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Technical Meeting on Nuclear Heating Theory and Data

Summary Report of an IAEA Technical Meeting

IAEA Headquarters, Vienna, Austria

19-22 April 2022

Prepared by

Marie Laure Mauborgne, Schlumberger Ltd., USA
Cedric Jouanne, CEA, France
Jean-Christophe Sublet, IAEA Nuclear Data Section

June 2022

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Objectives

The purpose of the event is to review the theory of nuclear heating, as well as the data it relies upon and their processing, usage, suitability, and appropriateness in novel and traditional applications. Prompt nuclear heating and damage, secondary radiation sources terms, are important parameters in any nuclear system or protocol, in particular in shielding, material irradiation, and earth and life sciences nuclear applications (https://conferences.iaea.org/event/260/).

The meeting is to bring together the different savant societies experts able to support the necessary enhancements, processes and data forms, foreseen for the multiple energy, non-energy, earth and life sciences applications to support high-fidelity Multiphysics simulation efforts.

Applications

Oil logging, space, agriculture, homeland security, nuclear propulsion & reactor & power, medical, interrogation technics, waste management, high energy physics

The main particles source and energy for those applications are 2, 7, 14 MeV neutron, Xray (< 400 KeV for oil and gas logging), γ flash radiography, white sources but also distributed ones in energy in the media or material, primary emitted, secondaries, and decaying.

The feedbacks from most applications to the active nuclear data communities is difficult if not inexistant, seldom at most. This is mostly due to the lack of knowledge transfer, direct, regular interaction between the communities. When non validated but verified data exists, the apathy of the established user community restrain further demands and feedbacks. The user's communities are not always capable to assess the quality, relevance of the data they often use blindly.

On the other side the active expert nuclear data community need to better promote the usage of new, better constrained, enhanced data sets and forms, capable of going beyond the legacy application & data set they provided. As the same nuclear data set is often used across many savant societies, those need to have a clear understanding of the relevance and applicability of certain of their forms to the need of their application. Not all applications are sensitive to reactor criticality simulation enhancements.

Summary

Certain applications that may be sensitive to doppler broadening, need to factor in the temperature dependence of nuclear events, mostly at low energy in the resonance ranges. For earth exploration this means up to 500K, interstellar from 10-100K, planetary like Venus around 700K, nuclear power and propulsion 350-550K, up to 2000K, superconductor technology 5K, etc.

From cradle to grave, the timescale of the nuclear events that generates heating plays an important role. If fission is a fast event, the decaying processes of the fission products will influence the time dependance of the heating response for years to come.

Burnup is an important technical factor for Spent Nuclear Fuel (SNF) decay. For spent fuel decay heat and dose, the predominant precursors for those responses vary with cooling time. At different cooling time the set of precursors evolve following their half-life. Some will decay away, while other will appear.

Simulation demonstrate that the set of decay heat precursors vary with time. After 100 years SNF cooling the minor actinides clearly become predominant. Before that timescale multiple set of a handfuls of fission products are predominant with time. The fission products ^{134}Cs and ^{137m}Ba seems to play a major role up to 35 years cooling time.

It is noticeable that very few direct measurements of the different types SNF decay heat has been made and/or are available worldwide. Those few measurements also do not overlap with the actual SNF park needs. It is also technically difficult to measure metallic fission products.

For oil logging, earth exploration rock characterization, the elemental data for capture and inelastic are needed. Using capture and inelastic allow to cover more element, differentiate between elements, and improve the statistic of the measurement. The elemental definition of rock matrix and fluid should include Si, Ca, Mg, Fe, Al, S and H, C, O, Cl. The probe is autonomous and can provide measurements during drilling. Its acquisition time need to be rapid in the seconds range but have enough counts to ensure precision. It should be noted that high energy gamma responses are more important as key signature differentiator during measurement.

The successive ENDF libraries: ENDF/B-VI, -VII, -VIII if they improved many aspects of the evaluated files, going from element to isotopic evaluation, by better constrained cross-section forms did not always fully embedded previous but thorough and validated knowledge on gamma production for particularly radiative capture.

As an example, outgoing gamma associated with the radiative capture reaction on Ca elemental in ENDF/B-VI.8 and given in MF-12/15 included gamma for thermal neutron for two continuum discreet rays at 6.4 and 4.4 MeV and for inelastic event two peaks around 8.0 MeV [1]. Those important signatures for general spectroscopy associated in fact only to the same reaction on the isotope Ca40 (97% weight), measured experimentally has unfortunately vanished in all the most recent isotopic libraries. Besides, such distinct signature also exists in the openly

available Prompt Gamma-ray Neutron Activation Analysis PGAA/EGAF databases [2] for the capture. While the compilation and dissemination of the data in the Baghdad Atlas [3] from inelastic scattering is another unique source of experimental information slowly been pushed in evaluation.

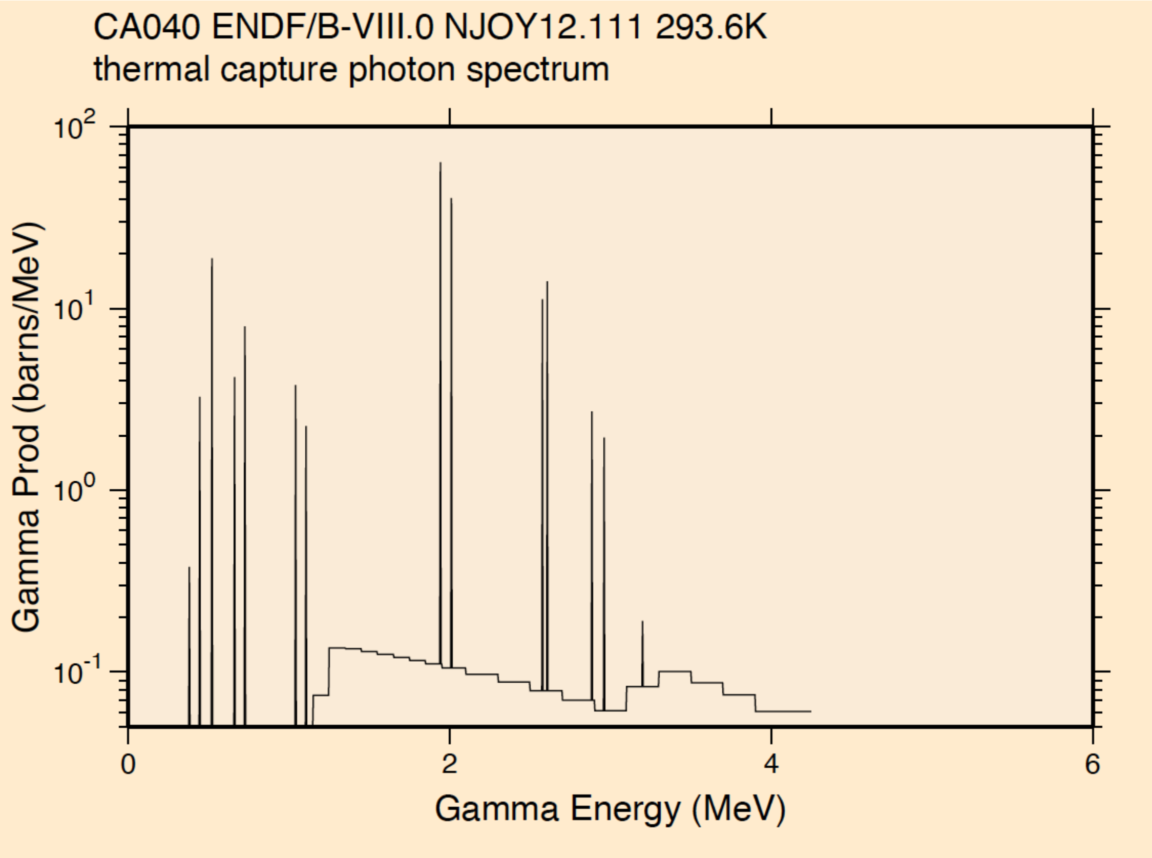

Figure 1 ENDF/B-VIII.0 Ca thermal gamma production MCNP Ace file

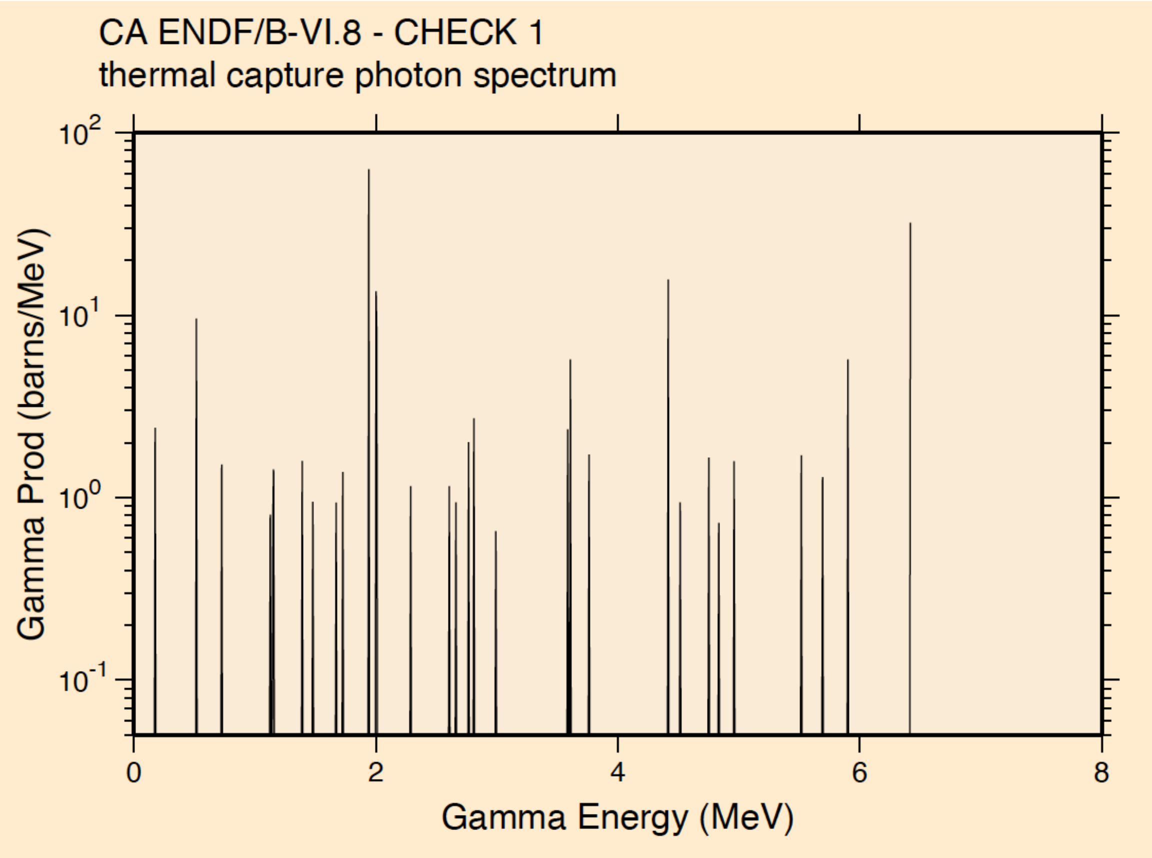

Figure 2 ENDF/B-VI.0 Ca thermal gamma production MCNP Ace file

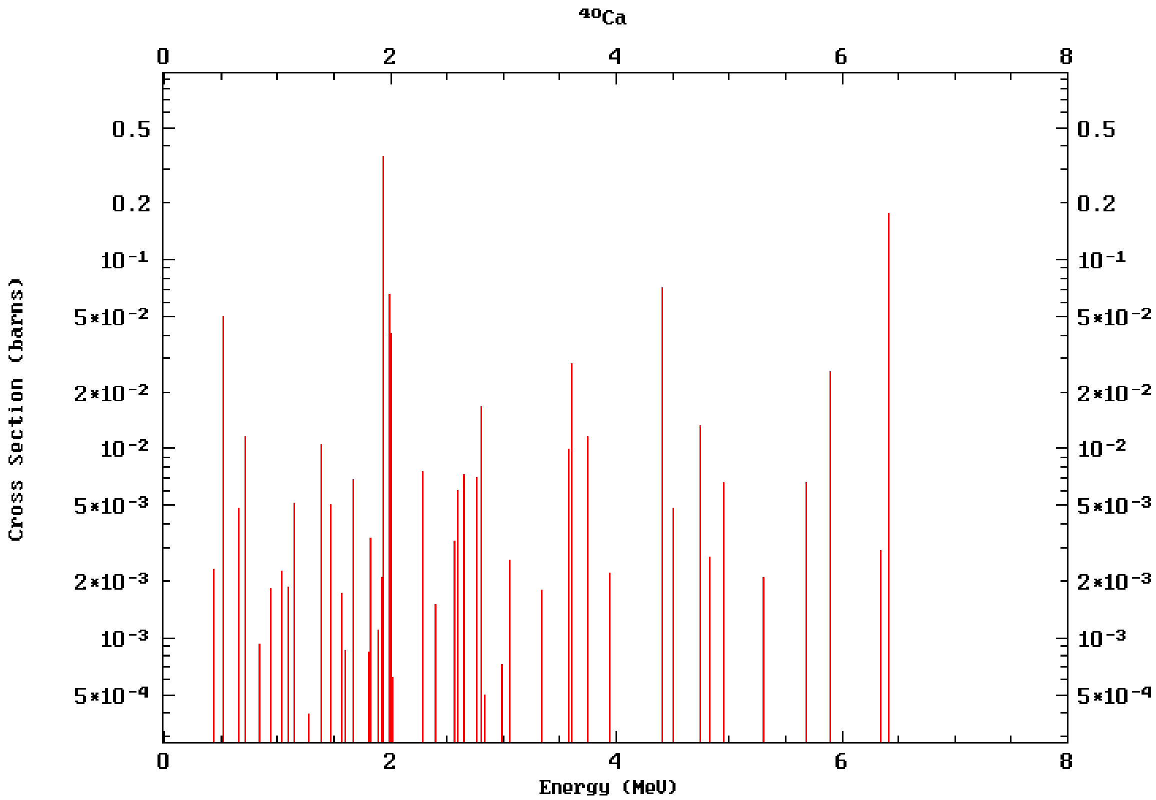

Figure 3 PGAA database Ca Gamma productions from https://www-nds.iaea.org/pgaa/pgaa7/index.html

This also could be seen in JEFF's series. For example, Ca and Mn evaluations seem to have lost a lot of information above 2.5 MeV. Such impediment certainly came during the evaluation processes from the shift of including elemental experimental gamma information to providing more physical but theoretical isotopic evaluations. With this knowledge active evaluators could easily revisit those aspects, benefit from past experiences. This in fact has already started in ENDF/B-VIII for Mn and many other in an upcoming, ongoing dedicated program.

There is a clear complicity, connivence between NJOY2016 application forms (ACE files) and the Monte Carlo code MCNP6 allowing that tandem to overcome most hurdles. This is a good way to respect the reaction kinematic of the secondary particles. Other Monte Carlo, such as TRIPOLI may run into more difficulty when relying on the ENDF's data, respecting evaluator's choice. An example could be when outgoing energy distribution is enforced as INT=22 (lin-lin unit base interpolation) by NJOY through ACER to serve MCNP when in fact given as INT=2 (lin-lin) in the evaluation. The best, physical choice been in that case is to have INT=22 in the file, a choice largely applied in the recently released JENDL-5 library.

When looking at different libraries, JEFF-4, JENDL-5, ENDF/B-VIII and TENDL-2021 there is a sometime a clear lack of completeness regarding the emitted particles outgoing data forms, that must include the gamma from many events. On that aspect TENDL-2021, and JEFF-4 by heritage, are the most complete, but carefully picked JENDL-5 or ENDF/B evaluations may still provide quality if not completeness.

A question mark remains, in the differentiation that can be made when interpreting evaluated data forms between discrete levels cascade gamma and isomeric state decaying ones. A clear difference in the event tempo (prompt, delayed and decay) and data storage needs to be made to prevent double counting in all cases.

The NJOY-20126's modules [4,5]: HEATR for Kerma heating neutron-gamma; GASPR for gas production (from explicit ENDF-6 form) and GROUPR for matrices (proton, deuteron, triton, He-3, alpha and a>4 residuals) are unique amongst all other openly available processing codes. This makes the application forms they compute also unique. An example from [6] can be given:

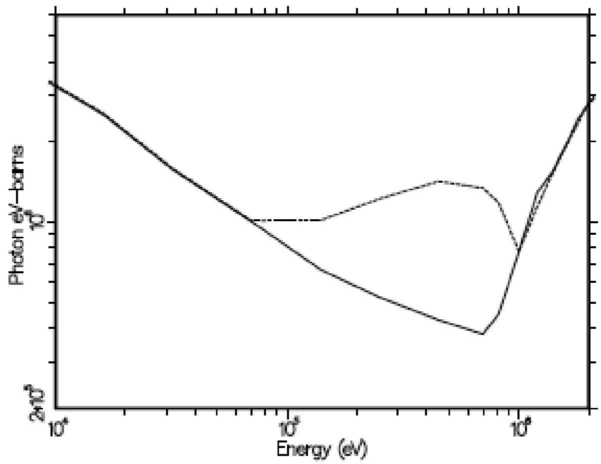

Figure 4 Computed photon energy production (dashed) compared with the kinematic value (solid) for ^{93}Nb

In Fig. 4 the original File 13 (photon production cross section) has grid points at 100 keV and 1 MeV. Interpolating across that wide bin gives a photon production rate that is much too large for energies in the vicinity of a few hundred keV. This will result in a large region of negative heating numbers. Since this is just the region of the peak flux in a fast reactor, niobium-clad regions could be cooled instead of heated!

Metastable nuclides with complete secondary distributions are increasingly more available in major libraries (513 m, 30 n in TENDL-2021), allowing for the calculation of their KERMA values. On investigation, the method by which NJOY calculates the heating for inelastic reactions is incorrectly handling the Q-values for metastable targets. It is unlikely that HEATR was originally written with such consideration in mind but a small correction in the original software could correct this mishandling.

The philosophy of Generalized Nuclear Data Structure [7] is to be particle and reaction agnostic, so as to allow the transport of any combination of particles and support of any type of reactions on all of them in the same transport simulation: multi particles in, multi particles out. GIDI+ is providing application data forms to the LLNL deterministic ARDRA and Monte Carlo MERCURY codes. For each reaction the available energy is stored: projectile kinetic energy + Q value and then for each outgoing particles its outgoing angle and energy average data forms stored in GNDS.

Event Generator Mode PHITS-EGM; sample all secondary particles from 2D sampling space at once considering energy & momentum conservation event by events. This feature can be triggered when a nuclear data library exists (JENDL, ENDF/B, JEFF and TENDL), below 20 MeV neutron-incident energy. In all events, the outgoing particles are generated by EGM while the reaction is sample from a particular library. This calculational method is analog; for each events the energy balance is fully respected. This method could lead to difference for capture heating response depending on the target nuclei, however those differences are small and will not significantly impact the energy integrated heating.

In the high energy region where many channels are open the PHITS-EGM method better allow to probe, differentiate the heating arising from all (n,p), (n,a), (n,n’), (n,np), (n,d), (n,2n), etc.

channels. However, if a particular nuclear data library does not include those reactions PHITS-EGM will not account for them.

PHITS-EGM include and evaporation model and a g-deexcite model called EBITEM. EBITEM is ENDSF-based isomeric transition and isomer production model. The nuclei are de-excited based on the scheme provided in the ENSDF database.

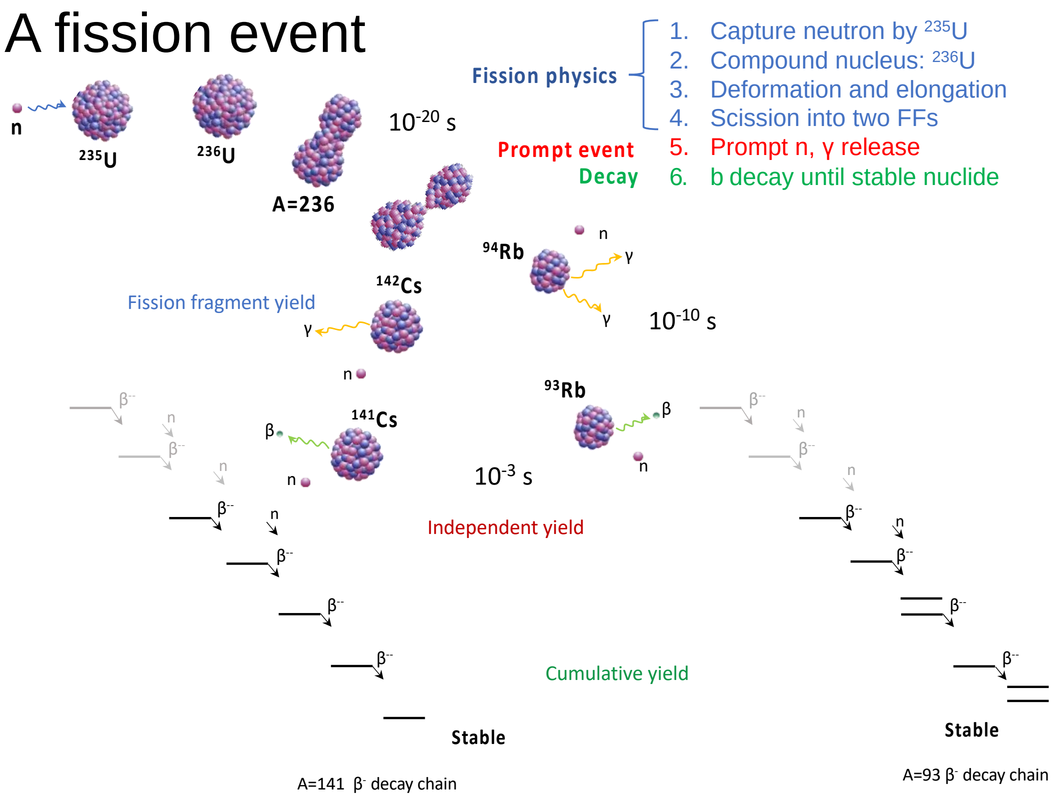

Figure 5 Decomposition of a fission event

Reactor feedback calculations require neutron flux distributions that are normalized to the specific power level of the reactor. Detailed power normalization methods rely on nuclide-specific energy release data in ENDF-format. Modern simulation code such as MC21 and Serpent propose a generalized framework for detailed energy deposition during radiation transport. Four different levels of energy deposition fidelity are proposed

- Constant eV per Fission event
- Local photon deposition
- Constant indirect energy release
- Fully coupled neutron/photon transport

Performance and conservatism push user to choose between the four above response types. However, extensive testing of such energy deposition frameworks showed unexpected results for some cases, particularly in the fast range and non-critical systems. The limitations in the

KERMA data format still prevents conservation of indirect energy release in most applications. Consideration should be given to improve the KERMA data representation in ENDF, by breaking up the data into more categories. Another feedback from those state-of-the-art simulation tools is that consistency in evaluation gives flexibility, diversity in heating response types. The subject of how to handle bremsstrahlung heating has been raised.

The remarks that materials test reactors simulation need better, more detailed data that nuclear power plant is also been made.

Recommendations

Clearly the research field, that recently benefited from serious simulation performance enhancements and acute scrutiny from diver's users, is in need of renovation. Such overall should allow to better answer the actual and next steps application needs.

Active evaluators should make the effort to account for past achievement and embed the experimental information on the detailed gamma production that have been collected. Their approach should embrace the needs of the broader non-nuclear communities, in terms of target and detailed forms, factor in the views of the non-nuclear power communities, novel applications toward what is a nuclear observable.

This subject is perfect to accommodate all evaluation projects and libraries in a unified manner, permit seamless, transparent collaboration on data, processes sharing. It allows the evaluated nuclear data forms to fit all uniformly.

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Meeting Room: CR2-C0213 (C Building, 2nd Floor)

Technical Meeting on Nuclear Heating Theory and Data (19-22 April 2022): Overview · Indico for IAEA Conferences (Indico)

Agenda

Tuesday, 19 April 2022

10:30 – 11:00	**Jean-Christophe Sublet and Arjan Koning**: Opening of the meeting; Welcome and introductions
11:00 – 12:00	Technical Discussions
12:00 – 14:00	Lunch Break
14:00 – 14:45	**Jean-Christophe Sublet:** NHtd white paper
14:45 – 15:45	**Shina Okumura**: Toward a consistent calculation of prompt and beta decay observables from fission fragment
15:45 – 16:30	**Dimitri Rochman:** Estimation of decay heat from Spent Nuclear Fuel: a PSI example
16:30 – 17:00	Discussions

Wednesday, 20 April 2022

10:00 – 12:00	Technical Discussions
12:00 – 14:00	Lunch Break
14:00 – 14:45	**Marie-Laure Mauborgne:** Missing secondary gamma ray lines in ENDF/B-VIII.0 library
14:45 – 15:45	**Cedric Jouanne:** KERMA calculation using TRIPOLI-4 and kinematics distributions of secondary particles.
15:45 – 16:30	**Jean-Christophe Sublet:** NJOY's heatr, gaspr, groupr usage, capability, and limitation
16:30 – 17:00	Discussions
18:30	Social event NENI am Prater

Thursday, 21 April 2022

10:00 – 12:00	Technical Discussions
12:00 – 14:00	Lunch Break

14:00 – 14:45	**Yosuke Iwamoto:** Comparative study of PHITS code and NJOY for recoil cross section spectra under neutron irradiation
14:45 – 15:30	**David Griesheimer:** A Generalized Framework for In-Line Energy Deposition in Monte Carlo Radiation Transport Simulations
15:30 – 16:15	**Bret Beck:** Using FUDGE and GIDI+ API to calculate energy deposition and other energy quantities
16:15 – 17:00	Discussions

Friday, 22 April 2022

10:00 – 12:00	Technical Discussions
12:00 – 14:00	Lunch Break
14:00 – 14:45	**Tim Gaines:** Neutron heating of metastables with NJOY
14:45 – 15:30	**Mark Gilbert:** Decay-heat validation of simulations with 14 MeV neutrons for fusion
15:30 – 16:00	Discussions and adjourn

Book of Abstracts

2

NJOY's heatr, gaspr, groupr usage, capability, and limitation

Author: Jean-Christophe SUBLET[1] [1]

IAEA

Corresponding Author: j.c.sublet@iaea.org

NJOY's heatr simulation of the energy-balance Kerma (kinetic energy release in material) provides a sensitive test of the consistency between the energy available from E+Q and the energy emitted as secondary neutrons and photons. The energy released by charged-particles and the recoil nucleus from an induced nuclear reaction is given by E + Q - E-bar-neutron - E-bar-gamma. Unfortunately, many nuclear evaluations are less than perfect in form and format and strange effects may occur, negative values or cooling instead of heating. In addition to computing the energy-balance heating, heatr also computes some kinematic limits that should bracket the energy-balance heating. The mod- ule prepares graphs showing the computed heating and its kinematic limits, for both neutron and photon. NJOY's gaspr extend all gas (a<4) production reactions while NJOY's groupr outputs light particle and residual production matrices. Recent applications have highlighted the needs for more detailed description of partials proton and alpha output channels while format consideration need to be carefully recognised when assembling evaluation with those same particles in the entrance channel. Added complexity occur when the material is composed of light nucleus, embedded in a compound environment or complex by nature.

3

NHtd white paper

Author: Jean-Christophe SUBLET[1] [1]

IAEA

Corresponding Author: j.c.sublet@iaea.org

The technical meeting on nuclear heating theory an data; prompt, delayed and decay radiation heat, secondary particle's energy productions and energy balance white paper describes the existent with regards to the field actual cover, capabilities, needs and challenges ahead. Heating is an important parameter in nuclear systems, particularly in unchartered R&D, while secondary radiation sources need to be better characterised, quantified, and qualified when they are required for an application. R&D is needed to support the necessary enhancements, processes, and data forms, foreseen for the multiple energy, non-energy, earth and life sciences applications and provision for high-fidelity Multiphysics simulation efforts.

4

Estimation of decay heat from Spent Nuclear Fuel: a PSI exam- ple

Author: Dimitri Rochman[1] [1]

PSI

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Spent fuel characterisation is crucial for the safe and economical handling and storage of high-level radioactive waste, such as Spent Nuclear Fuel (SNF). Among other quantities, the knowledge of SNF decay heat impacts the design of canisters and underground repository. How well do we know the SNF decay heat, through measurements and calculations? Part of the answer will be explored in this presentation, with a focus on the experience from realistic SNF decay heat calculations at PSI.

5

Missing secondary gamma ray lines in ENDF/B-VIII.0 library

Author: Marie-Laure Mauborgne[1] [1]

Schlumberger

Corresponding Author: mmauborgne@slb.com

In the oil field, exploration of the subsurface is essential to answer questions regarding the loca- tion, quantity, type, and producibility of hydrocarbons. Well logging provides measurements of the characteristics of rock formations and the fluids in their pore spaces to help identify and evaluate in- teresting reservoirs. Downhole nuclear measurements focus on formation properties such as natural radioactivity, formation density, and hydrogen content, as well as the identification of the elemental and mineralogical composition of the rock through spectroscopy using secondary gamma rays from capture and inelastic reactions.

While comparing modeling results with experimental ones, we surprisingly discovered discrepan- cies between them on a significant number of isotopes.
The recent focus on replacing tools based on radioisotopic sources with those based on DT neutron generators opens many opportunities for new measurements but highlights the deficiencies of cur- rent cross sections. Those cross sections are not of interest only for the oil and gas exploration but also for space exploration to enhance rock identification.

I will present recent results focusing on some key elements and also the improvement brought on Manganese cross section.

6

A Generalized Framework for In-Line Energy Deposition in Monte Carlo Radiation Transport Simulations

Author: David Griesheimer[1] [1] *Naval*

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Corresponding Author: david.griesheimer@unnpp.gov

A rigorous treatment of energy deposition in a Monte Carlo transport calculation, including coupled transport of all secondary and tertiary radiations, increases the computational cost of a simulation dramatically, making fully coupled heating impractical for many large calculations, such as 3-D anal- ysis of nuclear reactor cores. However, in some cases, the added benefit from a full-fidelity energy- deposition treatment is negligible, especially considering the increased simulation run time. In this presentation we discuss a generalized framework for the in-line calculation of energy deposition during Monte Carlo transport simulations. This framework gives users the ability to select among several energy-deposition approximations with varying levels of fidelity. The presentation describes the computational framework, along with derivations of four distinct energy-deposition treatments. Each treatment uses a unique set of self-consistent approximations, which ensure that energy bal- ance is preserved over the entire problem. By providing several energy-deposition treatments, each with different approximations for neglecting the energy transport of certain secondary radiations, the proposed framework provides users the flexibility to choose between accuracy and computa- tional efficiency. Challenges associated with ensuring energy balance in certain situations (e.g., qua- sistatic simulations, time-dependent simulations, and/or simulations involving coupled transport of multiple radiation types) are discussed and several unresolved issues related to energy balance are highlighted.

7

Comparative study of PHITS code and NJOY for recoil cross section spectra under neutron irradiation

Author: Yosuke Iwamoto[1]

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Because primary knock-on atoms (PKAs) create point defects and clusters in materials that are irradiated with neutrons, it is important to validate the calculations of recoil cross section spectra that are used to estimate radiation damage in materials. Here, the recoil cross section spectra of fission- and fusion relevant materials were calculated using the Event Generator Mode (EGM) of the Particle and Heavy Ion Transport code System (PHITS) and also using the data processing code NJOY2012-SPKA-6C with the nuclear data libraries TENDL2015, ENDF/BVII.1, and JEFF3.2. Heating numbers were also calculated using PHITS-EGM and compared with data extracted from the ACE files of TENDL2015, ENDF/BVII.1, and JENDL4.0. In general, the differences between the recoil cross section spectra of PHITS-TENDL2015 and NJOY-SPKA-6C-TENDL2015 were relatively small. From analyzing the recoil cross section spectra extracted from NJOY2012 + SPKA-6C, we found that the energy and angular recoil distributions for ^{72}Ge,^{75}As, ^{89}Y, and ^{109}Ag are incorrect in ENDF/B-VII.1, and those for ^{90}Zr and ^{55}Mn are incorrect in JEFF3.2. From analyzing the heating number, we found that the data in the ACE file of TENDL2015 for all nuclides are problematic in the neutron capture region because of incorrect data regarding the secondary gamma energy.Details are described in our paper [Y. Iwamoto and T. Ogawa, NIMB 396 (2017) 26-33.].

8

Neutron heating of metastables with NJOY

Author: Tim Gaines[1] [1]

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Metastable nuclides with complete secondary distributions are increasingly more available in major evaluations, allowing for the calculation of their KERMA values. When processing these metastable nuclides using NJOY's heatr module, negative total energy release values are being calculated for certain nuclides.

On investigation, the method by which NJOY calculates the heating for inelastic reactions is incorrectly handling the Q-values for metastable materials resulting in significant negative values equivalent to the metastable energy level which may be greater than the contribution from all other reactions. The cause for these values have been identified and further questions have been raised for the processing of metastable nuclides.

9

Decay-heat validation of simulations with 14 MeV neutrons for fusion

Author: Mark Gilbert[1]

Co-author: Jean-Christophe SUBLET [2]

[1] *CCFE*

[2] *IAEA*

Corresponding Authors: mark.gilbert@ukaea.uk, j.c.sublet@iaea.org

Nuclear inventory simulations have a vital role to play in the planning and execution of future fusion experiments and power plants. They are able to predict the transmutation (burn-up) of materials and also quantify their radiological response, including decay heat, by tracing the production (and decay) rates of radioactive nuclides. This information can be used to plan maintenance schedules at nuclear facilities, satisfy nuclear regulators during reactor planning, and quantify the waste disposal needs during reactor decommissioning.

The validity of inventory simulations must be verified to give confidence in the predictions. Here we describe an important experimental benchmark of decay heat measurements that test the quality of nuclear code predictions with the FISPACT-II inventory code and nuclear data libraries. The fusion (14 MeV) decay-heat measurements performed at the Japanese FNS facility, combined with detailed assessment techniques, focussed on the complex breakdown of decay-heat contributions from indi- vidual radionuclides, have been employed to compare and test results from different international nuclear data libraries.

On-load nuclear heating is also important during fusion reactor operations and is an indirect measure of the damage energy experienced by materials. We highlight the difference between fusion and fission conditions in this respect, we raises questions about the usefulness of fission irradiations to test fusion materials responses.

12

KERMA calculation using TRIPOLI-4 and kinematics distributions of secondary particles.

Author: Cedric Jouanne[1] [1] *CEA*

Saclay

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The calculation of the energies deposited by secondary particles in matter (KERMA) depends on a large amount of data: cross-sections and angular and energy distributions of the particles produced. The secondary particles can be transported or not depending on the simulation modes of the Monte Carlo codes. For the Monte Carlo code TRIPOLI-4, the particles taken into account for transport are: neutrons, photons, electrons and positrons. We will focus on neutrons and photons and explain the calculation modes of these simulated deposited energies.
In a second part, we will discuss the problems encountered with the use of recent neutron and photon transport libraries for the simulation of secondary neutron and photon.

13

Toward a consistent calculation of prompt and beta decay observ- ables from fission fragment

Authors: Arjan KONING[1]; Shin OKUMURA[1]; Kazuki FUJIO[2] [1] *IAEA*

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Accurate fission product yield (FPY) data consistent with fission observables in the evaluated nuclear data library are required for a broad range of nuclear energy applications in a wide energy range. For instance, delayed neutron yields, and gamma and beta decay energies released from the neutron-rich fission product undergoing beta decay should be consistent with the independent FPY.

In the nuclear reaction code, TALYS, a new feature to apply the Hauser-Feshbach statistical decay theory to the de-excitation of the fission fragment has been implemented by importing theoretical or phenomenological fission fragment distributions. The calculated independent FPY data are further assessed by examining beta-decay observables such as cumulative FPY, decay heat, and delayed neutron yields.

We present recent developments and calculated results by TALYS and beta-decay code.

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