

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

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Italian renaissance



Michelangelo, (c. 1511) the Creation of Adam

Simulation in space, energy and time



JK Atomic

nergy uthoritv





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/

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

<u>http://www-nds.iaea.org/fendl3</u>

• TENDL-2015 @

<u>https://tendl.web.psi.ch/tendl_2015/tendl2015.html</u>
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, α, γ, 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)



• Phase I (06-2006 – 03-2007)

ODE solver selection, pre-programming \blacksquare

• 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 II

- 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



- Here λ_i and σ_i are respectively the total decay constant and cross-section for reactions on nuclide i
- σ_{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
- λ_{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

FISPACT-II

Solver	Numerical - LSODES 2003			
Incident particles	α, γ, d, p, n (5)			
ENDF's libraries: TENDL-2015 & GEFY.5.2 ENDF/B-VII.1, JEFF-3.2, JENDL-4.0, CENDL-3.1 (~400 targets each)	 ✓ XS data (2809 targets) ✓ Decay data (3873 isotopes) ✓ nFY, sFY, otherFY ✓ Hazard, clearance indices, A2 			
Dpa, Kerma, Gas production, radionuclide yields	✓			
PKA, recoil, emitted particles spectra	v			
Uncertainty quantification and propagation UQP	✓ Variance-covariance			
Temperature (from reactor to astrophysics, plasma) 1 KeV ~ 12 million Kelvin	0, 294, 600, 900 K,5, 30, 80 KeV			
Self-shielding with probability tables and with resonance parameters	 Resolved and Unresolved Resonance Range 			
Energy range	1.0 10 ⁻⁵ eV – 30, 200 MeV,1GeV			
Sensitivity	✓ Monte Carlo			
Pathways analysis, routes of production	✓ multi steps			
Thin, thick targets yields	✓ 15			



- Large number of targets: 2809 from H¹ to Fl²⁸⁹ (Flerovium, mass 114)
- Broad energy range: 1.0 10⁻⁵ eV 200 MeV, 1 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 10⁶K)
- 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.
 - $\succ \alpha$, γ , 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.



2016 periodic table



Dawn Shaughnessy

Isotopic targets



Z (number of protons)



N (number of neutrons)

Isotopic targets



Z (number of protons)



N (number of neutrons)



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
 - CALENDF 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

cross-check

• NJOY12-064

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

ACE file

PREPRO-2015

ENDF file

- linear
- cross-check recent
 - sigma1
 - sixpack
 - activate
 - merger
 - dictin
 - groupie

Processed ENDF file

- CALENDF-2010
 - calendf
 - regroutp
 - lecritp



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 <u>transported</u>)
 - 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



- 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





Group structure: 1102



Group structure: 1102







Group structure: 1102



Peak and trough are well described



- 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



TENDL-2015 pendf, 200 MeV



(n, remainder) =mf3-mt5*mf6 above 30 MeV



TENDL-2015 pendf, below 30 MeV







NJOY generated MT's displayed by PREPRO





NJOY generated MT's displayed by PREPRO



TENDL-2015 pendf from mf3*mf6



Cross section channels above 30 MeV

Unique to PREPRO mf10-mt5



TENDL-2015 gendf, 200 MeV



Groupwise data from PREPRO-2015, MF-10 with isomers



TENDL-2015 gamma pendf, 200 MeV



2 24-Cr-52

24-Cr-52

30

24-Cr-52

24-Cr-52



- 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 α, γ, 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
 - \checkmark full set of covariance
 - $\checkmark\,$ probability tables in the RRR and URR
 - \checkmark 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 $D = CB/2 \sum_{i=1}^{\infty} \frac{1}{N} \sqrt{\gamma} = \frac{1}{\mu} \sqrt{\alpha} (E \sqrt{i}) / \mu \sqrt{m} (E \sqrt{i}) S \sqrt{\gamma} (E \sqrt{i})$
 - N_{γ} = number of γ energy groups,
 - μ_a = mass energy absorption,
 - μ_m = mass energy attenuation,
 - B =build-up factor,
 - S_{v} = rate of γ emission,
 - C' = conversion from MeV/kg/s to Sv/h
 - Dose from a point source
 - 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 & TENDL & ENDF/B, JENDL, JEFF





- 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 + CALENDF 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 & CALENDF
 ☑ 03/2012
- (5) EASY-II(13) = FISPACT-II & EAF's and TENDL's V&V libraries processed by NJOY, PREPRO & CALENDF
 ☑ 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

Ni	Z+2			(a, 3 n)	(a, 2 n)	(α,n)		✓ target Fe ⁵⁶
Co	Z+1			(p,n) β ⁻	(p, γ) (d,n)	(t,n)		5
Fe	Z	(n,4n) 37	(n,3n) 17	(n,2n) (γ,n) 16	(n,n') 4 K	(n,γ) 102	(t,p)	
Mn	Z-1	(n,2nt) 154	(n,nt; 3np) 33, 42	(n,t; nd; 2np) 105, 32, 41	(n,d; np) 104, 28	(n,p); β ⁺ 103		
Cr	Z-2	(n,2na) 24	(n,n'a) 22	(n,a; nh; pt) 107, 34, 116	(n,h; n2p; pd) 106, 44, 115	(n,2p) 111		
V	Z-3	(n,2npa) 159	(n,da; npa) 117, 45	(n,pa) 112		(n,3p) 197		
Ti	Z-4	(n,2a) 108						
		N-3	N-2	N-1	Ν	N+1	N+2	
		53	54	55	56	57	58	

n in \rightarrow Z always decrease

p, d, a in \rightarrow 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 GNUPLOT 5.0





Tungsten transmutation with FISPACT-II

Time: 0.000 seconds

Powered by GNUPLOT 5.0





 10^{6}