FISPACT-II & TENDL-2014
a system for modeling of n, d, p, γ and α activation and transmutation processes

J-Ch. Sublet¹, J. W. Eastwood², J. G. Morgan²,
M. R. Gilbert¹ and M. Fleming¹

¹UK Atomic Energy Authority, Culham Science Centre, Abingdon OX14 3DB, United Kingdom
²Culham Electromagnetics Ltd, Culham Science Centre, OX14 3DB, United Kingdom
Simulation in space, energy and time

**Boltzmann equation**
- transport
- time independent
- energy and spatial simulation
- primary response

**Bateman equation**
- inventory
- time dependent
- secondary response

- **Nuclear Data**
  - TENDL
  - EU
  - Number densities ($t_n$)
  - Prompt spectra
  - Reaction rates

- **API**
  - MCNP6
  - US
  - TRIPOLI
  - EU
  - SERPENT
  - EU
  - Carousels

- **EASY-II**
  - EU
  - Number densities ($t_n + \Delta t$)
  - Secondary, decay spectra
  - Irradiation conditions

**Application Program Interface**: interfaces to connect Boltzmann and Bateman solvers for non-linear t- and T-dependent transport
• Set of stiff Ordinary Differential Equations to be solved

\[
\frac{dN_i}{dt} = -N_i (\lambda_i + \sigma_i \varphi) + \sum_{j \neq i} N_j (\lambda_{ij} + \sigma_{ij} \varphi)
\]

• Here \( \lambda_i \) and \( \sigma_i \) are respectively the total decay constant and cross-section for reactions on nuclide \( i \)

• \( \sigma_{ij} \) is the cross-section for reactions on nuclide \( j \) producing nuclide \( i \), and for fission it is given by the product of the fission cross-section and the fission yield fractions, as for radionuclide production yield

• \( \lambda_{ij} \) is the constant for the decay of nuclide \( j \) to nuclide \( i \)
Analytical and Numerical Models

• Analytical models are mathematical solutions expressed in closed form. The solution to the equations used to describe the time evolution of a system can be expressed in terms of well-known mathematical functions whose numerical values can be computed accurately, reliably and quickly. Then the numerical values of solutions at any required times may be computed in principle, but not always in practice. For example, the accuracy of a solution may be severely limited by rounding error in floating-point arithmetic.

• Numerical models are used when analytical models are not available, or cannot be evaluated reliably. The approximate solution to a system of equations is obtained using an appropriate time-stepping procedure to evaluate the solution at a discrete sequence of desired times. Good procedures allow estimates of the numerical error to be obtained so that the accuracy of the solution is known. The mathematical solution is represented as a table of numbers generated by the numerical method and can be plotted as a graph.
The choice of an appropriate numerical method for any particular problem cannot be made naively. Decades of research in the field of numerical analysis has yielded a wide variety of methods, each suited to specific classes of problems:

- Euler integration; exponential, matrix exponential, Newton-Krylov implicit integrators; Markovian chains, first to fifth-order Runge-Kutta, etc …

In the case of the Bateman equations with constant coefficients:
- an analytical solution is available in principle, but cannot be evaluated in practice
- the solution can be expressed as a sum of exponential functions of time using the eigenvalues of the system matrix
- unfortunately, these eigenvalues cannot be computed reliably because of ill-conditioning
- if computable at all, the eigenvalues would take an unacceptably long time to evaluate

For inventory calculations, key characteristics of the system of equations are
- sparsity (most elements of the system matrix are zero)
- stiffness (contrasting timescales between the rapid decay of some nuclides and the length of the desired time interval)
• LSODES, Livermore Solver for Ordinary Differential Equations with general sparse Jacobian matrices
  - Backward Differentiation Formula (BDF) methods (Gear’s method) in stiff cases to advance the inventory
  - Adams methods (predictor-corrector) in non stiff case
  - makes error estimates and automatically adjusts its internal time-steps
  - Yale sparse matrix efficiently exploits the sparsity
  - ability to handle time-dependent matrix
  - no need for equilibrium approximation
  - handles short (1ns) time interval and high fluxes

• LSODES wrapped in portable Fortran 95 code
  - dynamic memory allocation
  - minor changes to Livermore code to ensure portability
### FISPACT-II features

<table>
<thead>
<tr>
<th><strong>FISPACT-II</strong></th>
<th><strong>Solver</strong></th>
<th>Numerical - LSODES 2003</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Incident particles</strong></td>
<td>α, γ, d, p, n (5)</td>
<td></td>
</tr>
<tr>
<td><strong>ENDF's libraries:</strong> TENDL-2014, ENDF/B-VII.1, JEFF-3.2 or JENDL-4.0</td>
<td>✔ XS data (2632 targets)</td>
<td>✔ Decay data (3873 daughters)</td>
</tr>
<tr>
<td></td>
<td>✔ Ingestion, inhalation indices</td>
<td>✔ A2 transport</td>
</tr>
<tr>
<td></td>
<td>✔</td>
<td></td>
</tr>
<tr>
<td><strong>Dpa, Kerma, Gas production, high energy yields, PKA spectra</strong></td>
<td>✔</td>
<td></td>
</tr>
<tr>
<td><strong>Parent/daughter Isomeric states</strong></td>
<td>m, n, o, ..., s, t</td>
<td></td>
</tr>
<tr>
<td><strong>Uncertainty</strong></td>
<td>✔ Variance-covariance</td>
<td></td>
</tr>
<tr>
<td><strong>Temperature</strong></td>
<td>0K, 294K, 600K, 900K,...30 KeV</td>
<td></td>
</tr>
<tr>
<td><strong>Self-shielding</strong></td>
<td>✔ Resolved and Unresolved Resonance Range</td>
<td></td>
</tr>
<tr>
<td><strong>Energy range</strong></td>
<td>1.0 $10^{-5}$ eV – 200 MeV</td>
<td></td>
</tr>
<tr>
<td><strong>Sensitivity</strong></td>
<td>✔ Monte Carlo</td>
<td></td>
</tr>
<tr>
<td><strong>Pathways</strong></td>
<td>✔ multi steps</td>
<td></td>
</tr>
<tr>
<td><strong>Thin, thick targets yields</strong></td>
<td>✔</td>
<td></td>
</tr>
</tbody>
</table>
• n-tendl-2014, multi temperature, 709 groups library; 2632 targets
  ✓ full set of covariance
  ✓ probability tables in the RRR and URR
  ✓ $\sigma$, dpa, kerma, gas, radionuclide production
  ✓ PKA spectra
• JENDL-4.0u, ENDF/B-VII.1, JEFF-3.2, 709 groups libraries; circa 400 targets each

• g-tendl-2014, 162 groups $\sigma$ library, 2626 targets
• p-tendl-2014, 162 groups $\sigma$ library, 2626 targets
• d-tendl-2014, 162 groups $\sigma$ library, 2626 targets
• a-tendl-2014, 162 groups $\sigma$ library, 2626 targets
Decay-2012, 3873 isotopes, all daughters (24 decay modes; 7 single and 17 multi-particle ones, e.g. $\beta^+\beta^+$ or $\beta$-$2n$)

Ingestion and inhalation, clearance and transport indices libraries, 3873 isotopes

JEFF-3.1.1, UKFY4.2 fission yields

EAF-2010 decay data: 2233 isotopes

EAF-2010 ingestion and inhalation, clearance and transport indices libraries, 2233 isotopes

EAF-2003 libraries; 293K, 774 targets (20 MeV)

EAF-2007 libraries; 293K, 816 targets (55 MeV)

EAF-2010 libraries; 293K, 816 targets (55 MeV)

EAF’s uncertainty files
Self shielding of resonant channels

- High Fidelity Resonances
- Thin and thick target yields
- Probability tables, sub-group method
Neutron self-shielding model

- thin and thick target yields
- accounts approximately for target geometry
- applicable to thick targets
- handles foils, wires, spheres and finite cylinders
- uses one physical length scale to represent the target: the “effective length” $y$

<table>
<thead>
<tr>
<th>Type ID</th>
<th>Geometry</th>
<th>Dimension(s)</th>
<th>$Y$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>foil</td>
<td>thickness (t)</td>
<td>$y=1.5t$</td>
</tr>
<tr>
<td>2</td>
<td>wire</td>
<td>radius (r)</td>
<td>$y=2r$</td>
</tr>
<tr>
<td>3</td>
<td>sphere</td>
<td>radius (r)</td>
<td>$y=r$</td>
</tr>
<tr>
<td>4</td>
<td>cylinder</td>
<td>radius (r), height (h)</td>
<td>$y=1.65rh(r+h)$</td>
</tr>
</tbody>
</table>
Epithermal Neutron Self-shielding Model

- theory of radioisotope production
- production rates and cross-sections
- saturation factors and practical yields

- model uses resonance parameters from the Resolved Resonance Range, RRR
- model includes the effects of neutron loss through radiative capture
- model includes effects of neutron energy diffusion through elastic scattering
one resonance in a pure target

- dimensionless parameter to combine the physical effective length with the nuclear parameters

\[ z = \sum_{tot} (E_{res}) y \sqrt{\frac{\Gamma_{\gamma}}{\Gamma}} \]

- where
  - \( \Sigma_{tot}(E_{res}) \) is the macroscopic cross-section at the energy \( E_{res} \) of the resonance peak
  - \( \Gamma_{\gamma} \) is the radiative capture width
  - \( \Gamma \) is the total resonance width
  - \( y \) “effective length”

- Self-shielding factor \( G_{res} \) is defined in terms of \( z \) only
Baumann, 1963; Yamamoto and Yamamoto, 1965; Lopes, 1991

\[ z = \sum_{\text{tot}} (E_{\text{res}}) \gamma (\Gamma / \Gamma)^{1/2} \]

**Experimental self-shielding factor**

- Co-59 Foils EAS62
- Co-59 Wires EAS62
- Au-197 Foils AXT63
- Au-197 Foils BAU63
- Au-197 Foils BRO64
- Au-197 Wires McG64
- Zr-94 Foils DeCOR87
- Zr-96 Foils DeCOR87
- Mo-98 Foils FRE93
- Mo-98 Wires FRE93
- Universal curve

**Target geometry**
Model development, first step (2)

\[ G_{res}(z) = \frac{A_1 - A_2}{1 + \left( \frac{z}{z_0} \right)^p} + A_2 \]

- this is the “universal sigmoid curve” for the model
- the parameters have been determined empirically to be a good fit to experimental data
- preferred values are:
  - \( A_1 = 1.000 \pm 0.005 \)
  - \( A_2 = 0.060 \pm 0.011 \)
  - \( z_0 = 2.70 \pm 0.09 \)
  - \( p = 0.82 \pm 0.02 \)
Model development, second step

- extend model to a group of separated resonances
- still considering a pure target: one nuclide
- assign a weight to each resonance

\[ w_i = \left( \frac{\Gamma_\gamma}{E_{res}^2} \cdot \frac{g\Gamma_n}{\Gamma} \right)_i \]

where

- \( \Gamma_n \) is the neutron scattering width
- \( g \) is the statistical factor, \((2J + 1)/(2(2I + 1))\)
- \( J \) is the spin of the resonance state
- \( I \) is the spin of the target nucleus
- form an average self-shielding factor from all resonances of interest

\[ \langle G_{res} \rangle = \frac{\sum w_i G_{res}(z_i)}{\sum w_i} \]
Model development, third step

- extend $\langle G_{\text{res}} \rangle$ to form the average for resonances of a mixture of nuclides
- assume the resonances of different nuclides do not overlap significantly
- make $\langle G_{\text{res}} \rangle$ energy dependent by taking averages separately for each energy bin used for the group-wise cross-sections
- use Fröhner’s simple expression for the peak cross-section of each resonance (not available from the Groupwise-ENDF data, but the MF-2 has been kept)
universal curve model provides an alternative to probability table self shielding

use $\langle G_{\text{res}} \rangle (E)$ to scale down energy-dependent cross-sections before cross-section collapse

$\langle G_{\text{res}} \rangle (E)$ reduces the neutron flux, so apply it to all cross-sections

target geometry specified with \texttt{SSFGEOMETRY} type length$_1$ <length$_2$>

use resonances from mixture specified with \texttt{SSFFUEL} or \texttt{SSFMASS}

PRINTLIB 6 now generates a table of all cross-sections with $\langle G_{\text{res}} \rangle$ reduction factors
Verification & Validation

• Validation of EASY-II and TENDL-2014, ENDF/B-VII.1, JEFF-3.2 or JENDL-4.0 nuclear data libraries through multi-faceted effort including variety of code applications

• Each of the following completed or will be by mid-2015:
  ▪ Detailed analysis of total heat measurements done at JAEA FNS
  ▪ Validation of all existing integro-differential activation experiments
  ▪ Simulation of complete set of material activations
  ▪ In-depth simulations of fission decay heat with break-down of nFY/decay/spectroscopic analysis
  ▪ Massive validation against library of integral data from integral resonance, astrophysics and fission sources

• No comparable system has undergone equivalent V&V
### FNS-00 5 Min. Irradiation - Ni

<table>
<thead>
<tr>
<th>Product</th>
<th>Pathways</th>
<th>$T_{1/2}$</th>
<th>Path %</th>
<th>E/C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Co62</td>
<td>Ni62(n,p)Co62</td>
<td>1.5m</td>
<td>99.8</td>
<td>0.90</td>
</tr>
<tr>
<td>Co62m</td>
<td>Ni62(n,p)Co62m</td>
<td>13.9m</td>
<td>100.0</td>
<td>0.89</td>
</tr>
</tbody>
</table>

**Product Pathways:**
- $61^\text{Fe}$
- $60^\text{mCo}$
- $62^\text{Co}$
**V&V: Decay power visualisation with EASY-II**

Time: 0.00 seconds
Total Decay Heat (kW/kg): 0.0

<table>
<thead>
<tr>
<th>Time (seconds)</th>
<th>Decay Heat (kW)</th>
<th>Heat Output (μW/kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>10^10</td>
<td>10^13</td>
</tr>
<tr>
<td>1</td>
<td>10^11</td>
<td>10^12</td>
</tr>
<tr>
<td>10</td>
<td>10^10</td>
<td>10^11</td>
</tr>
<tr>
<td>50</td>
<td>10^10</td>
<td>10^12</td>
</tr>
<tr>
<td>60</td>
<td>10^10</td>
<td>10^13</td>
</tr>
</tbody>
</table>

Simulation of SS316 irradiated in JAEA FNS
m - metastable state(s) > 50%

M.R. Gilbert & J.-Ch. Sublet CCFE-R(14)21 JAEA FNS Decay heat validation
M. R. Gilbert et al., "Inventory Visualisation techniques" Nucl. Sci. Eng (2014)
V&V: Integro-differential validation

- Inclusion of meta-stables substantially improves simulation accuracy

Sc$^{44}$m measured
Sc$^{45}$(n,2n)Sc$^{44}$m
$T_{1/2} = 58.6\text{h}$
- C/E distributions for integral measurements

- Top: TENDL-2014 outperforms EAF-2010 – the latter was specifically **tuned** to these!

- Bottom: all legacy libraries (ENDF, JENDL, JEFF shown) miss tremendous number of reactions entirely

- **TENDL will become standard**
V&V: Decay heat following a thermal pulse

- Simulation of complex fission burst decay experiments – Pu241 thermal ‘pulses’ above, with reconstruction of irradiation conditions
V&V: Decay heat following a thermal pulse

- Comparison between libraries for Pu241 total and gamma contributions to decay heat - note gamma deficiency

- ENDFB/JENDL include TAGS to correct $\gamma$

- FISPACT-II can track all nuclides for in-depth study

- Contribution to DH needs for $\nu_e +$ TAGS
Maxwellian-averaged astrophysics reactions

- High fidelity resonances and robust processing, with NJOY/PREPRO cross-checks

- Au\textsubscript{197}(n,g):
  - Gray=0K (background)
  - Red=5keV
  - Green=30keV
  - Blue=100keV

- RRs shown
MACS against KADoNiS

- Benchmarked against all KADoNiS database with multiple simulation methods (FISPACT-II, inter, maxwav) Au197:
  - Purple=inter
  - Black=maxwav
  - Missing low-E and negative res. diagnosed for various nuclides/libraries
  - RRR/URR improved w/HFR
• PKAs in Fe under DEMO conditions:

- **Elemental**
  - \( \alpha \)
  - \( p \)
  - Fe
  - Cr
  - Mn

- **Isotopic**

• Primary knock-on atom (PKA) evaluations using TENDL-2014 and FISPACT-II
• Necessary as input into materials modelling of radiation damage creation and evolution
• 2632 targets (H\textsuperscript{1} to Ds\textsuperscript{281})
• Target with $T_{1/2} > 1\text{s}$
• Cross section, 90 reaction types

\textbf{Target x 3}

\textbf{Validation: SACS}

\textbf{Decay x 1.7}

\textbf{n, p, d, α, γ}
\textbf{TENDL-2014}

\textbf{FISPACT-II}

\textbf{Decay-2012}

\textbf{Covariance}

\textbf{ENDF/B, JENDL, JEFF}

\textbf{UKFY-4.2}

\textbf{fission yield}

\textbf{Hazard indices}

\textbf{V&V, C/E integral and differential with uncertainty}

• Decay data: 3873 nuclides; 24 types
• All daughters with $T_{1/2} > 0.1\text{s}$
• Stables and isomeric states; g, m, n, o, ..
• The TALYS and Total Monte Carlo (TMC) methodology uses direct feedback from simulation to physical inputs

• TMC provides truly remarkable uncertainty analysis based upon simulation outputs – where legacy provides little/none

• TMC is as good as the simulation capability. The marriage of TENDL with FISPACT-II provides the most robust methodology

By bringing the disjoint nuclear data links, from evaluation to application, into a technologically-driven closed system we can provide complete, robust data forms and simulation superior to any legacy system
The EASY-II platform aims to develop 21st century observables for nuclear sciences and technology: stockpile, fuel cycle stewardship, source terms, materials characterization and life cycle management for all applications:

- Magnetic and inertial confinement fusion
- Advanced Fission, Gen IV and beyond
- Advanced energy and fuel systems
- High energy and accelerator physics
- Medical applications, isotope production
- Earth exploration, Astrophysics
- Homeland security
- ...

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