Validation of the Nuclear Data Evaluation Code CONRAD

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Plan

- Introduction
- Cross sections: Pu239(n,f), (n,n), Xe131(n,n)
- Observables: calculation vs. measurement
- Transmissions: Xe129, U238
- Capture Yields: U238, Au197, Mn55
- Conclusion, Outlook
CONRAD is a nuclear data evaluation code.

Adjustment of nuclear reaction parameters (RP, OMP, ...) for the calculation of cross sections and variance-covariance matrices from thermal range to several MeV.

Production of evaluated nuclear data files (JEFF).

Among others, use of differential and integral experiments for RLSF using marginalization (analytic or Monte Carlo) techniques.

In this short study, we will focus on the validation of theoretical cross sections and related observables (transmission, capture yield).
$^{239}\text{Pu}$ in RRR
- Fission cross section
- Reich Moore
- Doppler broadening @294K

$\Delta < 0.05\%$
$^{239}$Pu in RRR
- Elastic cross section
- Reich Moore
- Doppler broadening @294K

A bias is observed if the required accuracy in NJOY is set to 0.1%

No bias if the criteria is set to 0.01%

$\Delta < 0.05\%$
$^{131}$Xe in RRR
- Elastic cross section
- Multi Level Breit Wigner
- Doppler broadening @294K

$\sigma_{\text{CONRAD}} = \sigma_{\text{NJOY}}$

$\checkmark \sigma_{\text{CONRAD}}$

$\Delta < 0.05\%$
Transmissions + Capture yields: calculation

- Observables (transmission, capture yields) are functions of cross sections

Transmission: \[ T(E) = e^{-n\Sigma_t(E)} = e^{-\Sigma_t(E)L} \]

Capture yield: \[ Y(E) = Y_0(E) + Y_1(E) + Y_n(E) \]

Primary capture yield: \[ Y_0(E) = \left(1 - e^{-n\Sigma_t(E)}\right)\frac{\sigma_\gamma(E)}{\sigma_t(E)} \]

Single scattering correction: \[ Y_1^\infty(E) = \int_{-1}^{0} d\mu \left[ \frac{1 - e^{-\Sigma_t(E)L}}{\Sigma_t(E)} - \frac{1 - e^{-(\Sigma_t(E)L - \Sigma_t(E')L/\mu)}}{\Sigma_t(E) - \Sigma_t(E')/\mu} \right] \frac{\Sigma_c(E')\Sigma_s(E)p(\mu_c)}{\Sigma_t(E')} \frac{d\mu_c}{d\mu} \]

Single scattering correction (for infinite sample): \[ + \int_{0}^{1} d\mu \left[ \frac{1 - e^{-\Sigma_t(E)L}}{\Sigma_t(E)} \frac{e^{-(\Sigma_t(E')L/\mu)} + e^{-(\Sigma_t(E)L)}}{\Sigma_t(E) - \Sigma_t(E')/\mu} \right] \frac{\Sigma_c(E')\Sigma_s(E)p(\mu_c)}{\Sigma_t(E')} \frac{d\mu_c}{d\mu} \]

Single scattering correction (from SAMMY manual): \[ Y_1(E) = \frac{\int dxdy}{S} N \int dz \exp(-N\sigma_t(E)z) \int d\Omega \frac{d\sigma}{d\Omega} \sigma_c(E')N \int dq \exp(-N\sigma_t(E')q) \]

Not trivial; requires approximations (uniform + isotropic distribution of neutrons after 2 or more scatterings.)
Time of Flight technique \( (e^- \rightarrow \gamma \rightarrow {}^1_0n) \)

We would like to record neutrons as a function of energy but we measure gammas as a function of time.
In this kind of experiment (tof), we know “when” (time of flight) but not “where” (collision site) then the time spectrum is transformed in an energy spectrum using a fixed distance (the flight path F.P.).

The experimental resolution function (detector, moderator,…) is used in the calculations to reproduce the experimental results.

If we leave aside the experimental resolution (which can be neglected for various configurations), we must be able to calculate as precisely as possible the response (T(E), Y(E), …).
Monte Carlo simulation
Neutron transport in the sample (Implicit capture + Russian roulette)

\[ E = E(\tau, \delta) = E(\tau + t_0, \delta + d_0) \]

Simulation can be performed in several ways:
1. in time (Tof Varying with actual distance in the sample → actual energy \( E' \))
2. in time (Tof Varying with constant fixed distance, e.g. the flight path \( \delta \))
3. in time (Tof fixed with constant fixed distance, e.g. the flight path \( \delta \))
4. in energy (tally at energy just before capture \( E' \))
5. in energy (tally at incident energy \( E \))

1. ≡ 4. : identical to simulation in energy with MC transport codes (Tripoli4, Mcnp5, …)
2. ≈ Experimental result
3. = 5. = Analytical (p.7)

2. and 3. are difficult to distinguish (experimentally) → effect observed for unusually thick targets!!
$^{129}$Xe transmission

$\tau_{\text{CONRAD}} = \tau_{\text{REFIT}}$

![Graph showing transmission as a function of energy (eV) with data points and fitted curves labeled REFIT, CONRAD, and data (IRMM).]
$^{238}\text{U}$ @36.6 eV
- Primary capture yield
- $T = 294$ K

$n \approx 1.595 \times 10^{-3}$ at/b
$e = 0.5$ cm

$E = 36.68$ eV
$\Gamma_n = 34.1$ meV
$\Gamma_\gamma = 23.0$ meV
$^{238}\text{U} \text{ primary capture yield (ANalytical / MC schemes)}$

$^{238}\text{U} @36.6\text{eV}$
- Primary capture yield
- $T = 294\ \text{K}$

$Y_0^{\text{AN.}} = Y_0^{\text{MC}}$

$\checkmark \ Y_0^{\text{CONRAD,MC.}}$
$^{238}\text{U} @ 36.6\text{eV}$
- Primary capture yield
- $T = 294\ \text{K}$

$Y_{0\text{AN.}} = Y_{0\text{MC}}$
$^{238}$U @36.6eV @294K
- Single scattering correction $Y_1$

$Y = Y_0 + Y_1 + Y_n$

"infinite sample approximation for single scattering correction $R_S \gg R_B$"

$Y_{1,\infty}^{AN.} = Y_1^{MC}$
$^{238}\text{U} \text{ @36.6eV @294K}$
- Single scattering correction $Y_1$

$$Y_1 = Y_1^f + Y_1^b$$

backward and forward contributions
\( E'(E = 37.4, \mu = +1) = 37.4 \text{ eV} \)
\( \rightarrow \sigma_i \approx 120 \text{ } b \) : 'low' proba. of interaction
\( \rightarrow \) capture after forward scattering \( \downarrow \)
\( E'(E = 37.4, \mu = -1) = 36.8 \text{ eV} \)
\( \rightarrow \sigma_i \approx 6800 \text{ } b \) : 'high' proba. of interaction
\( \rightarrow \) capture after backward scattering \( \uparrow \)

\( E'(E = 36.8, \mu = +1) = 36.8 \text{ eV} \)
\( \rightarrow \sigma_i \approx 6800 \text{ } b \) : 'high' proba. of interaction
\( \rightarrow \) capture after forward scattering \( \uparrow \)
\( E'(E = 36.8, \mu = -1) = 36.2 \text{ eV} \)
\( \rightarrow \sigma_i \approx 120 \text{ } b \) : 'low' proba. of interaction
\( \rightarrow \) capture after backward scattering \( \downarrow \)
$^{197}$Au multiple scattering corrections (infinite sample) (Sammy ANalytical / Conrad ANalytical / MC schemes)

$^{197}$Au @4.9 eV
- Capture yields
- $T = 294$ K

“not so usual sample”
$n \approx 2.9 \times 10^{-3}$ at/b
$e = 5. \text{ cm}$ !!
$R_s = 40. \text{ cm}$ …

… to check $Y_{1,\infty}$ against SAMMY

Compared with SAMMY:
- $Y_0$ CONRAD, AN
- $Y_{1,\infty}$ CONRAD, AN
- $Y_{\text{tot}}$ CONRAD, MC.

$E = 4.9$ eV
$\Gamma_n = 15.2$ meV
$\Gamma_\gamma = 122.5$ meV

Analytical $Y_n$ is a crude approximation here
\begin{itemize}
\item $^{55}\text{Mn} \@ 337.3 \text{ eV}$
\item Capture yields
\item $T = 294 \text{ K}$
\end{itemize}

Compared with SAMSMC:
\begin{itemize}
\item $Y_0^{\text{CONRAD,MC.}}$
\item $Y_1^{\text{CONRAD,MC.}}$
\item $Y_n^{\text{CONRAD,MC.}}$
\item $Y_{tot}^{\text{CONRAD,MC.}}$
\end{itemize}

\begin{itemize}
\item $E = 337.3 \text{ eV}$
\item $\Gamma_n = 22. \text{ eV}$
\item $\Gamma_\gamma = 310 \text{ meV}$
\end{itemize}
✓ not so bad compared with experiment without any resolution function.

(analyt. solution fails \( Y_n \), zero K Scatt. Ker., ...), See WG36, WPEC May 2011, P. Schillebeeckx)
Conclusion

CONRAD code is validated for the calculation of doppler broadened

- **cross sections** (RM, MLBW) in the RRR but also at higher energy (not discussed here).
- **transmissions**
- **capture yields** : $Y_0$, $Y_1^\infty$ (analytical), $Y_0$, $Y_1$, $Y_n$, $Y_{tot}$ (Monte Carlo)

through NJOY, REFIT, SAMMY, SAMSNC codes.

Outlook

Additional comparisons have to be performed, especially:
- test the SVT and DBRC target velocity sampling methods (in preparation),
- find a target candidate as thick as possible to disentangle the different MC simulations/analytical calculations compared with experiment.
Thank you for your attention