FISPACT-II & TENDL: developments to model high-energy activation, transmutation processes and radiation damage source terms

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<table>
<thead>
<tr>
<th>Position</th>
<th>Element</th>
<th>Atomic Number</th>
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<td>Argon</td>
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- **Periodic Table of the Elements**

- Elements are arranged in increasing order of atomic number.
- Periods represent rows, and groups represent columns.
- Each element includes its atomic number, symbol, and atomic weight.
Nuclear landscape: Isotopic targets

TENDL-2015 [2809 (544) target nuclides (isomers)]
ENDF/B-VII.1 [423 (10) target nuclides (isomers)]
255 stable nuclides
TENDL: from MF-1 to MF-40, 200 MeV

- **MF-1**: Description + fission parameters
- **MF-2**: Resonance parameters (Reich-Moore or Multi-level Breit Wigner)
- **MF-3**: Cross sections $n_{tot}$, $(n,\text{el})$, $(n,\text{non})$, $(n,\text{inl}_i)$, ..., $(n,\gamma)$, $(n,p_i)$, $(n,\alpha_i)$
- **MF-4**: Elastic angular distribution (Legendre Polynomials)
- **MF-5**: Fission neutron spectrum
- **MF-6**: Double differential distributions and spectra for $(n,2n)$, ..., $(n,\alpha_i)$
- **MF-8-10**: Isomeric cross sections
- **MF-12-15**: Gamma yields, angular distributions and spectra
- **MF-31-32-33-34-35, 40**: $\nu$bar, Resonance parameter, cross section, angular distribution and fission neutron spectrum, radionuclide production.
The making of TENDL: T6 infrastructures

- T6: at the origin of TENDL: combination of 6 codes plus utilities
- Allow to loops over nuclear science \(\Rightarrow\) variance-covariance
TENDL’s advantages

- All targets isotopes in the same evaluated data forms, $10^{-5}$ eV to 200 MeV, with variance-covariance (MF-31 to 40), isomers as target ($T_{1/2} > 1$ s) and daughters ($T_{1/2} > 0.1$ s)
- 8th version, “putting 69 nuclear physics codes to work”

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<tr>
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<th>Neutron</th>
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<th>Deuteron</th>
<th>Triton</th>
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<th>Photon</th>
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The TENDL infrastructure combines other methods:

- **(fast) TMC**: Total Monte Carlo for uncertainty propagation

- **BMC**: Bayesian Monte Carlo for model parameter updates and sampling

- **HFR**: Resonance parameters for all targets isotopes consistent with the fast neutron range: Level Densities, Optical Model Parameters, Gamma-ray Strength Function,…
Processing steps: three codes

- NJOY12-082
  - reconr
  - broadr
  - unresr
  - thermr
  - heatr
  - gaspr
    - purr
    - acer
    - groupr

- PREPRO-2015
  - linear
  - recent
  - sigma1
  - sixpack
  - activate
  - merger
  - dictin
  - groupie

- CALENDF-2010
  - calendf
  - regroup
  - lecritp
  - ....

ENDF file

Processed ENDF file

ACE file

PT file

Single script for an entire library

cross-check

Processed ENDF file

Single script for an entire library
TENDL-2015 pendf, 200 MeV

90 reaction types

\((n, \text{remainder}) = mf3 - mt5 \times mf6\) above 30 MeV
Gas production

NJOY generated Gas production MT’s displayed by PREPRO

appm of He 4 = 1.13E+03
appm of He 3 = 1.30E-02
appm of H 3 = 1.43E-18
appm of H 2 = 2.07E+01
appm of H 1 = 1.18E+03
NJOY generated KERMA and DPA MT's displayed by PREPRO

12
NJOY generated gas production MT’s displayed by PREPRO

Gas production

- appm of He 4 = 1.13E+03
- appm of He 3 = 1.30E-02
- appm of H 3 = 1.43E-18
- appm of H 2 = 2.07E+01
- appm of H 1 = 1.18E+03
TENDL-2015 pendf from mf3*mf6

Unique processing to PREPRO-2015 mf10-mt5, with isomers

Cross section channels above 30 MeV

$A < 4$ and $A > 4$ productions cross sections
TENDL-2015 proton \([\text{Al}^{27}]\)

Yields for \(\text{Al}^{27}(p,\text{tot})\)

- 30 MeV
- 50 MeV
- 75 MeV
- 100 MeV

\(Z\) (number of protons)

\(N\) (number of neutrons)

Target \(\text{Al}^{27}\)

- \(10^{-6}\)
- \(10^{-5}\)
- \(10^{-4}\)
- \(10^{-3}\)
- \(10^{-2}\)
- \(10^{-1}\)
- \(10^0\)
- \(10^1\)
- \(10^2\)
- \(10^3\)
- \(10^4\)
- \(10^5\)
- \(10^6\)

50 MeV nuclide yields for \(\text{Al}^{27}(p,\text{tot})\)

100 MeV nuclide yields for \(\text{Al}^{27}(p,\text{tot})\)
TENDL-2015 proton [Sn120]

Yields for Sn120(p,tot)

30 MeV nuclide yields for Sn120(p,tot)

Z (number of protons) vs. N (number of neutrons)
In $^{56}$Fe: at low incident energy only elastic channels is important

Number of contributing channels increases dramatically at higher energies (MeV range)

TENDL results
• A more complex example with two recoiling species: $^{27}\text{Al}(n,\alpha)^{24}\text{Na}$
• A separate set of recoil vectors (blue) for the recoiling $^4\text{He}$
• @ higher energy than heavy $^{24}\text{Na}$ recoil (mass partition)
Q positive (7.3 MeV) means that the alpha energy can be much higher than the energy of the incident neutron.
Actinide decays and consequent (α,Xn) reactions for reactor fuel materials UO₂, UC, UF₆, PuO₂ and PuF₄

Only two libraries for Alpha induced!
17 targets in JENDL

TENDL-2015 is also been used in fuel denaturing studies
TENDL-2015 p-incident up to GeV
Random walk uncertainty

Decay power: FNS JAERI

FNS-00 5 Min. Irradiation - Ni

Heat Output [µW/g]

Time after irradiation [minutes]

Product Pathways $T_{1/2}$ Path % E/C
Co62 Ni62(n,p)Co62 1.5m 99.8 0.90
Co62m Ni62(n,p)Co62m 13.9m 100.0 0.89

missing path, but also metastable longer lived
When you do not account for isomer production channels….

The responses are missed entirely!!

Hunt for the isomers

Most are lost in seconds, minutes…
Capture reactions

- Neutron capture and other reactions are exothermic, allowing the reaction at any incident energy.
- These reactions possess resonance structure which often determines reaction rate (aside from thermal spectra systems).
- Either the resonances have been measured, we statistically resolve them or (in non-TENDL) we get unphysical straight lines…
Astrophysics reaction rates

0 Kelvin and kT=30 keV broadened cross-sections

ENDF/B-VII.1 and JENDL-4.0 seriously overestimate whatever the temperature

Temperature-dependent averaged cross-sections:
Astrophysical 5-80 keV

FISPACT-II forms: 1102 groups
The KADoNiS database includes some 357 nuclides over 11 Maxwellian-averaged temperatures for RR comparison.

Broadened cross-sections

Temperature-dependent averaged cross-sections
• Provide the user with the most sophisticated incident-particle nuclear data from the TENDL-2015, ENDF/B.VII.1, JENDL-4.0, CENDL-3.1 and JEFF-3.2 international libraries, which are complemented with the latest decay and fission yield data, including the most recent GEFY-5.2 libraries.

• Code features include self-shielding factors, broad temperature dependence, thin/thick target yields, robust pathway analysis, Monte-Carlo sensitivity and uncertainty quantification and propagation using full covariance data.

New features
• Allows the user to specify any output gamma group structure for decay sources
• Now with the ability to use arbitrary (ebins) incident group structure
• FISPACT-II to output the uncertainty from all depletion processes for a set of specified nuclides
• Creates data outputs and plot scripts with break-downs for all individual dominant nuclides (as opposed to integral quantities)

http://fispact.ukaea.uk/
TENDL-2015 includes about 2809 isotopes, why not going beyond?
- Understanding that nuclear data are pdf and not only $\sigma \pm \Delta \sigma$,
- Develop T6 to include other evaluation tools?
- 8000 isotopes (astrophysics)
- 1 GeV?

Example of what happens when model goes to the neutron drip line (Hauser Feshbach is not applicable anymore)
• Completeness, predictability, simultaneity
  – 6 incident particles, number of targets, isomers (targets and daughters), energy range (10^{-5} eV to 200 MeV) total and partials cross section, with variance-covariance, double differential data, all emitted spectra (particles and recoils)

• Reliability, regularity, robustness
  – For all applications (not a particular one) extensive V&V: fission, fusion, astrophysics, medical, high energy, earth explorations, safeguard, safety, security, …

• The only nuclear data library able to go outside the proverbial validations domains (differential and integral), scout the nuclear landscapes, fulfil the (often difficult to specified) data needs