Modelling with EMPIRE
nuclear reaction code and
nuclear data evaluation
OUTLOOK

☑ Background: ND for energy applications
☑ New U-238 evaluation
  ➢ Nuclear reaction modelling in EMPIRE
  ➢ Differential data
  ➢ Integral and quasi-differential data
☑ Nuclear data validation using SPA cross sections and dosimetry libraries
☑ Challenges
Do we need another $^{238}$U evaluation?

**OECD/NEA WPEC Subgroup 26 Final Report:**

“Uncertainty and Target Accuracy Assessment for Innovative Systems Using Recent Covariance Data Evaluations”,

M. Salvatores (coordinator), R. Jacqmin (monitor),


The request for improved cross sections and emission spectra and their accuracies for neutron induced reactions on $^{238}$U is an important issue that emerges in several of cases studied. High accuracy requirements were placed on inelastic cross-sections $^{238}$U(n,inl) in the whole energy range up to 20 MeV …

A. Santamarina, ND-2013, target uncertainty 5% (current ~ 15%)
Evaluated $^{235}\text{U}(n,f)$ vs. STD cross section

$^{235}\text{U}(n,f)\text{ SPA}(^{252}\text{Cf}) = 1224 \pm 5\, (0.4\%)$

IAEA STD $^{235}\text{U}(n,f)$
DOES EVAL.FISSION AGREES with STDs?

\[ ^{238}\text{U}(n,f) \text{ SPA in } ^{252}\text{Cf} = 318.5 (0.6\%) \]

\[ 
\begin{align*}
\text{Ratio to ENDF/B-UII.1: } & \quad \text{U-238}(n,f) \\
\text{ENDF/B-UIII.1: } & \quad \text{U-238}(n,f) \\
\text{JEFF-3.1.2: } & \quad \text{U-238}(n,f) \\
\text{JENDL-4.0: } & \quad \text{U-238}(n,f) \\
\text{ROSFOFD-2010: } & \quad \text{U-238}(n,f) \\
\text{CENDL-3.1: } & \quad \text{U-238}(n,f) 
\end{align*}
\]
7. For the low energy range (<3 MeV) the compound decay introduces additional degrees of freedom (level densities, strength functions, fission, width fluctuations). For better understanding the compound nuclear reaction mechanism on actinides a simple system must be studied. Predictions for neutron induced reactions on $^{238}$U below 1 MeV should be compared.

$^{238}$U(n,f) and $^{238}$U(n,γ) – fitted in STD

$^{238}$U(n,γ) SPA in $^{252}$Cf: $67.5 \pm 0.7$ mb (1.0%)

$^{238}$U(n,f) SPA in $^{252}$Cf: $318.5 \pm 2.1$ mb (0.6%)

$^{238}$U is the ideal test nucleus for elastic/inelastic studies


First problem:
Elastic and inelastic cross sections
DISCREPANCIES in $^{238}\text{U}(n,\text{inl})$

![Graph showing discrepancies in $^{238}\text{U}(n,\text{inl})$.](image)

- **Discrete Lev.**
- **Continuum ~ 1.3 MeV**

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IAEA Nuclear Data Section
DISCREPANCIES in $^{238}$U(n,${\text{in}}_L$)

![Graph showing discrepancies in neutron capture cross-sections for $^{238}$U.

The graph illustrates the ratio of various nuclear reaction data sets to ENDF/B-VII.1 for $^{238}$U(n,${\text{in}}_L$) as a function of incident energy (MeV). The data sources include ENDF/B-VII.1, JEFF-3.1.2, JENDL-4.0, ROSFOND-2010, and CENDL-3.1. The figure highlights significant differences and discrepancies across the energy spectrum, particularly at lower and higher energies, indicating areas where further research and data refinement might be needed.]

Joint ICTP-IAEA Workshop on Nuclear Reaction Data for nuclear power applications, 22-26 Sept. 2014, Trieste

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+ recent relevant modelling advances

- **Dispersive Lane consistent coupled-channel OMPs**: neutron inelastic scattering to discrete levels;
- **DIR-CN interference effects (as predicted by Moldauer)**;
- neutron inelastic scattering treatment;
- **improved fission formalism (descriptive capability)**

*J.M. Quesada *et al.*, EPJ Web of Conferences 42 02005 (2013)
J.M. Quesada *et al.*, ND2013 conference
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DCCOMP: rigid rotor with soft-rotor corrections

$^{238}\text{U}$

Diagram showing energy levels and transitions for $^{238}\text{U}$.
nonelastic cross sections

\[ \sigma_R - \sigma^{2+} - \sigma^{4+} \]
Impact of octupolar band
Inelastic angular distributions $E_n=1.5$ MeV

- $3^-$ 732 keV
- $1^-$ 680 keV
- $4^+$ 148 keV
- $2^+$ 45 keV
total (and 1\textsuperscript{st} lev) inelastic cross sections

DCCOMP + mult. band coupling

CN-DIR Interf.
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**new physics: DIR-CN interference**

Engelbrecht-Weidenmuller transformation [1]

Cross sections [mb] vs. energy [MeV]

- dir-CN interference
- elastic
- 1st level (44.9)
- 2nd level (148)
- no interference

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EMPIRE: Nuclear Reaction Model Code System for Data Evaluation

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IAEA Nuclear Data Section
elastic $\mu$-bar (P1 component)
Elastic angular distribution 720 keV

impact on reflectors
Neutron emission spectra (2-6 MeV)

- 6.02 MeV
- 4.25 MeV
- 2.03 MeV
EMPIRE: Nuclear Reaction Model Code System for Data Evaluation

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The origin of the nuclear energy is the difference of binding energy.

Hill-Wheeler formula for the Transmission coefficient through a parabolic barrier:

\[
T_i = \frac{1}{1 + \exp\left(\frac{2\pi}{\hbar \omega_i} (E_{fi} - E^*_i)\right)}
\]
FISSION BARRIERS

Shell correction dependence on Z,N and the dependence of the LD potential on the fissility parameter \((E_c/2E_s)\) make fission barrier specific to each nucleus;

- inner barriers almost constant 5-6 MeV for the main range of actinides; fall rapidly in Th region;

- secondary well’s depth around 2 MeV;

- outer barriers fall quite strongly from the lighter actinides (6-7 MeV for Th) to the heavier actinides (2-3 MeV for Fm).
\[ T_f = T_{dir} + T_{ind} = T_{dir} + T_{abs} \frac{T_B}{T_A + T_B} \]

\[ T_f = T_{dir} + T_{ind} = T_{dir} + T_{abs} \frac{T_{BC}}{T_A + T_{BC}} \]

\[ T_f = T_{dir} + T_{ind_1} + T_{ind_2} \]

**imaginary part:**

\[ W = -\alpha [E^* - V_f] \]

\[ T_{abs} = T_{dir} \frac{e^{2\delta} - (1-T_2)e^{-2\delta}}{T_2} - T_2 \]
Using integral data ($k_{\text{eff}}$) in the evaluation
ICSBEP Benchmark Summary Results
Integral parameter intercomparison

Delta k-eff (pcm)

Benchmark

NEA ICSBEP criticality benchmarks
Using quasi-differential data in the evaluation
RPI experimental setup

simple & easy to model geometry

Angle dependent cross sections: 29°

(n,el)  
(n,n') cont  
(n,f)  
(n,2n)
RPI benchmark: 29°
Angle dependent cross sections: $153^0$

- $(n,el)$
- $(n,n')$ cont
- $(n,f)$
- $(n,2n)$

Cross Section (barns) vs. Energy ($10^6$ eV)
RPI benchmark: 153°
OTHER CHALLENGES: PFNS

92-U-235(N,F),DE thermal neutrons

Ratio to Maxw. (T=1.32 MeV)

outgoing neutron energy (eV)

ENDF/B VII;U-235 thermal
2013 Vorobyev
2010 Korotkov
1989 Wang Yufeng
1985 Starostov
1985 Lajzai
1983 Nefedov1*
1983 Nefedov2*
1983 Starostov*
OTHER CHALLENGES: $^{235}\text{U}$ th. nubar

$v (^{252}\text{Cf}) = 3.782$

Frehaut & Shackleton p.201
 Reaction modelling of neutron scattering on $^{238}$U nucleus

- Dispersive CC OMP coupling all levels up to $E_n=1$ MeV
- Use of integral and quasi-differential benchmarks as part of the evaluation process

- EMPIRE advanced Hauser-Feshbach treatment includes:
  - Dispersive coupled-channel optical models
  - CN anisotropy
  - Direct effects on the CN emission
  - Multi-humped fission barrier with absorption

- Additional data challenges: PFNS and nubar