R&D in Nuclear Data for Reactor Physics Applications in CNL (CNL = Canadian Nuclear Laboratories)

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Improvement of TSL (Thermal Scattering Laws, or $S(\alpha, \beta)$ data)

New Evaluations for $\text{D}_2\text{O}$, $\text{H}_2\text{O}$, $\text{UO}_2$, $\text{ThO}_2$, ...

New Models, Measurements, and Testing (Benchmarking)

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Retired: K. Kozier, D. Altiparmakov, B. Wilkin, ...

Nuclear Science Division, CNL, Chalk River, Canada
From AECL to CNL

AECL is divided into:

• CANDU Inc. (← Toronto Reactor division of old AECL)
• CNL (← Chalk River Labs of old AECL)
• AECL (or R-AECL)

CNL will be managed following Canadian GoCo model
(∗GoCo = Government-owned, Contractor-operated)

“Restructuring of AECL’s Nuclear Laboratories”


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CNL (AECL) Reactor Physics Computational Scheme

- Evaluated nuclear data
- Cross section processing
- Library data
- Reactor lattice
- Condensation and control devices
- Two-group data
- Full core reactor

ENDF/B Data → NJOY

Multigroup Data → Continuous Data

WIMS-AECL

WIMS Utilities

DRAGON

Homogenized XS

Incremental XS

RFSP

MCNP

Reference Calculations

TSUNAMI

Sensitivity & Uncertainty Analysis
CNL libraries applied for ZED-2, NRU (Chalk River) and CANDU-type PHWRs
Importance of accuracy of ND and TSL: case study (e.g., in n spectra with optimal moderation by D$_2$O)

Impact of particular ENDF/B-VII.0 data on ZED-2 reactor simulation (left);
1 mk = 100 pcm
Effect of particular ENDF/B-VII.0 data on MCNP calculation of 37-element CANDU lattice cell
D. Altiparmakov, PHYSOR-2010
TSL for heavy and light water: interaction of thermal neutrons with liquid $D_2O$ / $H_2O$ at different $T$ and $p$

- Discrepancy for heavy water in modern evaluated ND libraries: in integral values, at neutron energy $E$ near $E_{th} = 0.0253$ eV, for liquid $D_2O$ at room temp. $T$, we have $(Exp. - Calc.) / Calc. \approx -8.4\%$ (using ENDF/B-VII.0 $S(\alpha_i \beta)$ for D-in-D$_2$O and Free Gas for $^{16}O$)

- What to do?
  TSL evaluation is a model of thermal neutron interaction with a condensed medium (liquid, solid) based on QM and Stat. Phys.; converted into dimensionless tables $S(\alpha_i, \beta_j; T_n)$ following ENDF format. So, improve modeling, improve numerics, ...

- How to improve modeling?
TSL for heavy water (FY 2014/2015)
interaction of thermal neutrons with liquid D$_2$O at room T

- Developing **new** TSL evaluations for water (CNL, Canada and CAB, Argentina): based on combining **Mol. Dynamics (MD)** simulations (GROMACS) and experimental data

- The resulting new **models** are formulated as LEAPR input files for LEAPR module of NJOY99 (**up396 with additional patches**)
NJOY = nuclear data post-processing code, LANL, USA
Benchmarking

Integral experiments: $k_{\text{eff}}$, also reaction rates, spectral indices
TSL for heavy water (FY 2014/2015)
interaction of thermal neutrons with liquid D$_2$O (at room T)

• **Testing**: using Crit. Safety Benchmarks with D$_2$O, overall, it is an **improvement** in $k_{\text{eff}}$ C/E if ENDF/B-VII.0 D$_2$O $S(\alpha,\beta)$ → **new** D$_2$O $S(\alpha,\beta)$ (we call it CAB models)

• We expect that $k_{\text{eff}}$ (CAB D$_2$O) < $k_{\text{eff}}$ (B-VII.0 D$_2$O), but what is the difference $dk = k_{\text{eff}}$ (B-VII.0 D$_2$O) − $k_{\text{eff}}$ (CAB D$_2$O) = ?; **cases with** $dk > \Delta k_{\text{Bench}}$ of special interests

answer for ZED-2 reactor: $dk \approx 100$ pcm, $dk < \Delta k_{\text{Bench}}$, *ZED2-HWR-EXP-001* benchmark (28-element NU UO$_2$ bundles, at room T, evaluator = J. Atfield, CNL)
Discuss: how accurately do we model criticality (critical zero-power assemblies), i.e., $k_{eff} = ?$ $k_{eff} = 1.0$, in theory. In practice (i.e., in modeling), ..... 

- we have a Bias (in $k_{eff}$)
- CVR bias: assume we have cooled and voided critical cases, then:

  Is any dependency / trend of $k_{eff}$ bias upon voiding of the coolant in a crit. assembly?

  Is it possibly to decrease the experimental (benchmark) uncertainty by factor of ... $(3-5)$?
**TSL for heavy water (FY 2014/2015)**

interaction of thermal neutrons with liquid D\(_2\)O (at room T)

- **Testing**: using Crit. Safety **Benchmarks** with D\(_2\)O, overall, it is an **improvement** in \(k_{\text{eff}} \ C/E\) if ENDF/B-VII.0 D\(_2\)O \(S(\alpha, \beta) \rightarrow \) CAB D\(_2\)O \(S(\alpha, \beta)\)

- We expect that \(k_{\text{eff}} (\text{CAB D}_2\text{O}) < k_{\text{eff}} (\text{B-VII.0 D}_2\text{O})\), but what is the difference \(dk = k_{\text{eff}} (\text{B-VII.0 D}_2\text{O}) - k_{\text{eff}} (\text{CAB D}_2\text{O}) = ?\), and check: \(dk < \text{or} > \Delta k_{\text{Bench}} ?\)

**answer for** ZED-2 reactor critical core (CNL, Chalk River):

\(dk \sim 100 \text{ pcm}\) using **LEW-MET-THERM-003** benchmark, note H-in-H\(_2\)O for r.gr. heavy water

This is NU U metal in Al cladding, at room T, evaluator = J. Atfield (CNL)
TSL for heavy water (FY 2014/2015)
interaction of thermal neutrons with liquid $D_2O$ (at room $T$)

LEW-MET-THERM-003: ZEEP rods in ZED-2 reactor in CNL, Chalk River:
art of modeling materials (J. Atfield): conversion of mass-spec data into MCNP data
Example:
benchmark $k_{\text{eff}} = 1.0000 \pm 0.0033$
impurity worth $\approx 4$ mk (e.g., $1.00371 - 0.99953 \approx 4.2$ mk, std. dev $[k_{\text{eff}}] = \pm 0.00004$)
compare with $S(\alpha,\beta)$ sensitivity: $dk$ (CAB vs. B-VII.0) $\approx -1.9$ mk ($= 0.99761 - 0.99953$)
TSL for heavy water (2014/2015, 2015/2016) interaction of thermal neutrons with liquid D$_2$O at different $T$ and $p$

- Inconsistency for heavy water TSL in modern evaluated ND libraries:
  - if $T > T_{\text{room}}$ ($p = 1$ atm), what happens with $\sigma_s(E; T)$?
  - D$_2$O moderator $T$ in CANDU-6: $\approx 68$ deg. C ($\approx 341$ K)
  - D$_2$O moderator $T$ in some ZED-2 experiments up to $\sim 50$-60 deg C. What for?

Moder. T coefficient of reactivity is an important parameter in CANDU reactor physics analysis.

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TSL for heavy water (2014/2015, 2015/2016)
interaction of thermal neutrons with liquid D$_2$O at different $T$ and $p$

- Inconsistency (?) for heavy water in modern evaluated ND libraries:
  if 100°C > $T$ > $T_{\text{room}}$ (p = 1 atm), what happens with $\sigma_s(E; T)$?
- New experimental results at 50 deg. C ($\sim$ 323 K): J.I. Márquez Damián and D. Baxter
- What can we do to improve $S(\alpha, \beta)$ for D$_2$O at 100°C > $T$ > 10°C (at p = 1 atm)?
- New (improved) models $\rightarrow$ NJOY (LEAPR) $\rightarrow$ ACE files & testing (benchmarking) using MCNP, migrate to GROMACS 5.0, NJOY99 $\rightarrow$ NJOY2012, MCNP5 $\rightarrow$ MCNP6 & SERPENT (student-friendly MC)
TSL for heavy water: 
new & improved models $\rightarrow$ new evaluation

New **evaluation** (in ENDF format) can be based on combining **molecular dynamics (MD)** simulations and reliable **experimental data**, and the resulting new **models** can be implemented in / have to be compatible with / **LEAPR** module of **NJOY** (nuclear data post-processing code, LANL, latest is **NJOY 2012**)

The **key points** for building new $S(\alpha,\beta)$ **models** are:

1. use of molecular (**self**)diffusion for translational motion of liquid $\text{H}_2\text{O} / \text{D}_2\text{O}$ (instead of **free gas approximation (FG)** used in **all** evaluated ND libraries);
2. continuous **vibrational spectra** computed from molecular dynamics (**MD**) simulation at a given thermodynamic state of the liquid, $(p, T)$ and density $\rho(p, T)$, (instead of derived / adjusted spectra from neutron scattering experiments);
3. a more precise description of the structure of liquid: e.g., models for D and O in $\text{D}_2\text{O}$ based on **experimental results** (instead of using the **incoherent approximation** in ENDF/B-VI or the Lennard-Jones **model** for D-D structure in JEFF 3.1 and ENDF/B-VII.0 $\rightarrow$ ENDF/B-VII.1)
4. better **numerics** (e.g., extended grid(s), $\alpha_i$, $\beta_j$, $T_n$, and NJOY data processing options revisited, and we need NJOY patches in leapr and thermr; )
5. **ACE files** to be generated for **testing/benchmarking** with MCNP5, MCNP6, and SERPENT

The resulting scattering kernels & cross sections will be an improvement over existing evaluations: they are compared with **measurements** of double differential scattering cross sections, quasi-elastic neutron scattering measurements, angular distributions of out-scattered neutrons, average cosine of the scattering angle (mu-bar), and total cross sections;

**Need to do all this at different** $(p, T)$
New TSL for heavy water and benchmarking: References


Neutron Scattering on Water using triple axis spectrometer at NRU reactor n beam at CNL (Chalk River)

Sample sizes: 0.1 mm to 3 mm

Triple axis spectrometer

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New Measurements at NRU to reduce ND uncertainties to improve Reactor Safety

Differential scattering cross section of D₂O.
Beam energy is 44 meV
(except for that the result from C5 is at E₀ = 41.44 meV).

- G. Bentoumi, G. Li, B. Sur, and Z. Tun (Canadian Neutron Beam Centre)

Absolute differential cross section (in barn/sr) for Light water, at E₀ = 41 meV, Beyster's data: ±5%.
New Measurements at NRU to reduce ND uncertainties to improve Reactor Safety

NRU measured differential cross sections of $D_2O$ (Beam energy is 44 meV)
and $S(\alpha,\beta)$ functions of $H_2O$ (using samples with different widths), after multiple-scattering corrections, all at room T

**Importance:**
- Safety and operating margins for nuclear reactors are crucially dependent on the availability and accuracy of nuclear data that are used for modeling, in particular for safety analysis and licensing applications

**Objectives:**
1. Carry-out new experiments at neutron beam facilities, such as NRU and (?) SNS (ORNL), and also at ZED-2 (CRL), to accurately measure the relevant nuclear data parameters
2. Investigate the discrepancy between the information obtained experimentally and existing nuclear data evaluations
3. Compare new experimental results with predictions based on new models
TSL for UO$_2$: phonon PDOS + coh. elastic

Phonons in actinides: active area of research, Judy Pang et al., Phonon density of states and anharmonicity of UO$_2$, PHYSICAL REVIEW B 89, 115132 (2014)

In reactor physics, for safety and licensing application: fuel temperature coefficient of reactivity (FTC); $T$ can go $\sim$ 2000 K
MCNP Results: Criticality Calculations, $k_{inf}$ vs. $T_f$

PHWR typical fuel bundle with UO$_2$ fuel near the middle of burn-up
D. Altiparmakov and D.R.
CNL Collaborations in Nuclear Data R&D

• Member of **CSEWG, USA**
  CSEWG = Cross Section Evaluation Working Group
  (responsible for the U.S. Evaluated ND Files ENDF/B, latest = ENDF/B-**VII.1**, 2011)

• Participation in **WPEC** sub-group activity under **OECD/NEA (EU)**
  WPEC = Working Party on International Nuclear Data Evaluation Co-operation,
  https://www.oecd-nea.org/science/wpec/
  e.g., sub-group 40:
  **The CIELO Collaboration: Neutron Reactions on** ¹H, ¹⁶O, ⁵⁶Fe, ²³⁵,²³⁸U, and ²³⁹Pu,
  https://www.oecd-nea.org/science/wpec/sg40-cielo/

• Continue our collaboration with scientists from Neutron Physics Department,
  **Centro Atómico Bariloche (CAB), Argentina**: New TSL evaluations for D₂O, H₂O
  and testing them using International Benchmarks (Crit. Saf. and Reactor Phys.)

• **INERI USA-Canada R&D Collaboration, 2015 - ... :**
  **new collaborations** with US scientists (ORNL, LANL, ..., academia): ?
TSL ( $S(\alpha,\beta; T)$ ) of water in a nutshell: from MD to RP

\[ \rho_{\text{MD}}(E) \text{ and } \rho_{\text{RP}}(E) \text{ for D-in-D}_2\text{O, } T = 300 \text{ K} \]

\[ 0.5 \times \rho_{\text{MD}}(E) \text{ for O-in-D}_2\text{O, } T = 300 \text{ K} \]