Precursors and decay events with EASY-II

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CCFE is the fusion research arm of the United Kingdom Atomic Energy Authority. This work was funded by the RCUK Energy Programme [grant number EP/I501045] .

- FISPACT-II is a modern engineering prediction tool for activation-transmutation, depletion inventories, etc.
- The EASY-II system has been guided by TALYS n-TAL collaboration, which provides *complete* nuclear data libraries.
- FISPACT-II was designed to be a functional replacement for FISPACT-2007 but significant development has produced a substantially superior, more mature code
- a, g, d, p, n-Transport Activation Library: TENDL-2014 from the TENDL collaboration, but also ENDF/B, JENDL, JEFF
- Nuclear data processing done with (including cross-checks) NJOY (LANL), PREPRO (LLNL), and CALENDF (CEA-CCFE)

- All problems are multi-physics but usually decomposed into single physics ones
- The nuclear data, processing steps answers the needs of single physics codes (mainly reactor physics)
- Advanced simulation methods rely upon multi-physics codes with complex feedback
- This *requires* integrated, multifaceted processing steps able to deliver rich, interconnected type of nuclear data forms and correlated uncertainty
- This in turn requires the basic nuclear data to be complete but unique, robust, technological based with variancecovariance for every quantities across all energy ranges and decay schemes

Physics

Set of stiff Ordinary Differential Equations to be solved

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

- Here λ_i and σ_i are respectively the total decay constant and cross-section for reactions on nuclide i
- \bullet 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_{ii} is the constant for the decay of nuclide j to nuclide i

- 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
	- **I** 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

7

- n-tendl-2014 (2013), multi temperature, 709 groups library; 2632 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, 709 groups libraries; circa 400 targets each
- g-tendl-2013, 162 groups xs library, 2629 targets
- p-tendl-2013, 162 groups xs library, 2629 targets
- d-tendl-2013, 162 groups xs library, 2629 targets
- a-tendl-2013, 162 groups xs library, 2629 targets

- \checkmark Decay-2012, 3873 isotopes (23 decay modes; 7 single and 16 multi-particle ones)
- \checkmark Ingestion and inhalation, clearance and transport indices libraries, 3873 isotopes
- \checkmark JEFF-3.1.1 DD and FY, UKFY4.2 fission yields, GEF
- \checkmark ENDF/B-VII.1 DD and FY (??)
- \checkmark JENDL FPD/FPY (??) 2011
- \checkmark EAF-2010 decay data: 2233 isotopes
- \checkmark EAF-2010 ingestion and inhalation, clearance and transport indices libraries, 2233 isotopes
	- \checkmark EAF's uncertainty files
- Decay-2015, at the assemblage level

FISPACT-II versus FISPACT-2007

EASY-II &TENDL & ENDF/B-VII, JENDL-4.0, JEFF-3.2

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 \triangleright For all targets nuclei, incident particles and daughters

- Cross sections, angular distribution, emitted spectra
- Half life, masse, energy levels and schemes
- Decay schemes and energies
- Spontaneous, induced fission yields (single/cumulative)
- Resonance Integrals, Maxwellian, thermal
- Correlated uncertainty
- Spallation products
- Inhalation, ingestion hazards
- Transport, clearance indices

14 MeV neutrons are generated by a 2 mA deuteron beam impinging on a stationary tritium bearing titanium target; Fusion Neutron Source

FNS Neutron spectra, neutron fluence monitored by 27 Al(n, \imed{math})Na²⁴

Two experimental campaigns: 1996 and 2000; 74 materials

Table 1: Irradiated sample materials

Decay power: FNS JAERI Ni

Decay power: FNS JAERI Ni Decay heat validation

Decay power simulation with EASY-II

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 CULHAM CENTREZ M.R. Gilbert & J.-Ch. Sublet CCFE-R(14)21 JAEA FNS Decay heat validation
FUSION ENERGYS M. R. Gilbert et al., "Inventory Visualisation techniques" Nucl. Sci. Eng (2014)

Thermal ²³⁵U pulse generates a large inventory...

Time after irradiation (s)

Fission decay heat TAGS

Blue = Greenwood nuclides and WPEC SG 25 P1, P2, P3 are priority 1, 2, 3 nuclides with requested TAGS by subgroup 25

- Selection of experiments usually used in validation of decay heat simulations
- Tobias is meta-analysis with exp from 1950s onward and modification of uncertainties to make fits

- Many fission decay heat experiments
- Different fission rate calculation methodologies
- Many nuclides: U235, U238, Pu239, Pu241, Th232, Np237
- Even more experimental fluxes ORNL 'thermal flux' \neq Karlrushe 'thermal flux' \neq LANL 'thermal flux' \neq ...
- Even more irradiation schedules
	- **Dickens 1 s irrad followed by 2 s waiting**
	- Akiyama 10 s irrad followed by 6 s waiting
	- Karlrushe 200 s irrad followed by 15 s waiting
- 'Correction factors' in experiments to get burst function, fission rate normalisation, capture correction, epithermal contribution …

• Each major library contains different sets of nuclides within decay sub-libraries, nFY and sFY

- nFY is function of incident neutron energy
	- ! Number of bins and placement chosen for simple applications
	- ! 3 nFY incident-energies *will not be sufficient* for more demanding analysis
- How do we obtain high-fidelity fine-grid nFY(E)??

- nFY in calculations are cumulative over 1ms pulse and thermal with mono-energetic 0.025 eV
- To focus on decays **all nFY data here = JEFF3.1.1 nFY**
- Calculations employ cumulative fission yields and are *necessarily "contaminated" with the decay data used*
- Small differences in decays of precursors can dramatically affect longer-term decays and heat
- **Future work**: will consider single fission event calculations to probe short timescale affects not possible in cumulative

Decay heat following a pulse of thermal neutrons

- All measurements shown. Under-estimation of gammas consistently
- Potential contamination from capture events and chain fissile decays!!

• Better agreement with JENDL-4 and ENDF/B-VII for **gamma**

- Below are the dominant nuclides and their *gamma* heat contribution at 250s after pulse for 241 Pu_{th} in kW (normalised relative to ENDF/B-VII)
- The Tc nuclides are very different for JEFF-3.1.1dd!
- Non-negligible Cs140 and Sb133 increases for JENDL

- Below are the dominant nuclides and their *beta* heat contribution at 250s after pulse for 241 Pu_{th} in kW
- Sb133 beta same while gamma different for JENDL?
- Tc differences reflected in beta as well

- 250s after pulse for $^{241}Pu_{th}$ in kW (x10 vs previous slides)
- Typically gamma +/- is reflected in beta -/+ *but not all!*
- Total should add, but sometimes do not
- The more nuclides considered, the more differences found!

• Compared against Tobias U235 thermal pulse compilation

- Comparison with gamma heat shows clear discrepancies
- *Nota bene* No Lowell data in Tobias for short time-scales, Tobias overestimates below 100s
- <20 s Generally larger uncertainties with fewer measurements and more corrections/modifications

- C/C comparisons
- Below are the dominant nuclides and their *gamma* heat contribution at 4s after pulse for $235U_{th}$ in kW
- JENDL Rb94, Y96, Nb102m \leftrightarrow Nb102 (all have both)

- Below are the dominant nuclides and their *beta* heat contribution at 4s after pulse for $235U_{th}$ in kW
- JENDL: Y96 reallocated to gamma and Nb102(m) switch
- Rb94 differences but suspiciously little Rb92 difference

- Comparison with gamma shows clear discrepancies
- *Nota bene* again no Lowell data included in Tobias
- Better simulation with TAGS results, recently added in JENDL 4.0 and ENDF/B-VII.1, not JEFF-3.1.1 decay files !!

Dominant nuclide heat production for 239 Pu_{th}

- Below are the dominant nuclides and their *gamma* heat contribution at 800s after pulse for $239Pu_{th}$ in kW
- Again Tc 104/5 different feeding for JEFF-3.1.1
- Sr93 jumps by 30% between ENDF and JENDL

Dominant nuclide heat production for $239Pu_{th}$

- Below are the dominant nuclides nuclides and their *beta* heat contribution at 800s after pulse for $239Pu_{th}$ in kW
- Tc differences reflected in beta
- Suspiciously little difference in Sr93 beta, given gamma

- All fast fission results from YAYOI reactor by Akiyama *et al*
- Simulation using 400 keV pulse to access fast fission nFY
- Below are MeV/fission of ²³⁸U_f pulse gamma and C/E
- Discrepancies after \sim 2 hours (\sim 1E4s) may be outside error?
	- ! No TAGS made for this time-period

Gamma discrepancies in fast fission vs Akiyama

- These are **gamma** C/E
- Other fast fission data shows similar disagreements
- Mainly due to beta/gamma (mis)allocation

0.86

100

1.08

1.06

 1.04

1.02

 0.98

0.96 0.94

 0.92

 0.9

 0.88

C/E Gamma Decay Heat

• JEFF-3.1.1dd missing TAGS

1000

 $Time(s)$

Akivama uncertainty

IENDL4

10000

- Decay data application (nuclear fuel) responsible for purposeful and systematic overestimation in *e.g.* ANSI/ ANS-5.1
- Discrepancies between simulations with different dd show data is not accurate enough for sophisticated applications
- Uncanny agreement in γ , β and total heat values where individual nuclide contributions are substantially different
- Cumulative nFY should be re-examined to ensure no contamination with incomplete decay data
- Decay heat experiments are filled with complexity and care must be taken when making comparisons with simulations

- FISPACT-II capabilities:
	- ! Can calculate based on arbitrary pulses and longer irradiations
	- ! Any ENDF-6 formatted library can be used for calculations
	- \blacksquare Full uncertainty treatment $-$ if given by the data
	- **Handles arbitrary combination of nFY and sFY, DD**
	- **Tracking heat contributions and pathways for nuclide production**
- EASY-II with TENDL (or other capable library) has the ability to use fission yields of arbitrary incident neutron energy
	- ! Potentially required for correct beta feeding (and emitted neutrino spectrum)

- Are decay files 'evaluated' averages or are the averages calculated from the decay schemes??
-
- Appropriate decay scheme
- How to account and compensate for missing levels
- Decay data for isomers?

- High energy gamma lines transport further
- Low energy beta equates high energy anti-neutrino
- Missing gamma lines impact on doses

Questions

21st century multi-particle/system inventory code package for stockpile, fuel cycle stewardship, source terms, materials characterization and life cycle management for:

- Magnetic and inertial confinement fusion
- Fission Gen II, III+, IV plants and piles
- High energy and accelerator physics
- Medical applications, isotope production
- Earth exploration, Astrophysics
- Homeland security, material sciences
- \bullet
- Able to access rich, multifaceted nuclear data forms and their uncertainties.

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

