

FISPACT-II: AN ADVANCED SIMULATION PLATFORM FOR INVENTORY AND NUCLEAR OBSERVABLES

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ABSTRACT

The inventory code FISPACT-II, when connected to the nuclear data libraries TENDL-2014, ENDF/B-VII.1, JENDL-4.0u or JEFF-3.2, forms a simulation platform for modeling activation, transmutation processes and simulating radiation damage sources terms. The system has extended nuclear data forms which have been the subject of recent validation efforts including inventory simulations, fission and fusion decay heat. Summaries of key findings are presented and comments are made on the major nuclear data libraries.

Key Words: **Nuclear Data, Inventory evolution, Bateman equations, Nuclear observables, ODE solver**

1. INTRODUCTION

Knowledge of the nuclide inventory of fission fuels and fusion reactor materials is essential for many applications. Depending on the time-scales involved, these range in fission from fuel/cladding behaviour and loss-of-coolant accidents (LOCAs) to waste classification and decommissioning processes. For fusion, these data are required for a variety of aspects including operation, maintenance planning, sensitive equipment damage and decommissioning.

The challenges for fusion are tremendous: higher-energy neutron reactions, an inability to pre-select the reaction channels of importance and limited nuclear data (of sufficient quality) has necessitated the creation of technological simulation tools which handle *all* nuclides, decays, reaction channels and tracks them with a code system designed to be as general-purpose and flexible as possible. This challenge has resulted in a powerful, modern code; FISPACT-II, which can access any ENDF-6 formatted nuclear data and generates a variety of un-engineered¹ outputs.

The advantage of FISPACT-II is that it is not burdened by the compensations and restrictions of legacy codes. The ability to access any nuclear data and follow any target/reaction/decay on some 2632 targets

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¹As compared with industry-standard codes which (as is proper) include many compensations to ensure accurate results irrespective of limitations in nuclear data, technological barriers or lack of physics knowledge.

and 3875 radionuclides (including all known isomeric states) allows FISPACT-II to simulate outside the proverbial box: fixed fissile systems, limited fission yields and/or reactions on the products, restrictions on incident particles, energies, emitted data, targets, decay chains and of course fixed nuclear data.

To build confidence in a relatively new, modern code verification and validation is required. This has been the subject of considerable effort at the UK Atomic Energy Authority, resulting in a variety of V&V reports of which fission and fusion heat and inventory simulations are discussed in this paper.

2. FISPACT-II

FISPACT-II [1] is a completely new inventory code – designed, written, tested and verified over a period of five years. It is written in object-style Fortran-95, using dynamical memory allocation and so may be readily adapted to any energy group structures. FISPACT-II currently works with every major ENDF-6 formatted nuclear data library (see below). It contains four major subsystems:

1. Extraction, reduction, manipulation and storage of nuclear and radiological data forms from the nuclear data library files, including cross sections, recoil spectra, and discrete decays lines.
2. Construction and solution of the rate equations to determine the time evolution of the inventory under different irradiation scenarios. These scenarios can include single or multiple irradiation pulses with arbitrary spectra/duration/particles, as well as multi incident-particle simulations.
3. Computation and output of derived primary and secondary radiological quantities.
4. Subsidiary calculations to identify the key reaction and decay reaction chains, together with the associated quantification and propagation of uncertainties. This subsystem also includes the ability to consider reduced model calculations and to perform Monte-Carlo sensitivity calculations in combination with library substitutions.

3. NUCLEAR DATA LIBRARIES

The new code system has benefited from the maturation of modern nuclear data libraries, now expected to include a full set of variance-covariance information and the amalgamation of the capabilities of the most recent release of three processing codes PREPRO, NJOY and CALENDF. Although the nuclear data forms available to the FISPACT-II inventory code are complete and complex in nature they mainly rely on an ENDF-6 format frame structure and this tremendously simplifies all further utilitarian operations such as plotting, comparison, concatenation and data manipulation in general. The nuclear data forms encompass group cross-sections (fine 660 groups below 30 MeV), resonance parameters with covariance, probability tables, recoil daughter and emitted particle spectra matrices, spontaneous and particle-induced fission yields, and decay data, as well as biological, clearance and transport indices. The libraries available within the FISPACT-II platform are:

- **ENDF/B-VII.1** [2] American library containing nFY and decay files
- **JENDL-4.0u** [3] Japanese library containing nFY and decay files

- **JEFF-3.2/3.1.1** [4] European library containing nFY and decay files
- **TENDL-2014** [5, 6] General-purpose libraries for 5 incident particles and all targets with $t_{1/2} > 1$ s. Produced with the T6, TALYS-based code package [7].
- **GEFY-4.2**[8, 9] Centre d'études nucléaires de Bordeaux Gradignan GEF-based fission-fragment yield library, where each file includes data for 49 incident energies from 0.0253 eV to 20 MeV.
- **UKDD-12** UKAEA decay data file built from EAF-2007 decay data [10] with inclusion of some updates and an increased set of short-lived nuclides to cover further TENDL daughter nuclides

Table I. Overview of the number of nuclides which have files within each nuclear data library.

Library	n-Incident	Decay	nFY	sFY
TENDL-14	2632	—	—	—
GEFY-4.2	—	—	119	109
UKDD-12	—	3875	—	—
ENDF/B-VII.1	423	3818	31	9
JENDL-4.0u	406	1380	31	9
JEFF-3.2/3.1.1	472	3854	19	3

4. VERIFICATION AND VALIDATION

A unique assortment of verification and validation efforts have been undertaken for FISPACT-II, using both fission [11] and fusion [12] decay heat experiments, integro-differential verification of the nuclear data used for a variety of neutron spectra [13], astrophysical Maxwellian-averaged cross-sections with fully broadened/collapsed data [14] and a combination of statistical and non-threshold verifications for the integrated nuclear data [15].

4.1. Fission Decay Heat and Inventory Predictions

Decay heat and inventory calculations for irradiated fission fuels are two of the most essential capabilities for a code such as FISPACT-II. A comprehensive World review of fission pulse and finite-irradiation experiments was performed and simulations using all nuclear data permutations were performed to validate the code and data against decay heat results from thermal and fast fission of $^{233,235,238}\text{U}$, $^{239,241}\text{Pu}$, ^{232}Th and ^{237}Np . The measurements were taken from the labs of eight countries, including several different measurement techniques for both spectroscopic and calorimetric heat, with irradiations and cooling times ranging from fractions of a second to over one year.

The results for a few of the simulations are shown in Figure 1. The agreement between the simulations and experimental results are generally good, but fairly large variation between simulations with different nuclear data libraries is apparent for both specific nuclides, cooling times and for the β/γ decay

heat apportionment. While the last is due largely to the well-known Pandemonium effect², the adoption of decay data taking advantage of recent (and not-so recent) TAGS measurements is not uniform amongst the major libraries.

To better probe the origin of these various discrepancies, FISPACT-II was used to compare specific heat contributions from each inventory component for each fissile at various cooling times. By fixing the fission yield data and comparing results with different decay data (or fixing decay and varying nFY), ratios against the reference indicate the variation in the files which matter to the observable in question, fission decay heat.

4.1.1. Comments on ²³⁵U

These are the most numerous in experiments and total heat measurements are generally in good agreement for pulse and longer irradiations. Scatter in experimental results remains somewhat problematic, particularly around 10 s and 1000 s cooling. The mixing of datasets within statistical meta-analyses is essential for industry standards such as the ANSI/ANS-5.1 decay heat standard, Tobias standard and others. It should be noted that these unfortunately absorb all of the systematic errors in the experimental methods employed, which should be of particular concern for the Tobias data which draws from experiments over nearly 40 years. Some effort may be made to eliminate outliers or re-evaluate experimental errors, but this is not a substitute for superior experiments.

The lack of TAGS-related decay data β/γ corrections within JEFF-3.1.1 and the (largely built from JEFF decay files) UKDD-12 results in considerable over-prediction of beta heat for many cooling times and under-prediction of gamma. This can be seen in virtually all comparisons with experiment over any irradiation duration. Particularly large discrepancies between libraries exist for the first 200 s cooling, which were probed by performing inventory comparisons with different libraries. While more details and specific inventories are provided in the report and its supplements, the major heat contributors such as ^{92,93}Rb have large differences depending on TAGS adoption and other significant nuclides such as ¹⁴¹Cs, ^{144,145}La, ¹⁴⁹Ce (and many others) show large differences between libraries which have adopted new data. Disagreement in isomeric productions, for example with ^{102,102m}Nb, also generate non-negligible partial heat differences.

4.1.2. Comments on ²³⁹Pu

In many respects similar to ²³⁵U, ²³⁹Pu shows generally good agreement between total heat experiments and simulation, except for around 2-10 s cooling where the standard compilation data gives a 10% higher result. A smaller discrepancy is also found around 1000-2000 s cooling. While the former is not common to other experiments, the latter appears to be a confirmed difference between simulations with all data libraries and all experiments considered.

As with ²³⁵U, incomplete adoption of TAGS data and some differences in implementation have resulted in non-negligible gamma heat under-predictions and beta heat over-predictions – particularly

²Incomplete knowledge of high-energy, low-probability gamma decays (generally due to limitations of HPGe detectors) has resulted in incorrectly low average gamma energy per decay for many nuclides. This results in over-allocation to beta heat and inaccuracies in local heating within simulations. International effort to correct these has been ongoing for more than two decades, but the analysis is challenging and data trickles slowly into decay files.

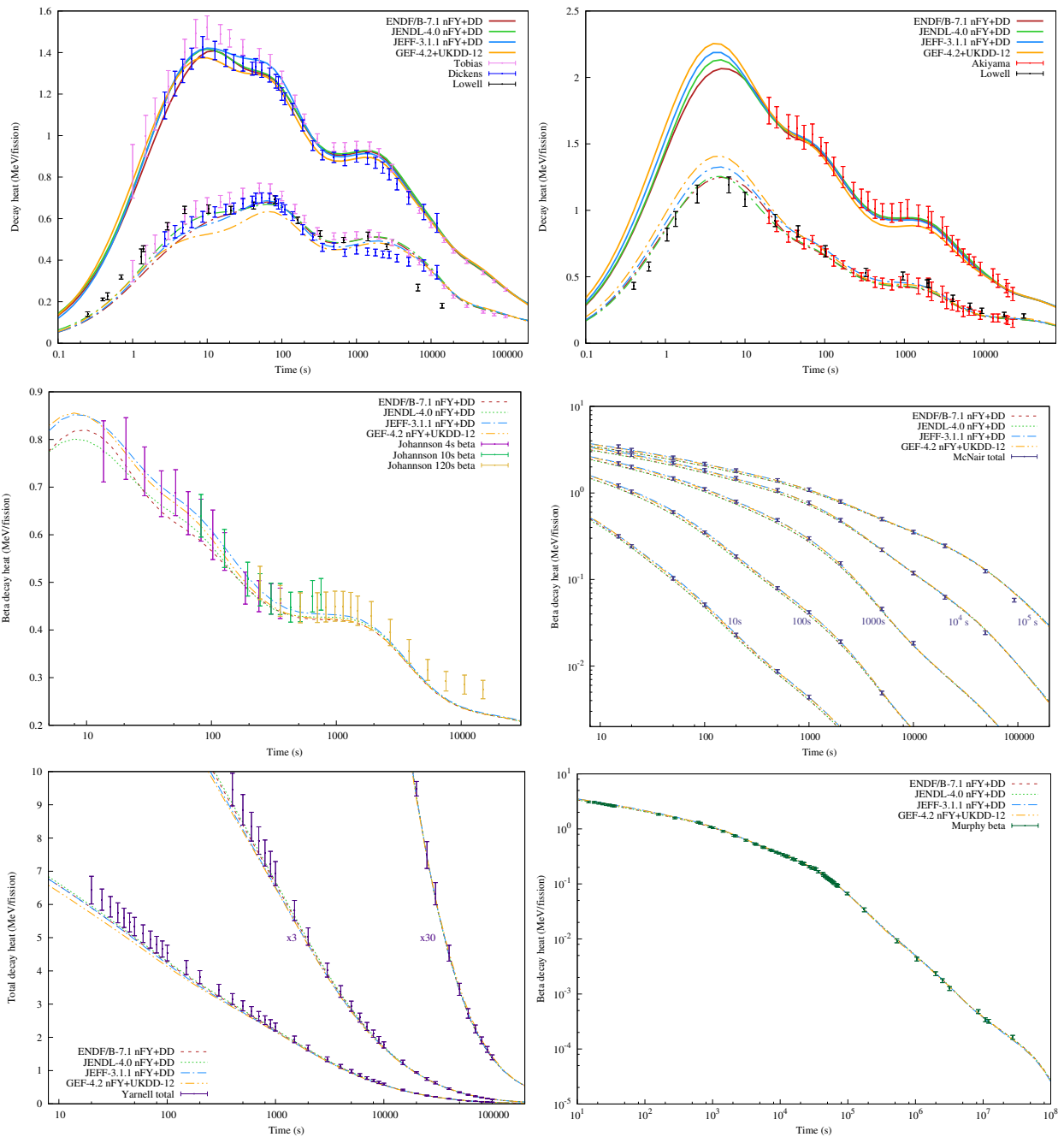


Figure 1. Example figures from [11] showing FISPACT-II simulations using various nuclear data for (read left to right): (1) ^{235}U thermal fission pulse total and gamma heat against ORNL Dickens, UM Lowell and Tobias compilation data, (2) total and beta heat from ^{238}U fast pulse against JAEA YAYOI reactor and UM Lowell data, (3) various thermal irradiations of ^{235}U from Studsvik beta decay heat, (4) beta heat from 10-10⁵ s irradiations from the UK AWRE Herald reactor of ^{239}Pu , (5) calorimetric measurements of ^{233}U irradiation for 2×10^4 s from LANL and (6) beta heat from ^{239}Pu irradiation for 10⁵ s at UKAEA Zebra fast reactor.

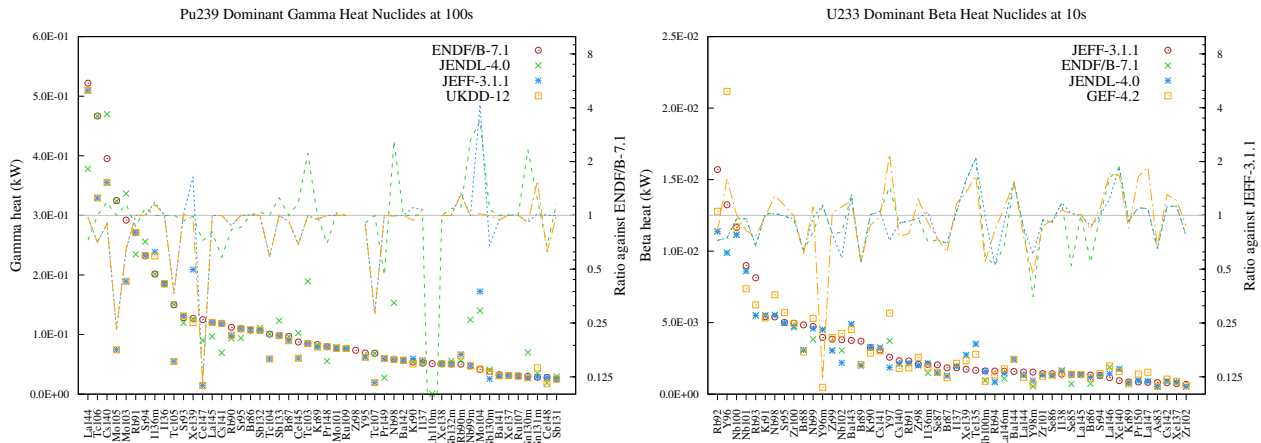


Figure 2. Nuclear data comparisons made using FISPACT-II simulations with varied nuclear data. **Left:** comparison of ^{239}Pu thermal gamma heat by nuclide with various decay data libraries and ENDF/B-VII.1 reference. **Right:** comparison of ^{233}U fast beta heat by nuclide with various nFY libraries and JEFF-3.1.1 reference.

with JEFF-3.1.1 and UKDD-12.

4.1.3. Comments on ^{238}U

Only a handful of fast fission pulse experiments are available for comparison. While for cooling times greater than 10 s both the UM Lowell and JAEA YAYOI data shows very good agreement with simulation, large differences between simulations with varied nuclear data appear for shorter cooling times. These are reflected in both total and partial spectroscopic heat due to disagreements in the fission yield files, most notably in the $^{98,99}\text{Y}$ and $^{96,97}\text{Sr}$. It is worth noting that these are only the ‘top of the iceberg’ and that yields for nuclides with $t_{1/2} < 1$ s are generally quite scattered.

4.1.4. Comments on ^{241}Pu

^{241}Pu is another good example where total decay heat simulations are in good agreement with the experimental data from ORNL, but incomplete TAGS adoption gives low gamma heating for the JEFF-3.1.1 and UKDD-12 decay data libraries. While measurements on different nuclides are required for the various fissionable nuclides, there is considerable overlap and those new data for ^{235}U and ^{239}Pu have a considerable impact on ^{241}Pu . The GEFY-4.2 data is also responsible for significant under-prediction of the total heat between 5-100 s cooling due to disagreements in yields for multiple nuclides. Examples can be found in the report and supplements.

4.1.5. Comments on ^{232}Th and ^{233}U

As essential data for thorium fuel-cycle reactors, the decay heat knowledge for these systems have not benefited from the many dozens of high-quality experiments for U-Pu systems. The most important data compared with FISPACT-II simulations came from YAYOI fast reactor irradiations and the ^{233}U was generally in good agreement with simulations using TAGS-corrected decay data. No data with

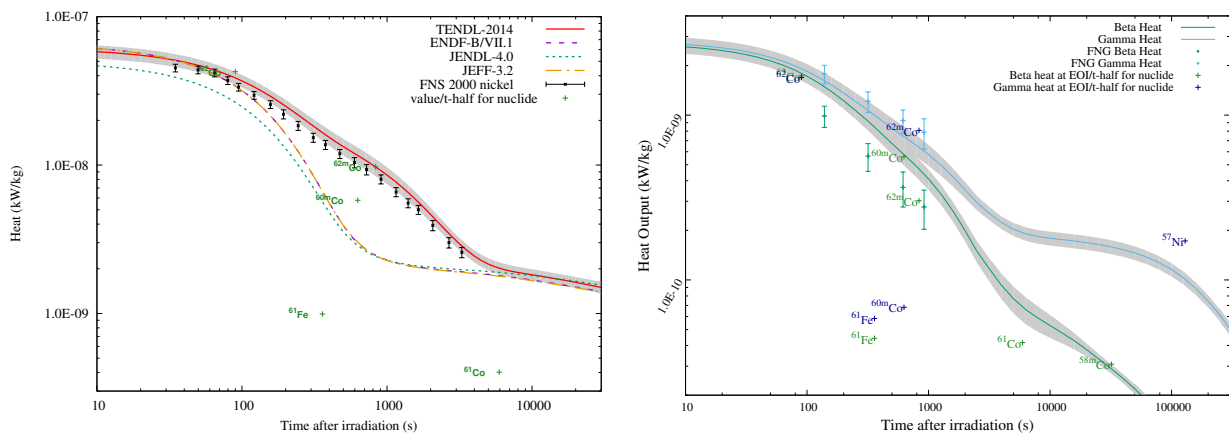


Figure 3. Comparisons of fusion D-T neutron irradiation of Ni decay heat experiments from FNS (left) and FNG (right) against simulations using TENDL-2014 and other nuclear data libraries. Note the absence of ^{62m}Co production in all but TENDL-2014, which results in a near order-of-magnitude error between 1 minute and 1 hour cooling.

corrections for the ^{233}Th capture product were available for the ^{232}Th decay heat pulse³.

Unfortunately while the decay data are largely shared by the more well-studied systems, the fission yield data are not as well-studied and comparisons between the major libraries show unfavourable discrepancies in many of the major products. It is curious that the total heat values appear to agree between libraries while the individual inventory values do not.

4.2. Fusion Decay Heat and Cross Section Predictions

Fusion devices such as magnetic-confinement plasma reactors (*e.g.* JET and ITER) produce 14 MeV neutrons when operating in D-T modes. These neutrons irradiate machine components, transmuting nuclides into unstable radionuclides and generating decay heat throughout the machine. Experimental data for applications above the fission neutron spectrum are more limited and the well-known neutron-induced data libraries are often incomplete for these energies, with missing channels, limited isomeric production and incomplete covariance data (to name a few issues). Complete files for activation studies are required, and provided by the TALYS-based TENDL-2014 libraries. Both total heat and spectroscopic heat have been the subject of measurements using neutron sources from deuteron beams into tritiated targets, such as the Japanese Fusion Neutron Source (FNS) and Italian Frascati Neutron Generator (FNG). These have been the subject of validation work using FISPACT-II and nuclear data libraries [12] including TENDL-2014, with examples shown in Figure 3. The lack of the $^{62}\text{Ni}(n,p)^{62m}\text{Co}$ isomeric production in all but the TENDL library results in a large under-prediction.

A variety of accelerator-based neutron sources using deuteron beams onto tritium, beryllium and lithium have been used to generate neutron spectra up to and above 50 MeV. A meta-validation against

³The authors are aware of figures of corrected data and have been informed by colleagues that these have been performed by Akiyama *et al*, but no tabulated data or detailed methodologies were available.

the experimental data collected from numerous campaigns has underlined the need for a technological nuclear data solution, as provided by TENDL [13].

5. DAMAGE FUNCTIONS FOR MATERIALS SCIENCE

Alongside the extensive V&V efforts for FISPACT-II, there have also been additional developments to extend the application-space of FISPACT-II beyond the traditional observables: nuclear activation, transmutation, and burn-up. One such technological advance has been the development of software routines that can calculate so-called damage source terms based on the available nuclear data and the nuclide inventory predicted by a FISPACT-II calculations. Such functions, which describe the type and energy distribution of the recoiling particles after nuclear interactions, are vital inputs for the modelling and simulation of the damage induced in materials. They provide information about the primary knock-on atoms (PKAs) that initiate the cascades of atomic displacements that produce the extended lattice defects in irradiated materials, which can have dire consequences for the performance and hence lifetimes of nuclear components.

A code, SPECTRA-PKA [16], which is part of the FISPACT-II platform, has recently been developed to read and process the recoiling and emitted (*e.g.* α -particles and protons) particle cross section matrices obtained from NJOY, collapse these with a neutron field to define PKA spectra for each reaction channel of a particular target nuclide, and combine such results for a complex nuclide inventory. Figure 4 shows the example of the time $t = 0$ result (*i.e.* before any transmutation has taken place) for SiC under the fuel-assembly-averaged neutron spectrum of a typical pressurized-water reactor (PWR) fission power plant. The same figure can also be generated as a function of irradiation times. Figure 4a shows the PKA spectra summed as a function of the recoiling nuclides, while in Figure 4b this summing has been taken one stage further to produce PKA spectra as a function of element, which is perhaps the most useful form for materials simulation where the differences in mass between isotopes of the same element are not normally considered.

6. CONCLUSION

The new and advanced features of FISPACT-II, with enhanced nuclear data forms, provide robust simulation capabilities, which can be generally applied to any nuclear system. By remaining general-purpose, code results can be used for various applications without compromising predictive power when moving between physical regimes. The utility of this approach can be seen in the fission pulse experiments, where partial gamma/beta heats are poorly simulated with legacy methods. While total heat was never badly predicted due to compensations, local heating simulations (due to difference in gamma/beta heat diffusivity) and other advanced applications (neutrinos) could not be performed with accuracy.

Experimental results covering the decays and inventory benchmarking activities from fusion and fission events are useful to probe the databases and can be used to develop simulation guidance and uncertainty quantification and propagation in decay heat and inventory predictions for all applications with the inventory code FISPACT-II and its attached libraries. The ability to read any and all nuclear data libraries, particularly the general-purpose TENDL with variance-covariance and technological GEFY fission yields, affords a unique capability to probe and contrast data in the effort to increase nuclear

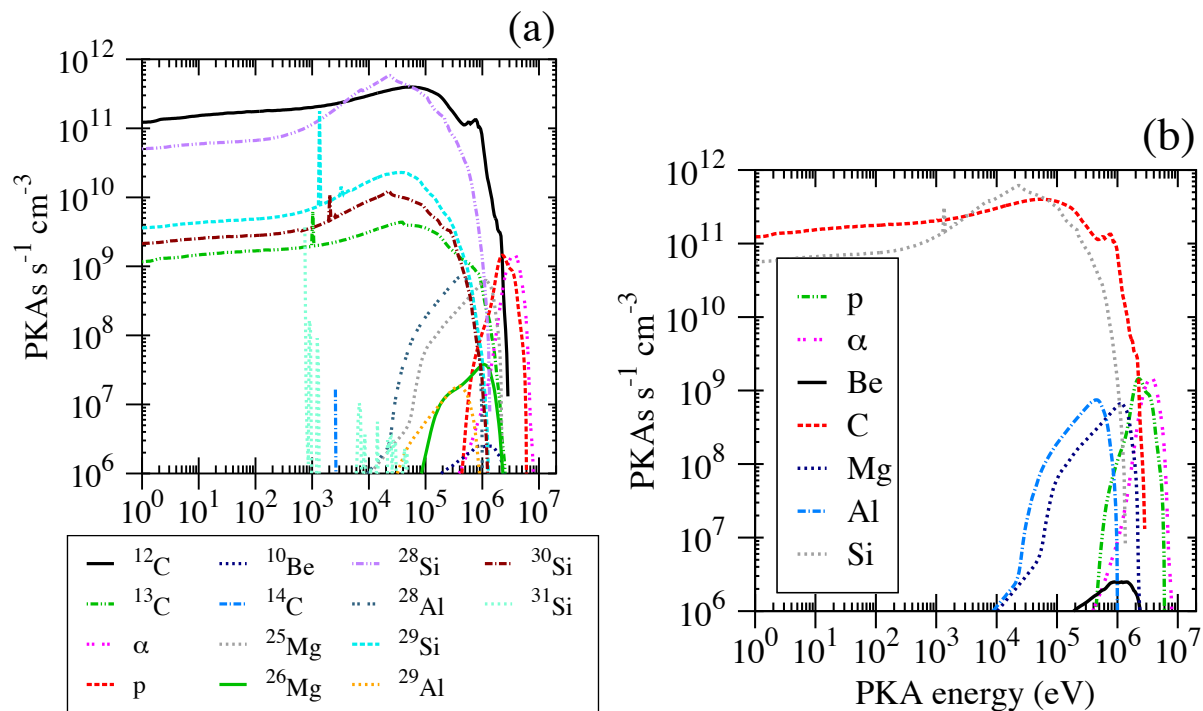


Figure 4. The (a) isotopic and (b) elemental primary knock-on atom (PKA) spectra calculated for SiC under the fuel assembly neutron spectrum of a typical PWR fission reactor using SPECTRA-PKA[16] with TENDL-2014.

data robustness for all applications. By offering the ability to probe nuclear data libraries, evaluators may target the areas of greatest need and provide analysts the tools to improve simulation accuracy.

This latest modern simulation platform is capable of meeting the present and future nuclear simulation and material science requirements in terms of activation, transmutation, depletion, burn-up, decays, source terms and inventory. It can help probe the nuclear model code capabilities away from the valley of stability, interrogate nuclear observables and provide robust simulation capabilities for all present and future applications.

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