Chapter 5: Applications
Fission simulations
• FISPACT-II is distributed with a variety of fission yields and decay data, just as incident particle cross sections, etc.

• Fission is **by default turned off** and must be included with the following keywords:
  - USFISSION – turns on fission
  - FISYIELD – selects the fission yield files to read
  - FISCHOOSE – turns on fission for the given nuclides

• The default fission yields are read from mt=454, the independent fission yields. To use the cumulative mt=459 add the **keyword**: CUMFYLD
Fission within FISPACT-II

- Fission (*fy_endf* and *sf_endf*) are handled within the ARRAYX processing process with decay.

- Note that (n,f) reactions will populate without the full ARRAYX data, but not produce the yields.
The standard modern fission yields are all distributed with FISPACT-II, including ENDF/B, JEFF, JENDL.

- These have at most three incident energies: thermal (0.0253 eV), fast (~400-500 keV) and 14 MeV.
- Fission yields are very sensitive to incident energy, particularly at higher energies – also note multi-chance.
- For thermal reactors, this may be fine, but not for many others.

Simulation of fission yields has become much more sophisticated in past 10 years, particularly with codes such as GEF and FREYA.
The GEF code has been developed (and much of the physics within it!) by several physicists.

We cite those below (and their collaborators), from which we take the following material.

It is a fast, freely available code with surprisingly complex capabilities.

Karl-Heinz Schmidt,
Beatriz Jurado,
Christelle Schmitt

Nucl. Data Sheets 131 (2016) 107
There is also considerable added theory in the model! And the semi-empirical parameters are fit to experimental data

• The JEFF-3.1.1 thermal Pu239 is shown below, there is also a 400 keV file but nothing more.
The GEFY-5.2 Pu239 file

Pu-239 2.53E-02 eV

UK Atomic Energy Authority

Stable nuclides

Mass distribution

10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}

GEFY-5.2 Pu239 nFY at 2.53E-02 eV

N (number of neutrons)

Z (number of protons)
In many cases outside this ‘application range’, GEF remains at least one of the best simulation codes.
• Extensive chi-squared analysis against mass yields and evaluated files have demonstrated power of the system.
Advanced GEF applications

- GEF possesses many advanced features, such as A-dependent nu-bar, TKEs, covariances etc. Not currently employed since no standardised format – watch this space!

FISPACT-II with fission yields

- FISPACT-II condenses the fission yields as a function of energy with the incident particle spectrum, producing effective yields which account for full multi-chance (when using GEF).

- A full decay library is required and FISPACT-II will issue warnings for missing decays.

- **BEWARE:** missing data is a common issue for legacy libraries – employing independent yields without checking the decays will leave nuclides ‘in the sink’.
FISPACT-II can employ normalisation through two methods:

- **FLUX** – given in standard incident particles per cm\(^2\) per second
- **POWER** – normalise flux to match a power output in W/cm\(^3\). The power per incident particle is given by the full collapse of KERMA based on user-supplied reactions (total, only fission, fission plus specific channels, etc)

Note that as the nuclide inventory changes, the energy release per kg of target will change (for example with depletion of U235)

- Correct for changes in nuclide inventory with repeated use of the **POWER** keyword
Example: In-Cycle Fission Reactor

- Examples of % reactor power after shut-down following:
  - Left – LWR fuel with frequency of power renormalisation ranging over 2/year to 1/day
  - Right – Variation over burn-up, showing effect on Pu239/240 isotopic inventory ratios
• In realistic simulations, renormalisation and spectral modification are necessary, so multiple **POWER** uses must be combined with new **GETXS**

• **GETDECAY** is typically not required since the decays and fissions are unaffected, unless the proportion of fissions as a function of energy are significantly changed
  - This would require massive spectral shift – not partial fuel burn

• In addition, re-self-shielding is typically required, particularly as fuel composition and/or poison inventories change
Time evolution of spectrum

Original spectrum in CASMO-586
Converted spectrum in UKAEA-586

Neutrons per unit lethargy vs. Energy (eV)

BWR MOX+Gd
Burn-up step 1
• FISPACT-II accommodates multiple collapses using multiple spectra with the FILES file

• xs_endf and prob_tab must be re-specified for each – potentially with updates if desired
• Self-shielding and collapses can be run in multiple ways, depending on user input, for example:

  ▪ Users may specify for each and run individual collapses – followed by one simulation which reads each

  ▪ Users with all spectra can include multiple collapses during a single simulation

    ▪ Directly coupled Boltzmann-Bateman can be done for each step with new inputs

• Power normalisation can be set constant to re-calculate flux given inventory and kerma values
Charged incident particles, high-energy and residuals
• FISPACT-II can handle the incident nuclear data for five particles, which are selected using the PROJECTILE keyword

- PROJECTILE 1 neutrons (default if not stated)
- PROJECTILE 2 deuterons
- PROJECTILE 3 protons
- PROJECTILE 4 alphas
- PROJECTILE 5 gammas

• For neutrons, the 709 group data are used (and 1102, 586 in development versions)

• For charged particles, the 162 group is used instead
  - Note that GETXS 1 162 must be used as well
• Above 30 MeV, reaction channel uniqueness breaks down as a functional description within ENDF6
  ▪ Too many reactions for < 200 mt values
  ▪ Many reactions give equivalent products
  ▪ Only total residual production tends to have experimental data

• At 30 MeV TENDL changes from specific-mt descriptions to mt=5 mf=10 yield data

• These include summation over all reaction channels and condense the data into yield x cross-section for production of each residual nuclide
F-56 deuteron irradiation

30 MeV

Yields for Fe056(d,tot)

Target Fe-56

N (number of neutrons)

Z (number of protons)

10^{-6}

10^{-5}

10^{-4}

10^{-3}

10^{-2}

10^{-1}

10^{0}
• TENDL contains additional knowledge of fission cross sections which are stored and read by FISPACT-II above 30 MeV

• These exist for neutron-induced reactions as well as proton, deuteron, alpha, gamma…

• The remaining data required for these are fission yields. While these are not supplied in the standard FISPACT-II distribution, approximate files can be generated by any suitable code (e.g., GEF)
  - FISPACT-II can read these (in ENDF6 format) within the same fy_endf directory irrespective of incident particle
Total Monte-Carlo
• FISPACT-II has a powerful pathway-based uncertainty method which allows UQP for target nuclides produced through reactions.

• Depletion uncertainty of fuels also can be determined from full covariance treatment with the code

• An alternative, powerful method for uncertainty quantification is the Total Monte-Carlo, based on semi-empirical model parameter variation in the nuclear data generation

• Multiple ‘random’ (not random, but based on random parameter sampling) files are used for simulation and observables are statistically collapsed
The key ingredient is a set of nuclear data files which reflect sampling of input parameters and nuclear data uncertainty.

These may include reaction data, fission yields, decays, etc.

For reactions, the TMC method has been extensively developed by the TENDL/TALYS/T6 project.

For fission yields, GEF has been used for UQP, particularly using semi-Bayesian methods.
TENDL Nuclear data methodology = T6

Applications code (eg FISPACT) → UQP
• The fission yields are sensitive to various input parameters which have some uncertainty – this is translated to yield uncertainties.
• TENDL-2015 (and several earlier distributions) contain sampled files, eg:

https://tendl.web.psi.ch/tendl_2015/neutron_html/Sn/NeutronSn120.html

• These come with full parameter information for complete reproducibility and statistical tests
• For fission yields

• For thermal scattering
  https://tendl.web.psi.ch/tendl_2015/randomThermalScattering.html

<table>
<thead>
<tr>
<th>List of isotopes</th>
<th>Date</th>
<th>Description</th>
<th>Data size</th>
</tr>
</thead>
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<td>Z=90, $^{239}$Th</td>
<td>(16/10/2015)</td>
<td>0.0253 eV, 500 ENDF files (11 Mb)</td>
<td></td>
</tr>
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<td>Z=90, $^{239}$Th</td>
<td>(21/08/2015)</td>
<td>spontaneous fission, 2 ENDF files (40 kb)</td>
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</tbody>
</table>
• The ability to fully read any of these files allows repeat simulation and collapse – particularly unique for full TENDL

• Simply point to different directories for sampled files within the FILES file

```
# collapsed cross section ${i}
fluxes fluxes
xs_endf ${fisp_folder}ENDFdata/TENDL2015data/tal2015-n/gxs-586-600_sample_${i}.
prob_tab ${fisp_folder}ENDFdata/TENDL2015data/tal2015-n/tp-586-600_sample_${i}
collapxi COLAPX${i}
collapxo COLAPX${i}
```

• Alternatively use the covariance data provided within TENDL (and processed by FISPACT-II), which is based on the same parameter variation
Sampling of the files and repeated simulation results in different simulated quantities, such as this Nd148 inventory after 40 GWD/tn burn-up in a BWR-MOX assembly. Statistics on these results gives the full TMC uncertainty.
• Independent covariances intuitive based on simulation of fission events (independent correlation chart for Nd148 GEFY-5.3 U5_th)

Target nuclide: Nd148

This is 1 ‘column’
Comments on covariances

- Cumulative covariances and covariances from full irradiation scenarios show completely different trends (assembly 40 GWD/tn)

![Graph showing correlation values for neutron numbers and stable nuclides]

Target nuclide: Nd148

- Z (number of protons)
- N (number of neutrons)
- Correlation value
FISPACT-II can be used to fully sample random independent (or cumulative) yield files with any decay library, propagating uncertainties through full fuel life-cycle.*

*Taken from upcoming NDS paper D. Rochman et al.
• Coupling FISPACT-II covariance UQP for reaction rates with TMC we can provide coupled uncertainties:

  – From unc. of fissions and production of fissionable nuclides
  – From unc. in fission yields
  – And the coupled nFY + RR unc.

Takahama SF97-1 after 45 MWd/ TU

Bands x10 for visualisation
• Since TENDL-2012 the NRG libraries have entered the secluded world of criticality benchmarking – also superseding the terminated EAF libraries (last EAF-2010)
• TENDL uniquely contains covariance information
• TENDL provides for all applications: transport, burn-up, inventory, transmutation, dosimetry, astrophysics,…
• TENDL-2015 has fully benefited from TENDL-2008, -09 (EAF), -10, -11, -12, -13, -14, V&V and the T6 technological construction framework
• n-TENDL-2015 nuclear data libraries already outwit in many aspects the regional majors: ENDF/B, JENDL, JEFF,…
• However, low z isotopes still will need to come from R-matrix theory and the actinides from carefully nurtured TALYS model

TENDL-2015: reliable, V&V libraries for all applications
FISPACT-II:

• A powerful predictive activation-transmutation-burnup, radiation source term prediction tool
• Identifies and quantifies important reactions and decays
• Uses full TENDL-2015 covariance data
• Uncertainty estimates:
  • pathways to dominant nuclides
  • Monte-Carlo sensitivity
  • reduced model + Monte-Carlo sensitivity
• Uncertainty on all responses: number density, activity, decay heat, dose rate, inhalation and ingestion indices, ….

http://www.ccfe.ac.uk/fispact.aspx