ENDF/B-VIII.0

D. Brown for the
Cross Section Evaluation Working Group
ENDF/B-VIII.0 was released on 2 Feb. 2018 by the Cross Section Evaluation Working Group (CSEWG)

Integrates contributions for many sources

- Neutron Data Standards IAEA, NIST
- CIELO Pilot Project BNL led Fe, LANL led $^{16}$O and $^{239}$Pu, IAEA led $^{235,238}$U
- Many new and improved neutron evaluations (DP, Crit. Safety, NE, USNDP)
- New thermal scattering libraries (Crit. Safety, Naval Reactors)
- Charged particles USNDP (LLNL)
- New atomic data (LLNL)
- Success rests on EXFOR library IAEA project but USNDP (BNL) coordinates compilation of reaction data for Western Hemisphere

* ENDF/B-I was released in June 1968
ENDF/B-VIII.0 is our best performing and highest quality library yet

- Validate by simulating well characterized systems
  - Thousands of critical assembly benchmarks
  - 14 MeV & $^{252}$Cf(sf) source transmission
  - Many other tests
- Quality also assured by
  - ADVANCE continuous integration system at BNL
  - Annual Hackathons

FIG. 29. (Color online) The distribution of $C/E$, in units of the combined benchmark and statistical uncertainty. The normal distribution (in black) would be the perfect situation.
Library and evaluations detailed in Nuclear Data Sheets vol. 148 (2018)

- **ENDF/B-VIII.0**: D. Brown *et al.*, Nuclear Data Sheets 148, 1 (2018)
- **Neutron Data Standards**: A. Carlson *et al.*, Nuclear Data Sheets 148, 143 (2018)
- **$^{239}$Pu(n,g) measurement**: S. Mosby, *et al.*, Nuclear Data Sheets 148, 312 (2018)
Outline for remainder of talk

- We didn’t “change anyone’s answers”

- Big changes that “didn’t change anyone’s answers”: $^{235,238}U$, $^{239}Pu$, and $H_2O$

- Other important changes that “maybe changed answers”: $^{16}O$, natC, Fe, graphite

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UNCLASSIFIED
There are many ways to “get the right answer”

- E. Bauge, et al. (CEA-DAM)
- Swap portions of one evaluation for other until completely swapped
- Elastic & inelastic scattering provided biggest swing

<table>
<thead>
<tr>
<th>Quantity</th>
<th>$\Delta k_{\text{eff}}$ (1000’s of %)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fission</td>
<td>-138</td>
</tr>
<tr>
<td>Capture</td>
<td>+269</td>
</tr>
<tr>
<td>Elastic Scattering</td>
<td>-638</td>
</tr>
<tr>
<td>Inelastic Scattering</td>
<td>+522</td>
</tr>
</tbody>
</table>

How does $k_{\text{eff}}$ change when a BRC09 value is replaced by one from ENDF-VII.1?

The end result is a lack of confidence in modeling systems that significantly differ from the integral benchmark.

Figure from L. Bernstein
Situation “unchanged” in VIII.0

Pu-239 CEA-CIELO to LANL-CIELO

FIG. 28. (Color online) Simulations of criticality k-eff for 239Pu for two critical assemblies: a fast assembly (Jezebel, PMF-1), and a thermal assembly (PST-4). This figure shows that both LANL CIELO-1 (ENDF/B-VIII.0) and CEA CIELO-2 (JEFF-3.3) predict similar k-eff values, but do so for very different reasons. The changes in criticality are evident when individual cross section channels are substituted between the two evaluations.

M. Chadwick et al., Nuclear Data Sheets 148, 189 (2018)
Variation in C/E Values is Much Less Than Predicted by ENDF/B Covariances

- C/E
- SCALE 6.2 Covariance Library
- ENDF/B-VIII Beta 5 Covariance Library
- ENDF/B-VIII Beta 5 Covariance with SCALE 6.2
Variation in C/E Values is Much Less Than Predicted by ENDF/B Covariances

So, we engineered the mean values, but this is not reflected in the covariances.

M. Williams, CSEWG meeting, Nov 2017
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Large overlap in evaluations of Big 3

- Neutron Data Standards: $(n,f)$ cross section
- $P(\nu)$ for neutrons and gammas (Talou)
- Fission energy release (Lestone)
- PFNS & associated cov. (Neudecker)
- PFGS new, resolves long standing problem with fission gammas (Stetcu)
- Feedback from benchmarks
- Main differences: treatments of RR & Fast parts of evaluation
Each major ENDF release is built off the newest release of the Neutron Data Standards.

### TABLE XXXII. Neutron Data Standards.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Standards Energy Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^1$H(n,n)</td>
<td>1 keV to 20 MeV</td>
</tr>
<tr>
<td>$^3$He(n,p)</td>
<td>0.0253 eV to 50 keV</td>
</tr>
<tr>
<td>$^6$Li(n,t)</td>
<td>0.0253 eV to 1.0 MeV</td>
</tr>
<tr>
<td>$^{10}$B(n,$\alpha$)</td>
<td>0.0253 eV to 1 MeV</td>
</tr>
<tr>
<td>$^{10}$B(n,$\alpha$$\gamma$)</td>
<td>0.0253 eV to 1 MeV</td>
</tr>
<tr>
<td>C(n,n)</td>
<td>10 eV to 1.8 MeV</td>
</tr>
<tr>
<td>Au(n,$\gamma$)</td>
<td>0.0253 eV, 0.2 to 2.5 MeV, 30 keV MACS</td>
</tr>
<tr>
<td>$^{235}$U(n,f)</td>
<td>0.0253 eV, 7.8-11 eV, 0.15 MeV to 200 MeV</td>
</tr>
<tr>
<td>$^{238}$U(n,f)</td>
<td>2 MeV to 200 MeV</td>
</tr>
<tr>
<td>$^{252}$Cf(sf)</td>
<td>Prompt fission neutron spectra</td>
</tr>
</tbody>
</table>

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A. Carlson et al., Nuclear Data Sheets 148, 143 (2018)
**235U: Other cross sections adjusted to match fission**

![Graph 1: 235U(n,f)](image1)

![Graph 2: 235U(n,n')](image2)

![Graph 3: 235U(n,γ)](image3)

![Graph 4: 235U(n,2n)](image4)

(b) Fast neutron range above 100 keV.

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A. Carlson et al., Nuclear Data Sheets 148, 143 (2018)

Scattering data carefully re-evaluated for $^{238}$U

**FIG. 17.** (Color online) Neutron-induced reaction cross sections on $^{238}$U (top) and effect of the Engelbrecht-Weidenmüller transformation [179] on elastic and inelastic scattering on the first two excited levels of $^{238}$U (bottom). Experimental data in the top panel have been taken from EXFOR [91].

- Dispersive OMP tuned to major actinides
- Proper treatment of (in)elastic mixing though E-W transform
- Proper compound angular distributions
- ($n,n'_g$) data WAS NOT used

**FIG. 18.** (Color online) Calculated total and partial inelastic $^{238}$U(n,n') cross sections on 45 keV level compared with experimental and evaluated data files. Experimental data have been taken from EXFOR [91].

R. Capote et al., Nuclear Data Sheets 148, 254 (2018)
$^{239}$Pu received relatively smaller updates

- Resonances from WPEC SG-34, up to 2.5 keV
- Fast region not full evaluation
  - Capture fitted to new DANCE data (Mosby, et al.) & theory advances from Kawano
- Fission: new standards
- PFNS: evaluation based on Chi-Nu data
- Updated covariances

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**$^{239}$Pu $(n,\gamma)$ Cross Section (b)**

- Incident Neutron Energy (MeV)

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**$^{239}$Pu $(n,\gamma)$ Cross Section (b)**

- Incident Neutron Energy (MeV)
Light water used in LWR, PWR, many solution assemblies
Light water re-evaluated by Centro Atomico Bariloche (Argentina)

- CAB Light water model
- Molecular diffusion using a modified Egelstaff-Schofield diffusion model.
- A continuous spectrum derived from molecular dynamics simulations
- Alpha and beta grids were refined

**FIG. 125**. (Color online) Evaluated $^1$H$_2$O(n, total) total cross section at 293.6 K, compared with data retrieved from EXFOR and published by Zaitsev et al. [338].

**FIG. 126**. (Color online) Evaluated $^1$H$_2$O(n, total) total cross section at different temperatures, compared with data measured by Stepanov et al. [339, 340] at 0.2266 meV.
Rolls-Royce conducted a series of critical experiments at the Neptune facility to validate the ability to predict criticality for water-isolated arrays as a function of temperature [see Ref.].

Configurations were neutronically similar to spent fuel storage racks without poison inserts in flux trap.

Test was specifically designed to assess criticality safety issues for spent fuel rack configurations with water gaps.

In this configuration, undermoderated fuel assemblies can have a positive temperature coefficient of reactivity.

Water temperature varied from 20-60 °C.

MC21 Calculated $k_{\text{eff}}$ for Neptune Configuration C as a Function of Temperature Using ENDF/B-VII.1 Non-Moderator Libraries and Various H-H$_2$O TSL Libraries

The $k_{\text{eff}}$ temperature bias (over the 33°C range) is reduced from +70 pcm w/ ENDF-VIII.0(β4) H-H$_2$O to +20 pcm w/ -β5 H-H$_2$O. There is no statistically significant $k_{\text{eff}}$ temperature bias with ENDF-VII.1 H-H$_2$O.

Error bars represent the 95% confidence interval, or $2\sigma = 10$ pcm in each direction.
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* ENDF/B-I was released in June 1968
New $^{56}\text{Fe}$ evaluation really aimed at improving steel

- $^{56}\text{Fe}$ (CIELO)
- $^{54,57,58}\text{Fe}$
- $^{59}\text{Co}$
- $^{58-62,64}\text{Ni}$
- $^{12,13}\text{C}$ (Neutron Data Standards)

Steel PWR pressure vessel (wikimedia commons)
Resonances in $^{56}$Fe go back to Froehner

- Minor correction to the previous evaluations
- Fluctuations extend high in energy
Elastic & inelastic for $^{56}$Fe

Fluctuations imposed on inelastic scattering to the first and second excited states taken from experimental data.

Elastic obtained by subtracting the sum of all reactions from the total.

Cross Section (b) vs. Incident Neutron Energy (MeV) for $^{56}$Fe(n,inel) and $^{56}$Fe(n,elas).
Validation in critical assemblies

CIELO Iron Validation

$\Delta k_{\text{eff}}$ (pcm)

- ENDF/B-VII.1
- ENDF/B-VIII.0
- ENDF/B-VIII.0 + VII.1 $^{54,56,57,58}$Fe

Fast
Therm
Fast

M. Herman et al., CIELO meeting, IAEA, Vienna - Dec 16-22, 2017
Compared to ENDF/B-VII.1 irons, the new iron evaluations when coupled to the ENDF/B-VIII.0 library:

- improve performance of 12 benchmarks
- maintain the performance for 8.
- worsen the agreement for 4 benchmarks

Δ$_{k_{eff}}$ (pcm)
TREAT reactor@INL restarted Nov 14, 2017: need graphite

- Graphite moderated
- Materials testing
- Shut down in 1994
- After Fukushima, interest in restarting

TREAT Reactor (wikimedia commons)
**Graphite**

**Ideal “crystalline” graphite** consists of planes (sheets) of carbon atoms arranged in a hexagonal lattice. Covalent bonding exits between intraplanar atoms, while the interplanar bonding is of the weak Van der Waals type. The planes are stacked in an “abab” sequence.

- Hexagonal Structure
- 4 atoms per unit cell
- \(a = b = 2.46 \, \text{Å}\)
- \(c = 6.7 \, \text{Å}\)
- Density = 2.25 g/cm\(^3\)

**Reactor graphite** consists of ideal graphite crystallites (randomly oriented) in a carbon binder. It is highly porous structure with porosity level ranging between 10% and 30%.

**Nuclear Graphite (SEM at NCSU)**
Density = 1.5 – 1.8 g/cm\(^3\)
3.1.2.5 Fuel Pebbles

The graphite fuel pebbles have a diameter of 6.00 cm. A total of 9394 TRISO particles are randomly distributed within the graphite matrix of the fueled zone (diameter of 4.700 cm) of each fuel pebble (Figure 3.1-8). The fuel pebbles are located in the core cavity; their positions in each core configuration are described in more detail in Section 3.1.2.11. Each TRISO particle consists of four layers surrounding a UO$_2$ kernel. The fuel kernel has a diameter of 0.0502 cm. A graphite buffer layer (thickness of 0.00915 cm) surrounds the fuel kernel. An inner pyrolytic carbon (IPyC) layer (thickness of 0.00399 cm), SiC layer (thickness of 0.00353 cm), and outer pyrolytic carbon (OPyC) layer (thickness of 0.00400 cm) then each, in succession, surround the growing TRISO particle, as shown in Figure 3.1-8.

Figure 3.1-8. Fuel Pebble and TRISO Particle.

Calculation curtesy of S. Van der Marck

Main message

- ENDF/B-VII.1 was very good
  - $k_{\text{eff}}=1$ is “baked in”, which surprisingly is a problem for many customers
  - $k_{\text{eff}}=1$ but with really big uncertainty does mean we biased the mean somehow, but were conservative with our uncertainty estimates

- ENDF/B-VII.1 was good, but ENDF/B-VIII.0 is much better

- There is still a lot of room for improvement

Happy 50 ± 1 Anniversary!

* CSEWG formed in 1966
  ENDF/B-I released in 1968