Processing, validating and verifying modern activation-transmutation files

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Background; literature

• Unresolved Resonance Range cross section probability and self shielding factors, CEA-R-6227, 2009.

• ENDF Cross Sections are not Uniquely Defined, LLNL-TR-446331, June 2010.

• A Short History of ENDF/B Unresolved Resonance Parameters, LLNL-TR-461199, October 2010.

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• ENDF-6 Formats Manual, BNL-90365, June 2009
  – Format enhancements, new MT’s, …
Background; codes and Libraries

• Latest processing codes
  – NJOY99.364, 364 updates since April 2000
  – PREPRO-2010 new code and modules
  – CALENDF-2010 new code and modules
  – SAFEPAQ-II enhancements

  ➢ Bug correction, compliances, better physics. Not without impact on the processed data (libraries created with earlier version are less reliable)

• New Libraries
  – TENDL-2010, JENDL-4, ENDF/B-VII.1

  ➢ more consistency, checks, “new” better format
Background; processes

- The ENDF-6 format evolves: LRF-7, MT’s, radii,.. as the Utility codes to check it.
- The nuclear data files content evolves through bug correction but also better physics, model parameters, robust format frame, etc..
- The V&V, Verification and Validation processes are in place and working, finding many errors, bug, non compliance, non iniquity.
- Our computer power and graphics allows us to see more better and deeper.
- People now have the power to cross check, comparison are made… and results shared!!
And all this do not only apply to the cross sections excitation function but also to the:

- Resonance and model parameters
- Q values, isomeric branching ratio
- Emitted particles angular distribution
- Emitted particles spectra
- Raw ENDF file and/or processed ones

And this can be done

- On your own computer or on the web
- By your software tools or somebody else ones but interpretation differences persist
20 years or so ago

Once upon a time in the 90’s a modified local version of NJOY-94 was used on a ECN Petten computer to generate groupwise constant from tape 1 to 9 of the newly released (1993) JEF-2.2 library. The binary groupr output was send on tape by post to CEA Saclay. The tape could then be accessed by CEA Cadarache personnel to hopefully, finally produce and assemble an ERANOS library. The same binary file (byte to byte) is still in use by this NEA accessible code system. This same library also form the basis of the adjusted ERRALIB library. The all process took years....
CCFE’s processing tools (June 2011)

• SAFEPAQ-II (+)
  – An original CCFE software to assemble, process, verify and validate the EAF’s libraries

• NJOY99.364 (+)
  – A LANL nuclear data processing system

• PREPRO-2010 (+)
  – A IAEA/LLNL pre-processing system

• CALENDNF-2010
  – A probability table based processing system

➢ Every system has unique and useful capabilities

(+) mean with added, non (yet) official patch
### ENDF-6 format frame

<table>
<thead>
<tr>
<th>MF</th>
<th>Description for energy below 60 MeV</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>General information, comments</td>
</tr>
<tr>
<td>2</td>
<td>Resonance parameter, scattering radius</td>
</tr>
<tr>
<td>3</td>
<td>Total reaction channels</td>
</tr>
<tr>
<td>8</td>
<td>Flag, file pointer, dictionary</td>
</tr>
<tr>
<td>9</td>
<td>Isomeric branching ratio, for non threshold reaction</td>
</tr>
<tr>
<td>10</td>
<td>Split threshold reaction channels</td>
</tr>
<tr>
<td>32</td>
<td>Covariance of neutron resonance parameters</td>
</tr>
<tr>
<td>33</td>
<td>Covariance of neutron cross sections</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>MF</th>
<th>Description for energy above 60 MeV</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>Activation yields for MT-5</td>
</tr>
<tr>
<td>40</td>
<td>Covariance for radionuclides production yields</td>
</tr>
</tbody>
</table>
### 87 simple particles reactions

<table>
<thead>
<tr>
<th>MT</th>
<th>Particles</th>
<th>MT</th>
<th>Particles</th>
<th>MT</th>
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<td>182</td>
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<td>n’</td>
<td>102</td>
<td>g</td>
<td>160</td>
<td>7n</td>
<td>183</td>
<td>n’pd</td>
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<td>anything</td>
<td>103</td>
<td>p</td>
<td>161</td>
<td>8n</td>
<td>184</td>
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<td>158</td>
<td>n’dα</td>
<td>181</td>
<td>3nρα</td>
<td></td>
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</tr>
</tbody>
</table>

Only 6 of the new channels **do not** output a neutron

**Actual MT black (39)**

**New MT green (48)**

Approved during the Nov. 2010 CSWEG meeting

ENDF-6 Format Manual - July 2011 Revision
Processing steps: as one shell script

1. Format checks
2. MF-2 reconstruction, unionization and linearization
3. Doppler broadening
4. Nuclear heating and damage
5. URR processing
6. Gas production
7. Activation and yields processing
8. Multigroup constants
9. Graphical checks

Feeding into: TRIPOLI, MCNP, TART, ...
FISPACT-II, ACAB, ...
Processing sequences

1. Format checks: moder, dictin, fixup, calendf, crectj6
2. MF-2 parameters: recent, linear, reconr
3. Doppler: sigma1, broadr
4. Heating, damage: heatr
5. RR & URR: calendf, groupie, purr
6. Gas production: gaspr
7. Activation: activate, groupr
8. Multigroup: groupie, groupr
9. Graph checks: evalplot, plotr, viewr, complot and ZVView

All this is done respecting the ENDF-6 format
Processed files

- The end results are fully compliant ENDF-6 formatted processed files.
- All processing steps, sequences can be easily re-launched to account for any changes, modification, updates.
- Many intermediary steps, output listing or pre-processed files, add to the robustness of such system.

➢ The basic nuclear data and the processing steps are transferred to technology in a consistent and QA manner.
EAF-2010 in ENDF-6 format with PREPRO, ZView, EXFOR

60 MeV
SAFEPAQ-II at CCFE

Cr-52(n,2n)Cr-51

EAF-2010 in EAF format with SAFEPAQ-II

60 MeV

SAFEPAQ-II integral Validation
PREPRO-2010 & CALENDF-2010

MAT 9443

Total Cross Section

-27.40 To 62.88 %

Incident Energy (eV)

EAF-2010 in ENDF-6 format with complot
PREPRO-2010 (+) at CCFE

EAF-2010 in ENDF-6 format with evalplot

60 MeV
PREPRO & NJOY

MAT 7443
Total Cross Section 74-W-186

-99.66 To 8639. %

Min Ratio
Max Ratio

Cross Section (barns)

TENDL-2011 Prepro
ENDF/B-VII Njoy

Ratio

ENDF/B-VII Njoy/TENDL-2011 Prepro

200 MeV

ENDF-6 formatted files with complot
Principal cross sections

Cross section (barns)

Energy (MeV)

total
absorption
elastic
gamma production

ENDF-6 formatted file with NJOY plotr, viewr
PREPRO-2010 (+)

TENDL-2011 689 groups file with PREPRO

MAT 4025
Major Neutron
294 Kelvin Cross Sections
40-2r-90

Cross Section (barns)

Total
Elastic
Inelastic
(n,remainder)
(n,γ)

200 MeV
Conclusions

- All aspects to process, verify and validate modern transport activation-transmutation file have been outlined. It includes file format, numerical and physical contents, each processing sequences, intermediary steps, all processing codes used, leading to a processed file in ENDF-6 format.
- Every individual steps have already been achieved.

The Autumn 2011 will see the birth of new generation of nuclear data files feeding in new generation of activation-transmutation codes.