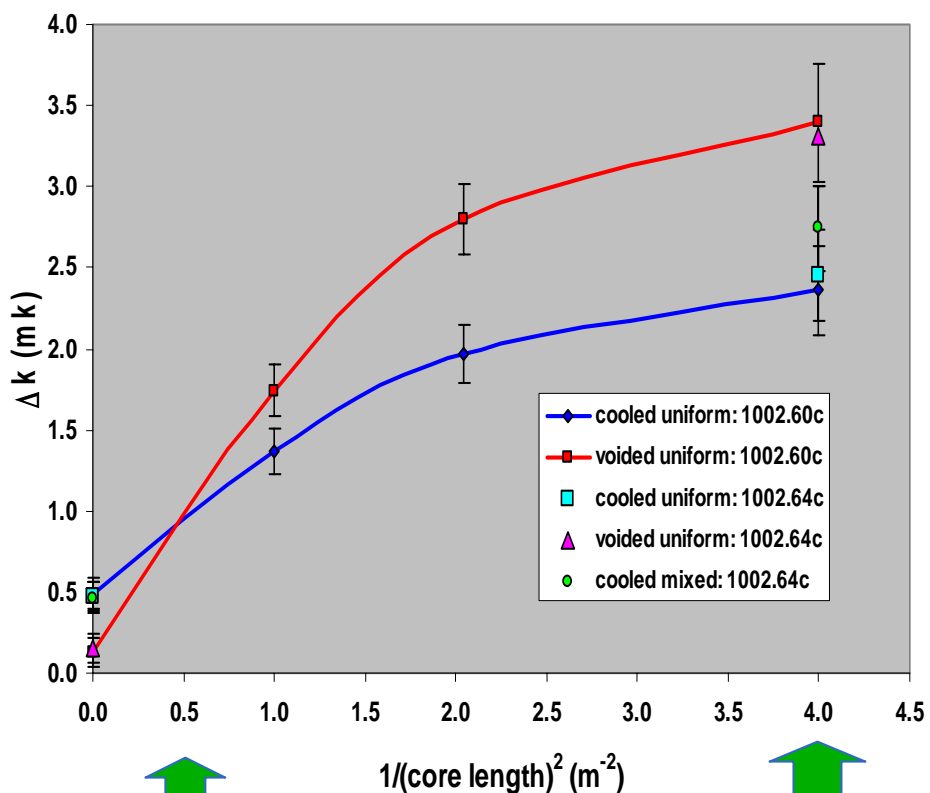




## Sensitivity of CANDU-SCWR numerical benchmark to $^2\text{H}$ data

- $\Delta k$ -[1002.64c – 1002.66c] increases with axial leakage & depends on coolant state
- Essentially a 1:1 correspondence between  $\Delta k$  & the change in calculated leakage

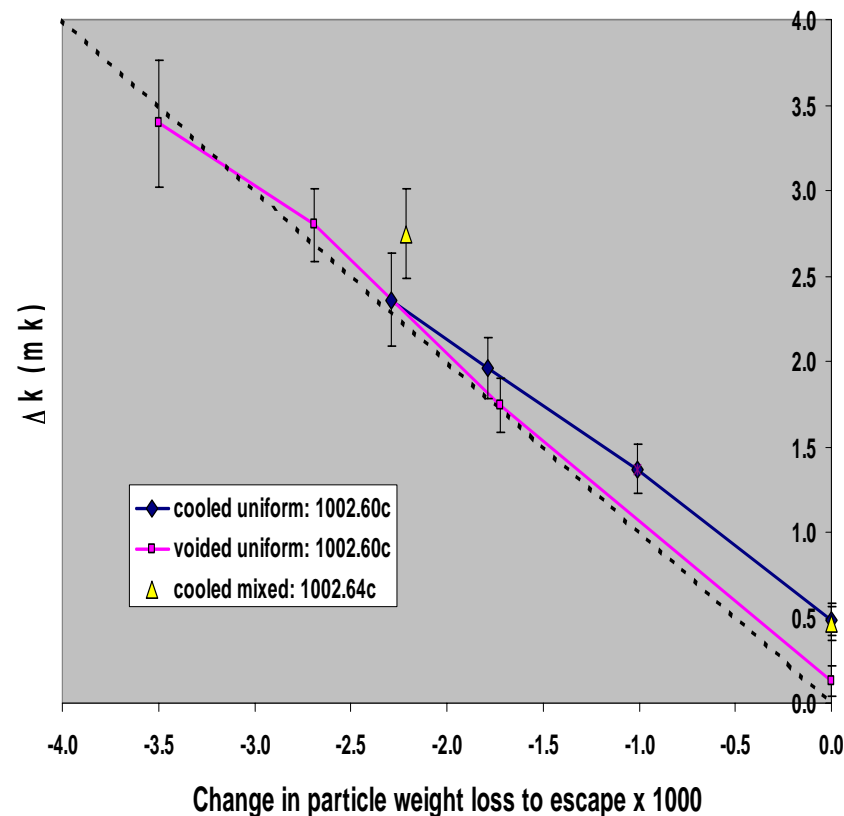
MCNP5  $\Delta k$  relative to 1002.66c vs  $1/(\text{core length})^2$



ZED-2

~HST-004,020 leakage

MCNP5  $\Delta k$  relative to 1002.66c vs change in leakage







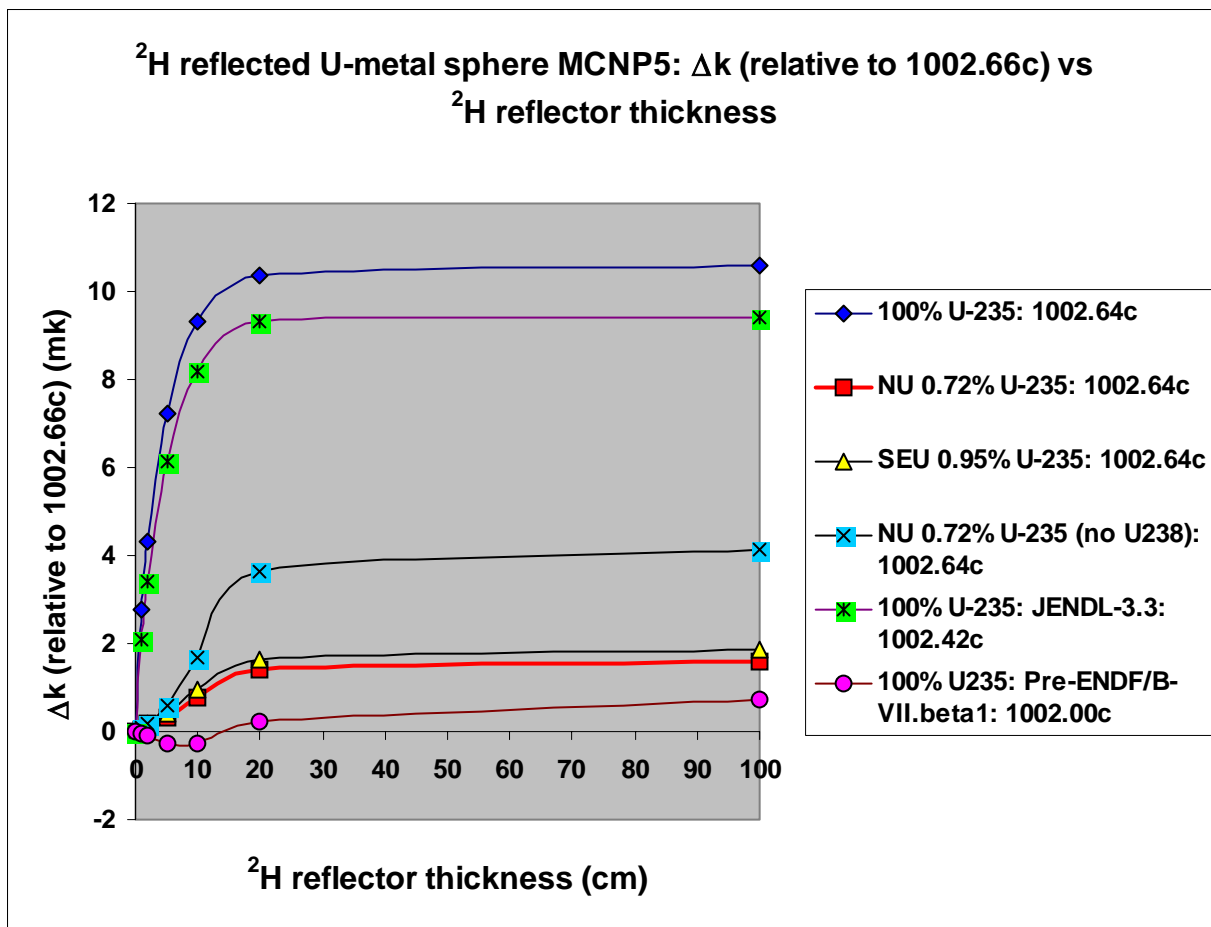
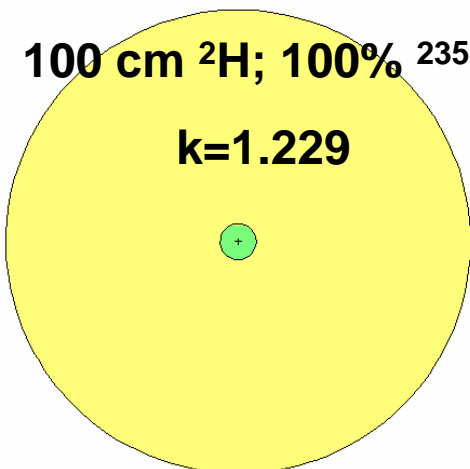
# Simplified $^2\text{H}$ benchmark to highlight reactivity impact of angular scattering

- $^2\text{H}$ -(at  $\text{D}_2\text{O}$  # density)reflected 8.4-cm radius U-metal sphere; no  $S(\alpha,\beta)$

0 cm  $^2\text{H}$ ; 100%  $^{235}\text{U}$   
 $k=0.997$



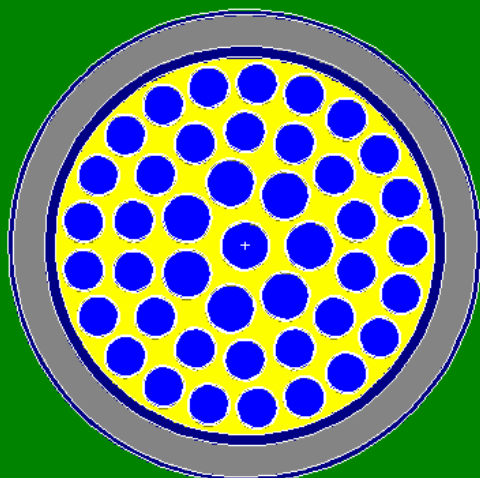
100 cm  $^2\text{H}$ ; 100%  $^{235}\text{U}$   
 $k=1.229$



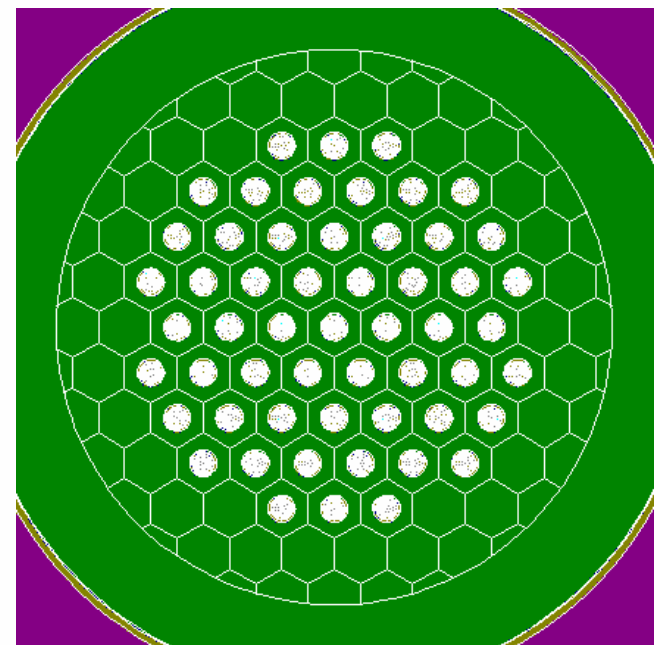
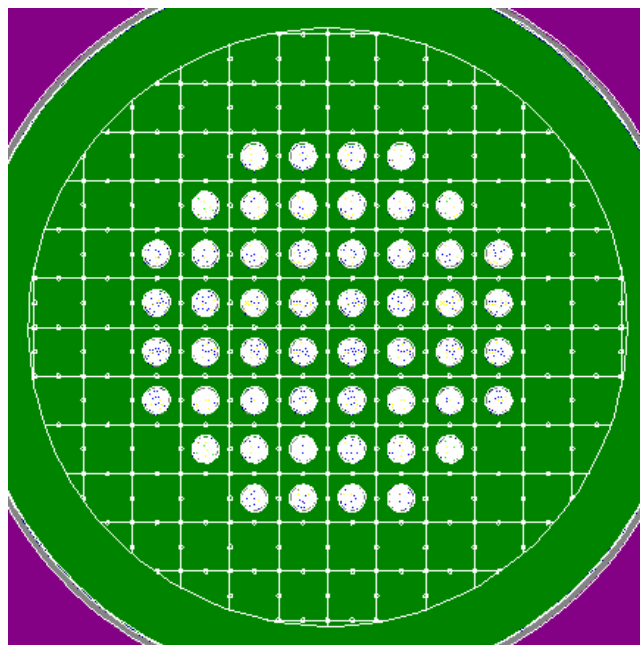


## Recent ZED-2 results

- Slightly Enriched Uranium (SEU): 0.95 wt%  $^{235}\text{U}$
- 43-element CANFLEX fuel geometry (greater subdivision)
- Square vs. hexagonal lattices; pitch = 20 to 24.5 cm
- $\text{H}_2\text{O}$  & air 'coolant'



CANFLEX



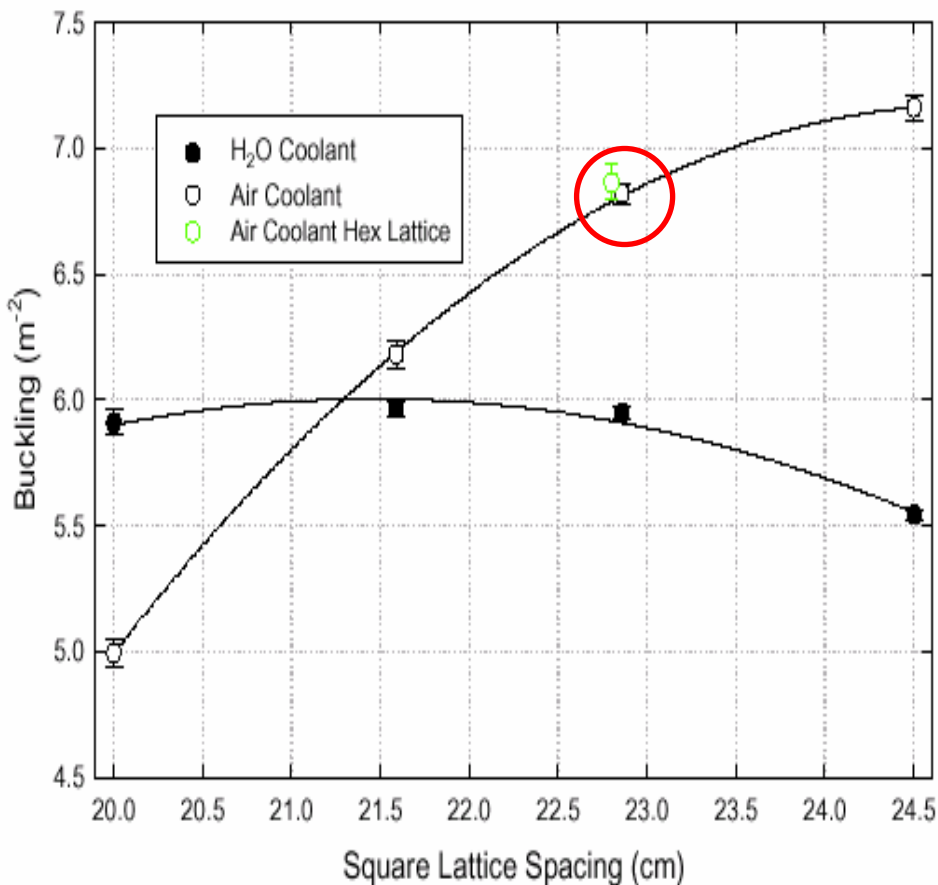
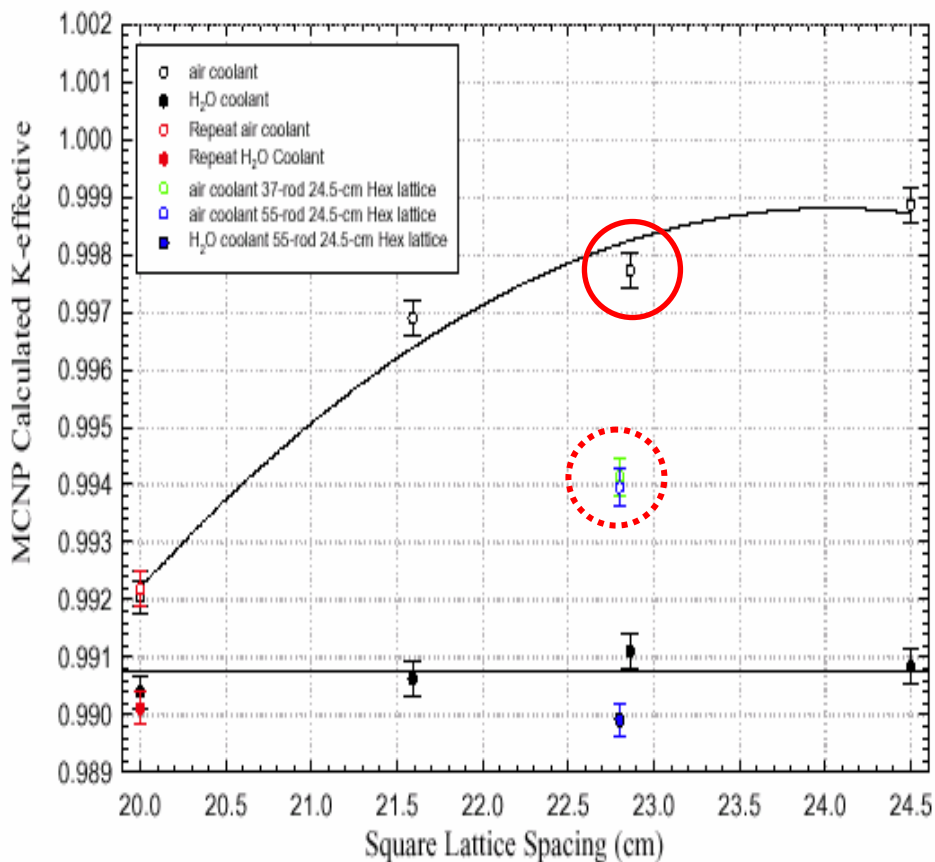


## Recent ZED-2 H<sub>2</sub>O CVR results for SEU CANFLEX fuel

- MCNP5 H<sub>2</sub>O CVR bias increases to **~+8 mk** with square lattice pitch
- Hexagonal-pitch data plotted at equivalent square lattice pitch
- MCNP5 shows different hex & sq. results, but expt. critical bucklings the same

CANFLEX SEU in ZED-2

**ENDF/B-VI.8** CANFLEX SEU in ZED-2

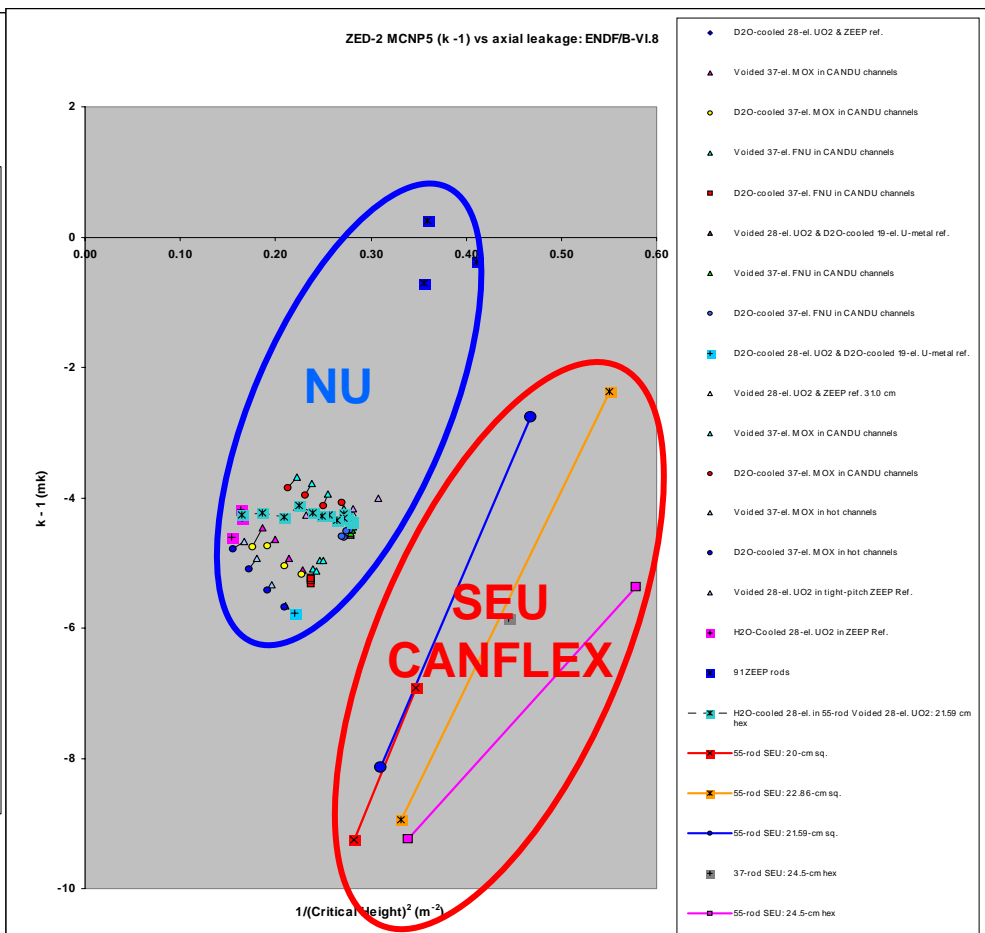
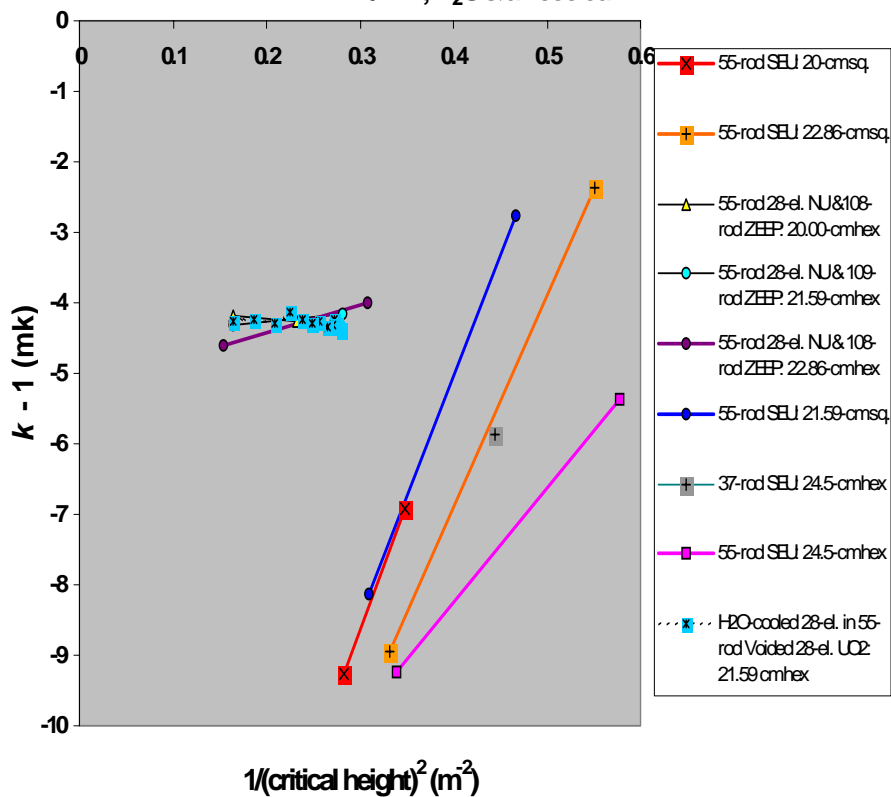




# Dependence of ZED-2 MCNP5 $k_{eff}$ on axial leakage

- New SEU ZED-2 H<sub>2</sub>O CVR measurements involve relatively large changes in axial leakage
- MCNP5  $k_{eff}$  increases with axial leakage, as before

ZED-2 MCNP5  $k_{eff}$  dependence on axial leakage:  
ENDF/B-VI; H<sub>2</sub>O & air cooled





# Summary/Conclusions

- Big difference in reactivity sensitivity of HST (~10 mk) & ZED-2 (<1 mk) NU results to ENDF/B-VI.5 & VI.4  $^2\text{H}$  data
- ZED-2 results show lower  $\text{D}_2\text{O}$  CVR bias (by ~0.6 mk) with newer ENDF/B-VI.5  $^2\text{H}$  data relative to ENDF/B-VI.4
- But, still a significant rising trend of  $(k_{\text{eff}} - 1)$  with leakage for both ZED-2 & HST criticals
- Numerical benchmarks with different  $^2\text{H}$  data show
  - CANDU-SCWR: reactivity sensitivity depends on leakage & presence/absence of low-density  $\text{H}_2\text{O}$  coolant
  - $^2\text{H}$ -reflected U-metal sphere: reactivity sensitivity depends on  $^{235}\text{U}$  enrichment ( $^{235}\text{U}$  # density & offset due to  $^{238}\text{U}$  captures) & reflector thickness (reduced leakage)
- MCNP5 results for new SEU CANFLEX ZED-2 measurements show a large (up to ~+8 mk)  $\text{H}_2\text{O}$  CVR bias that depends on lattice pitch & arrangement (square vs. hexagonal)
- **New  $^2\text{H}$  evaluation &/or angular scattering measurements needed?**



# Acknowledgments

- *Russ Mosteller* (LANL) provided pre-ENDF/B-VII for U & 1002.64c data **in ACE format**
- *Andre Trkov* (IAEA) provided new  $S(\alpha,\beta)$  for D<sub>2</sub>O & H<sub>2</sub>O
- *Radoslav Zajac* (BNL-NNDC) provided pre-ENDF/B-VIIbeta1 1002.00c data
- CRL ZED-2 experiment & analysis crew, particularly, Mike Zeller, Benoit Arsenault & Bruce Wilkin





# Reminder . . . . .

- **PHYSOR-2006** is 10 months away:  
**Sept. 10-14, Vancouver, BC, Canada**
- **Key dates:**
  - **Jan. 7, 2006**, 1000-word reduced-length paper due
  - **June 15, 2006**, full-length papers due
- See <http://www.cns-snc.ca/physor2006>
- **Technical Program includes:**
  - **Plenary:** Advances in Nuclear Data Libraries
  - **Covariance Data Generation for Nuclear Applications** (**Luiz Leal**, ORNL)
  - **Nuclear Safety Validation & Performance of ENDF/B-VII** (**Richard McKnight**, ANL)
  - **Nuclear Data** (**Mike Dunn**, ORNL)
  - **The International Reactor Physics Experiment Evaluation Project (IRPhEP)** (**J. Blair Briggs**, INL; **Ibrahim Attieh**, AECL)

	<p align="center"><b>CALL FOR PAPERS</b>  <b>PHYSOR-2006 TOPICAL MEETING</b>  <b>HYATT REGENCY VANCOUVER</b>  <b>VANCOUVER, BRITISH COLUMBIA, CANADA</b>  <b>SEPTEMBER 10-14, 2006</b></p>	
<b>Advances in Nuclear Analysis and Simulation</b>		
<p><b>Organizing Committee</b></p> <p><b>Honourary Chair</b> Dr. James Lake <i>Idaho National Laboratory</i></p> <p><b>General Chair</b> Dr. Ben Rouben <i>AECL</i></p> <p><b>Technical Program Co-Chairs</b> Dr. Ken Kozier <i>AECL</i> Prof. Chang Hyo Kim <i>Seoul National University</i> Dr. Russell Mosteller <i>LANL</i> Dr. Enrico Sartori <i>OECD/NEA</i></p> <p><b>Workshops</b> Dr. Wei Shen <i>AECL</i></p> <p><b>Publications</b> Dr. Adriaan Buijs <i>AECL</i></p> <p><b>Finance</b> Mr. Marv Gold <i>Candesco Research Corporation</i></p> <p><b>Facility Contact</b> Dr. Ben Rouben <i>AECL</i></p> <p><b>Student Program</b> Dr. Eleodor Nichita <i>University of Ontario Institute of Technology</i></p> <p><b>Registration</b> Ms. Denise Rouben <i>CNS</i></p> <p><b>Publicity</b> Dr. Mohamed Younis <i>AECL</i></p>	<p align="center"><b>ANS Sponsoring Division</b> Reactor Physics Division <b>Hosted by</b> Canadian Nuclear Society (CNS)</p> <p align="center"><b>International Co-Sponsors</b> Associazione Italiana Nucleare, Atomic Energy Society of Japan, Belgian Nuclear Society, Brazilian Nuclear Energy Association, British Nuclear Energy Society, Chinese Nuclear Society, Croatian Nuclear Society, Finnish Nuclear Society, French Nuclear Energy Society, Israel Nuclear Society, Korean Nuclear Society, OECD Nuclear Energy Agency, Romanian Nuclear Energy Association, Sociedad Nuclear Mexicana, Swiss Nuclear Society</p> <p align="center"><b>Technical Topics</b></p> <ul style="list-style-type: none"> <li>• Accelerator and Spallation Physics •</li> <li>• Advanced Reactor Designs • Alternative Concepts • Biomedical Applications •</li> <li>• Fuel/Core Design and Analysis • Fuel Cycle Physics •</li> <li>• Neutron Physics • Nuclear Data •</li> <li>• Reactor Analysis Methods • Reactor Physics •</li> <li>• Research Reactor Applications •</li> <li>• Space Applications • and Other Topics •</li> </ul> <p align="center"><b>Preliminary Plenary Session Topics</b> International Development of New Reactors Advances in Nuclear Data Emerging Nuclear Technologies and Applications Advances in Analysis Methods and Reactor Simulation</p>	<p><b>Important Dates:</b>  <b>January 7, 2006</b> Electronic Submission of 1,000-Word Reduced-Length Paper  <b>February 17, 2006</b> Notification of Acceptance to Authors  <b>June 15, 2006</b> Deadline for Submission of Final Full-Length Paper  <b>July 31, 2006</b> Early Registration Deadline</p> <p><b>Instructions for Reduced-Length Papers:</b></p> <ul style="list-style-type: none"> <li>– Describe work that is NEW, SIGNIFICANT, and RELEVANT to the nuclear industry</li> <li>– Use ~1,000 words, including Figures and Tables</li> <li>– Electronic submission via: <a href="http://www.cns-snc.ca/physor2006">http://www.cns-snc.ca/physor2006</a></li> </ul>
<p>For more information, please contact:          Dr. Ken Kozier, Atomic Energy of Canada Limited          Chalk River Laboratories, Chalk River, Ontario, K0J 1J0          Phone: +1-613-584-8811+ext.5059          E-mail: <a href="mailto:physor2006@aecl.ca">physor2006@aecl.ca</a></p>		



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The main logo features a large, stylized blue 'A' with a horizontal line through it and a small circle at the end of the line, followed by the letters 'AECL' in a bold, serif font.