FISPACT-II: an advanced simulation platform for inventory and nuclear observables “a renaissance”

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James W. Eastwood, J. Guy Morgan
Culham Electromagnetics Ltd
Michelangelo, (c. 1511) the Creation of Adam
Simulation in space, energy and time

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

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

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**Application Program Interface:** interfaces to connect Boltzmann and Bateman solvers for non-linear t- and T-dependent transport

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**Carousels**
- TRIPOLI
- Fr
- SERPENT
- Fi

**API**

**TENDL NL**

**Nuclear Data**

**Multifaceted interface**

**Material evolution**

**MCNP6 US**

**FISPACT-II UK**

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**UK Atomic Energy Authority**
Chapter 1
• Framework
• ODE solver
• Nuclear data processing steps and libraries
  ▪ Particles induced reactions
  ▪ DD, sFY, nFY, otherFY
  ▪ Hazard, transport, clearance indices

Chapter 2
• Reaction rates uncertainty quantification and propagation, variance-covariance
• Self shielding of resonant channels
  • Probability tables, sub-group method
  • Thin and thick target yields
  • Real-world application
Chapter 3
• Extended pathways search
• Verification and Validation, V&V
  – Differential
  – Integral

Chapter 4
• Applications
  – Scoping studies of material response
    • Activation, transmutation and primary damage response functions
  – Fission
  – High energy
  – Input into materials science
Chapter 5

• FISPACT-II & Libraries simulation software
• Future Roadmap
- ENDF/B-VII.1, JENDL-4.0, JEFF-3.2, CENDL-3.1 nuclear data: available through the NNDC
  - [https://www-nds.iaea.org/](https://www-nds.iaea.org/)

- EAF-2010 in ENDF-6 format = n-FENDL-3.0/A; d-FENDL-3.0/A and p-FENDL-3.0/A = part of d-TENDL-2011 and p-TENDL-2011
  - [http://www-nds.iaea.org/fendl3](http://www-nds.iaea.org/fendl3)

- TENDL-2015 @
    A project with yearly upgrade
• FISPACT-II is a modern engineering prediction tool for activation-transmutation, depletion inventories at the heart of the an enhanced multi-physics platform that relies on the TALYS collaboration to provide the nuclear data libraries.

• FISPACT-II was designed to be a functional replacement for the code FISPACT-2007 but now includes many enhanced capabilities.

• $d$, $p$, $\alpha$, $\gamma$, $n$-Transport Activation Library: TENDL-2015 from the TENDL collaboration, but also ENDF/B, JENDL, JEFF, CENDL and GEFY

• All nuclear data processing is handled by NJOY (LANL), PREPRO (LLNL) and CALENDF (UKAEA)
Development history (2009 - 2015)

- Phase I (06-2006 – 03-2007)
  ODE solver selection, pre-programming ✓

- Phase II (03-2009 – 03-2010)
  Release 0-20 alpha, 1-00 alpha, EASY-2010 benchmarking,
  CVS repository, software specification documents ✓

- Phase III (06-2010 – 09-2011)
  FISPACT-II (12) 1.00, User manual, EAF-2010 full integration,
  PT's self shielding factor method, CCFE internal distribution ✓

- Phase IV (10-2011 – 03-2012)
  EASY-II(12) R-2.00 first release ✓

- Phase V (06-2012 – 06-2013)
  V&V suites, EASY-II (13) R-2.10 release ✓

- Phase VI (06-2013 – 07-2014)
  V&V suites, EASY-II (14) R-2.20 release ✓

- Phase VII (07-2014 – 09-2015)
  V&V suites, FISPACT-II R-3.00 & Libraries release ✓
Ordinary Differential Equation solver
• 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 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, Chebyshev Rational Approximation, 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 advanced simulations

<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>$\alpha, \gamma, d, p, n$ (5)</td>
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<tr>
<td><strong>ENDF's libraries:</strong></td>
<td>✔ XS data (2809 targets)</td>
<td></td>
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<tr>
<td>TENDL-2015 &amp; GEFY.5.2</td>
<td>✔ Decay data (3873 isotopes)</td>
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<td>ENDF/B-VII.1, JEFF-3.2, JENDL-4.0, CENDL-3.1</td>
<td>✔ nFY, sFY, otherFY</td>
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<td>(~400 targets each)</td>
<td>✔ Hazard, clearance indices, A2</td>
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<tr>
<td><strong>Dpa, Kerma, Gas production, radionuclide yields</strong></td>
<td>✔</td>
<td></td>
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<tr>
<td><strong>PKA, recoil, emitted particles spectra</strong></td>
<td>✔</td>
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<tr>
<td><strong>Uncertainty quantification and propagation UQP</strong></td>
<td>✔ Variance-covariance</td>
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<tr>
<td><strong>Temperature (from reactor to astrophysics, plasma)</strong></td>
<td>0, 294, 600, 900 K,…5, 30, 80 KeV</td>
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<tr>
<td>1 KeV ~ 12 million Kelvin</td>
<td>✔ Resolved and Unresolved Resonance Range</td>
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<tr>
<td><strong>Self-shielding with probability tables and with resonance parameters</strong></td>
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<tr>
<td><strong>Energy range</strong></td>
<td>1.0 $10^{-5}$eV – 30, 200 MeV, ..1GeV</td>
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<tr>
<td><strong>Sensitivity</strong></td>
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</tr>
<tr>
<td><strong>Pathways analysis, routes of production</strong></td>
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<td><strong>Thin, thick targets yields</strong></td>
<td>✔</td>
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</table>
FISPACT-II features: ENDF’s libraries

- Large number of targets: 2809 from H\textsuperscript{1} to Fl\textsuperscript{289} (Flerovium, mass 114)
- Broad energy range: \(1.0 \times 10^{-5} \text{ eV} - 200 \text{ MeV}, 1 \text{ GeV}\)
- Five incident particles: a, g, d, p, n

- Covariance information on neutron entrance channels, uncertainty
- Pathways analysis, production routes, dominant contributors
- Self-shielding effects: channels, isotopic, elemental

- Sensitivity analysis, (Monte Carlo)
- Isomeric states and branching ratio (g, m, n, o, p, q,...., from RIPL)
- Consistent decay data and cross section data: energy levels

- Transport A2, clearance, inhalation and ingestion indices
- DPA, Kerma (primary and secondary), gas and radionuclide production
- Temperatures: 0, 294, 600, 900 K,.... and stellar 5 Kev, 30 Kev, 80 Kev (1 Kev = 12 \(10^6\)K)
- Thin, thick target yields
- V&V suites: fusion, fission, accelerator, astrophysics,..

For all nuclear applications
Partners: IAEA, PSI, UKAEA, CEA DIF, Uppsala University,..

Objectives: To create a set of modern baseline general-purpose files aimed at satisfying the radiation transport and activation-transmutation requirements for facilities in support of nuclear technology.

- $\alpha, \gamma, d, p, n$-TENDL libraries
- Multi applications, consistent libraries
- Complete variance-covariance information
- TALYS nuclear model
- T6 codes; TALYS, TAFIS, TANES, TARES, TEFAL and TASMAN, wrapped into a Total Monte-Carlo loop for uncertainty quantification
• From model parameters to code result quantities
• Allow physical parameters to impact the basic nuclear data and not an engineered localized adjustment, unable to account for compensation effects.
• With variance-covariance data based on experimental data and nuclear models, allowing design optimization of nuclear technology.
• Account for the processing (non unique) steps.
• Include, account for V&V Verification and Validation processes.
• Feedback of extensive validation and benchmark activities are automatically and rapidly, within a year not 10, taken into account.
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<td>Pu</td>
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<tr>
<td>95</td>
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<td>Cm</td>
<td>Curium</td>
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<td>Bk</td>
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<td>Cf</td>
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<td>Fermium</td>
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<td>Md</td>
<td>Mendelevium</td>
<td>258.58</td>
</tr>
<tr>
<td>102</td>
<td>No</td>
<td>Nobelium</td>
<td>259.101</td>
</tr>
<tr>
<td>103</td>
<td>Lr</td>
<td>Lawrencium</td>
<td>262.069</td>
</tr>
</tbody>
</table>

**Lanthanide Series**
- La (13) to Lu (71)

**Actinium Series**
- Ac (89) to Lr (103)
Isotopic targets

TENDL-2015 [2809 (544) target nuclides (isomers)]
EAF-2010 [821 (74) target nuclides (isomers)]
255 stable nuclides

Z (number of protons)

N (number of neutrons)
TENDL-2015 [2809 (544) target nuclides (isomers)]
ENDF/B-VII.1 [423 (10) target nuclides (isomers)]
255 stable nuclides
Nuclear data processing steps and libraries
• Legacy EAF’s format style libraries are being phased out, replaced by ENDF’s style libraries, however the physics input streams remain

• This has been made possible because of:
  ▪ November 2010 CSWEG ENDF-6 format extension
  ▪ NJOY-12 extensions: mf8, reconr basic, acer, gaspr…
  ▪ PREPRO-2015 extensions: sixpack, complot,…
  ▪ TENDL-2015 enhanced GP format framework: unequivocal, clear format cutoff @ 30 then to 200 MeV, then to 1 GeV.

• The development of the FISPACT-II inventory code
• Uniquely, uses three processing codes to prepare, shape its nuclear data forms:
  – NJOY – kerma, dpa, matrix, gas production & crosschecking
  – PREPRO – ENDF data file preparation, high energy
  – CALENDNF – probability table & crosschecking

• Advantages
  – Robustness, completeness
  – Redundancy
  – Portability, repeatability
  – Legacy and maturity

• Remarks: not all observables need processing to be usable
Processing steps: three codes

- **NJOY12-064**
  - reconr
  - broadr
  - unresr
  - thermr
  - heatr
  - gaspr
    - purr
    - acer
    - groupr

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

- **CALENDNF-2010**
  - calendf
  - regroup
  - lecritp
  - ....

Diagram:
- ENDF file
- cross-check
- cross-check
- PT file
- Single script for an entire library

**ACE file**
**Processed ENDF file**
**Single script for an entire library**
- **NJOY-12.064**
  - 0 Kelvin run
  - Single temperature *pendf*
  - Two *heatr* runs (7 + 4 responses, gamma local)
  - *Groupr* 1025 groups @ 30 MeV; p, d, t, alpha and he-3 + residual nucleus (A>4) production matrix, recoil matrix

  - *thermr*, free gas
  - Two more *heatr* run (7 + 4 responses, gamma transported)
  - *purr* (nbin=20, ladders=64)
  - Two *acer* (new cumulative angle distribution (law 61) and one for checking and ace data forms display)

The MCNP routes
• **CALENDF-2010**
  - 0 Kelvin run
  - Single temperature pendf, statistical resonance in the URR
  - Single temperature Probability Tables
  - PT in the RR and URR from 0.1 eV to the end of the URR for each isotopes
  - Group structure 615 @ 10 eV, 900 @ 5 MeV

Those PT tables as they are stored can be used by either FISPACT-II and TRIPOLI-4.9. They allow self-shielding treatment in the URR to be accounted for (300 pcm on Bigten @ 20-150 KeV)
• PREPRO-2015
  
  - 0 Kelvin run
  - Single temperature pendf, 294 Kelvin to... 100 KeV
  - **SIXPACK**: unique mf3-mt5/mf6 high energy processing
  - **ACTIVATE**: unique mf9 processing
  - Merge NJOY-12 dpa, kerma pendf responses
  
  - **GROUPIE** to:
    - 1102 gprs @ 1 GeV
    - 1067 gprs @ 200 MeV
    - 1025 gprs @ 30 MeV
    - 162 gprs @ 200 MeV (for charge particles)
  
  - mf-2 processed, but also kept in for further usage

The resulting pendf “tape” fully comply to the ENDF-6 format frame and many utilitarian process (display, merge, concatenate, etc. ) can be performed on such data forms
• For all 2809 TENDL target nuclides
• 1102 energy groups for all applications alike

- **Thermal**
  - 50 equal U per decade
  - Thermo: 237 gprs

- **Resonance fine**
  - Equal energy 0.025 eV
  - Resonance: 378 gprs

- **Resonance shielded**
  - 50 equal U per decade
  - Shielded: 285 gprs

- **Fast Fusion**
  - Equal energy 200 KeV
  - Fast: 125 gprs

- **Fast**
  - 50 equal U per decade
  - Fast: 27 gprs

- **High Energy**
  - Equal lethargy
  - High Energy: 50 gprs

- 1e-5 eV 0.55 eV 10 eV 5 MeV 30 MeV 100 MeV 1 GeV
  - 615 groups 378 groups 285 gprs 125 gprs 27 gprs 50 gprs

• 378 fine groups in the resonance range
• Resonance shielded data available in the RRR (0.1 eV) up to the end of the URR for all nuclides IDs
• Fast fine structure for accurate threshold reaction rate
Group structures

Cumulative number of energy bins

Incident energy (eV)

Energy bin width (eV)

Lethargy bin width

Incident energy (eV)
Group structure: 1102

MAT 6440

\( (n,\gamma) \) Cross Section

Resolved

<table>
<thead>
<tr>
<th>Max Ratio</th>
<th>Min Ratio</th>
</tr>
</thead>
</table>

- Resolved
- Max Ratio
- Min Ratio

Cross Section (barns)

- pointwise
- groupwise 1102

Ratio

- groupwise 1102/ pointwise

Incident Energy (eV)

- 4
- 10
- 100
- 1000
- 10000

Fine group to 10 eV  
Resonance shielded to end of URR

64-Gd-157

- 93.48 To 8940. %
Group structure: 1102

Fine group to 10 eV   Resonance shielded to end of URR
Group structure: 1102

Peak and trough are well described
Applications forms

- Pointwise forms, Temperature dependent
- Groupwise, T and sigma zeroes dependent, PTs
- Variance and covariance (on cross section)
- MF-2 resonance widths for shielding
- Matrices: n-n, n-g, n-prod and recoil
- All partials and total Kerma (7), dpa (4), gas production (5)

- FISPACT-II & SPECTRA-PKA nuclear data forms, groupwise with probability tables, uncertainty, n-prod/recoil matrices, responses
90 reaction types

(n, remainder) = mf3 - mt5 * mf6 above 30 MeV
MAT 2431
Neutron Production
294 Kelvin Cross Sections

Cross Section (barns)

Incident Energy (MeV)
Gas production

NJOY generated MT’s displayed by PREPRO
NJOY generated MT’s displayed by PREPRO

Total, partial Kerma

Total, partial Dpa
Cross section channels above 30 MeV

Unique to PREPRO mf10-mt5
Groupwise data from PREPRO-2015, MF-10 with isomers
• Multi-particle groupwise, multi-temperature libraries with NJOY12-064, PREPRO-2015, probability tables in the RRR & URR with CALENDF-2010

  ▪ For the inventory code FISPACT-II

• From $\alpha$, $\gamma$, $p$, $d$, $n$-TENDL-2015 & ENDF/B-VII.1, JEFF-3.2, JENDL-4.0u, CENDL-3.1

• FISPACT-II parses directly the TENDL’s covariance complex information

• Transport and activation application libraries now stem from unique, truly general purpose files
• n-tendl-2015, multi temperatures, 1102 groups library for 2809 targets
  ✓ full set of covariance
  ✓ probability tables in the RRR and URR
  ✓ xs, dpa, kerma, gas, radionuclide production

• JENDL-4.0u, ENDF/B-VII.1, JEFF-3.2, CENDL-3.1, 1102 groups libraries for circa 400 targets each

• γ-tendl-2015, 162 groups xs library, 2804 targets
• p-tendl-2015, 162 groups xs library, 2804 targets
• d-tendl-2015, 162 groups xs library, 2804 targets
• α-tendl-2015, 162 groups xs library, 2804 targets
✓ UKDD-2012, 3873 isotopes (23 decay modes; 7 single and 16 multi-particle ones)
✓ Ingestion and inhalation, clearance and transport indices libraries, 3873 isotopes
✓ GEFY 5.2, JEFF-3.1.1, UKFY4.2 fission yields
✓ ENDF/B-VII.1 DD and FY
✓ JENDL-4.0 DD and FY

Kept for compatibility, but with less capabilities:
✓ EAF-2010 decay data: 2233 isotopes
✓ EAF-2010 ingestion and inhalation, clearance and transport indices libraries, 2233 isotopes
  ✓ EAF-2010 libraries; 293K, 816 targets (55 MeV)
  ✓ EAF’s uncertainty files
• γ-dose rate
  ▪ From either contact (default) or point source
  ▪ Contact: dose rate at surface of semi-infinite slab
    \[ D = CB/2 \sum_{i=1}^{N_\gamma} \mu_a (E_{\downarrow i})/\mu_m (E_{\downarrow i}) S_{\gamma} (E_{\downarrow i}) \]

  - \( N_\gamma \) = number of γ energy groups,
  - \( \mu_a \) = mass energy absorption,
  - \( \mu_m \) = mass energy attenuation,
  - \( B \) = build-up factor,
  - \( S_{\gamma} \) = rate of γ emission,
  - \( C \) = conversion from MeV/kg/s to Sv/h

  ▪ Dose from a point source
    • \textbf{DOSE 2 x}
    • Point source of 1 g of material at a distance \( x \) (m)
• Biological hazard – HAZARDS
  - Estimates the biological impact to human beings
  - Library of dose coefficients
    - Determine the dose following ingestion or inhalation of 1 Bq of activity from each radionuclide
    - From ICRP and NRPB where available
    - Uses an approximation otherwise (1209 nuclides)

• Clearance indices – CLEAR
  - IAEA data coefficients determining when a radionuclide can be disposed of as if non-radioactive (clearance=1)
FISPACT-II roadmap

① FISPACT-2007+ & EAF-2010 in EAF format processed by SAFEPAQ-II ☑ 08/2010
② FISPACT-II(11) & EAF-2010 in EAF format processed by SAFEPAQ-II ☑ 01/2011
③ FISPACT-II(11) & EAF-2010 + CALENDLF PT’s ssf method, ENDF’s format and processing framework ☑ 09/2011
④ EASY-II(12) = FISPACT-II(12) & EAF’s and TENDL-2011 ENDF’s libraries processed by NJOY, PREPRO & CALENDLF ☑ 03/2012
⑤ EASY-II(13) = FISPACT-II & EAF’s and TENDL’s V&V libraries processed by NJOY, PREPRO & CALENDLF ☑ 06/2013
⑥ EASY-II(14) = FISPACT-II & EAF’s, TENDL’s, ENDF’s libraries, automated V&V processes ☑ 07/2014
⑦ FISPACT-II & TENDL’s, ENDF’s libraries, automated V&V processes ☑ 09/2015

Vigilant, thorough V&V stepped approach, weathered in five years
- Grid of reactions, MT numbers defined in ENDF-6 format

<table>
<thead>
<tr>
<th></th>
<th>Z+2</th>
<th>(α,3n)</th>
<th>(α,2n)</th>
<th>(α,n)</th>
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<tbody>
<tr>
<td>Ni</td>
<td>Z+1</td>
<td></td>
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<td></td>
</tr>
<tr>
<td>Co</td>
<td>Z+1</td>
<td>(p,n)β−</td>
<td>(p,γ)</td>
<td>(t,n)</td>
</tr>
<tr>
<td>Fe</td>
<td>Z</td>
<td>(n,4n) 37</td>
<td>(n,3n) 17</td>
<td>(n,2n) (γ,n) 16</td>
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<tr>
<td>Mn</td>
<td>Z-1</td>
<td>(n,2nt) 154</td>
<td>(n,nt; 3np) 33, 42</td>
<td>(n,t; nd; 2np) 105, 32, 41</td>
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<tr>
<td>Cr</td>
<td>Z-2</td>
<td>(n,2na) 24</td>
<td>(n,n′a) 22</td>
<td>(n,a; nh; pt) 107, 34, 116</td>
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<td>V</td>
<td>Z-3</td>
<td>(n,2npa) 159</td>
<td>(n,da; npa) 117, 45</td>
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<td>Ti</td>
<td>Z-4</td>
<td>(n,2a) 108</td>
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<tr>
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<td>54</td>
<td>55</td>
<td>56</td>
<td>57</td>
<td>58</td>
</tr>
</tbody>
</table>

n in ➔ Z always decrease
p, d, a in ➔ Z may increase
The emitted particles may differ, not the residual
The residual product may be another element
Tungsten transmutation with FISPACT-II

Powered by GNUPLLOT 5.0

Time: 0.00 seconds

Pure W irradiated in a DEMO FW armour spectrum

Total flux: $6.60 \times 10^{14} \text{ n cm}^{-2} \text{ s}^{-1}$

m - concentration dominated by metastable nuclide(s)

Tungsten transmutation with FISPACT-II

Time: 0.000 seconds

Pure W irradiated in a
DEMO FW armour spectrum
Total flux: $8.25 \times 10^{14}$ n cm$^{-2}$ s$^{-1}$

Powered by GNUPLLOT 5.0