

# **Technical Meeting on Nuclear Heating Theory and Data**

## **Report of Contributions**

Contribution ID: 2

Type: **not specified**

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

*Wednesday, 20 April 2022 15:45 (45 minutes)*

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  $E + Q - E_{\text{neutron}} - E_{\text{gamma}}$ . 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 module 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.

**Primary author:** Dr SUBLET, Jean-Christophe (IAEA)

**Presenter:** Dr SUBLET, Jean-Christophe (IAEA)

Contribution ID: 3

Type: **not specified**

## NHtd white paper

*Tuesday, 19 April 2022 14:00 (45 minutes)*

The technical meeting on nuclear heating theory and 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 uncharted 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.

**Primary author:** Dr SUBLET, Jean-Christophe (IAEA)

**Presenter:** Dr SUBLET, Jean-Christophe (IAEA)

Contribution ID: 4

Type: **not specified**

## Estimation of decay heat from Spent Nuclear Fuel: a PSI example

*Tuesday, 19 April 2022 15:45 (45 minutes)*

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.

**Primary author:** ROCHMAN, Dimitri (PSI)

**Presenter:** ROCHMAN, Dimitri (PSI)

Contribution ID: 5

Type: **not specified**

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

*Wednesday, 20 April 2022 14:00 (45 minutes)*

In the oil field, exploration of the subsurface is essential to answer questions regarding the location, 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 interesting 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 discrepancies 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 current 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.

**Primary author:** MAUBORGNE, Marie-Laure (Schlumberger)

**Presenter:** MAUBORGNE, Marie-Laure (Schlumberger)

Contribution ID: 6

Type: **not specified**

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

*Thursday, 21 April 2022 14:45 (45 minutes)*

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 analysis 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 balance 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 computational efficiency. Challenges associated with ensuring energy balance in certain situations (e.g., quasistatic 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.

**Primary author:** GRIESHEIMER, David (Naval Nuclear Laboratory)

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Contribution ID: 7

Type: **not specified**

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

*Thursday, 21 April 2022 14:00 (45 minutes)*

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  $^{72}\text{Ge}$ ,  $^{75}\text{As}$ ,  $^{89}\text{Y}$ , and  $^{109}\text{Ag}$  are incorrect in ENDF/B-VII.1, and those for  $^{90}\text{Zr}$  and  $^{55}\text{Mn}$  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].

**Primary author:** IWAMOTO, Yosuke (Japan Atomic Energy Agency)

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Contribution ID: 8

Type: **not specified**

## Neutron heating of metastables with NJOY

*Friday, 22 April 2022 14:00 (45 minutes)*

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.

**Primary author:** GAINES, Tim (AWE)

**Presenter:** GAINES, Tim (AWE)



Contribution ID: 9

Type: **not specified**

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

*Friday, 22 April 2022 14:45 (45 minutes)*

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 individual 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 raise questions about the usefulness of fission irradiations to test fusion materials responses.

**Primary author:** GILBERT, Mark (CCFE)

**Co-author:** SUBLET, Jean-Christophe (IAEA)

**Presenter:** GILBERT, Mark (CCFE)

Contribution ID: 12

Type: **not specified**

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

*Wednesday, 20 April 2022 14:45 (1 hour)*

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.

**Primary author:** Dr JOUANNE, Cedric (CEA Saclay)

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Contribution ID: 13

Type: **not specified**

## Toward a consistent calculation of prompt and beta decay observables from fission fragment

*Tuesday, 19 April 2022 14:45 (1 hour)*

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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**Presenter:** OKUMURA, Shin (IAEA)

Contribution ID: 14

Type: **not specified**

## **Using FUDGE and GIDI+ API to calculate energy deposition and other energy quantities**

*Thursday, 21 April 2022 15:30 (45 minutes)*

TBW

**Primary author:** Dr BECK, Bret (LLNL)

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