INL/CON-18-45015-Revision-1

The Combined Materials Experimental Toolkit (CoMET) Modern Information Management Tools for Nuclear Materials Research with NSUF

October 2018

Changing the World's Energy Future

Brenden J. Heidrich, Dain P. White, Kaecee Holden, Jordan Argyle

Idaho National Laboratory

INL is a U.S. Department of Energy National Laboratory operated by Battelle Energy Alliance, LLC

INL/CON-18-45015-Revision-1

The Combined Materials Experimental Toolkit (CoMET) Modern Information Management Tools for Nuclear Materials Research with NSUF

Brenden J. Heidrich, Dain P. White, Kaecee Holden, Jordan Argyle

October 2018

Idaho National Laboratory
Idaho Falls, Idaho 83415

http://www.inl.gov

Prepared for the
U.S. Department of Energy
Under DOE Idaho Operations Office
Contract Unknown

www.inl.gov

Idaho National Laboratory

Experiment Design with Confidence: CoMET

Jordan Argyle,[1] KaeCee Holden,[1] Shannon Hurley,[1] Kelley Verner,[1] and Brenden Heidrich[2]

[1]University of Idaho, [2]Nuclear Science User Facilities, INL

NSUF Nuclear Science User Facilities

Introduction

NSUF is developing an online expert system called the Combined Materials Experimental Toolkit (CoMET) to facilitate research project design and proposal writing. CoMET connects NSUF resource databases with proposal-writing and scoping tools, including reference material, to facilitate collaborative, informed proposal writing. Among the tools included are three scoping calculators. The first is a Neutron Damage Calculator, which estimates the material damage (DPA) incurred based on time spent in a specific reactor position. Using this irradiation time, the second, a Radioactivity Calculator, estimates the radioactivity levels and gamma dose rates of sample materials post-irradiation. The third calculator also uses output from the Neutron Damage Calculator to estimate temperatures reached within experimental capsules during irradiation. This poster will focus on these three calculators in CoMET.

Method

Multiple steps were necessary to collect the data needed for these calculators:

1. Calculate multi-group neutron flux profiles for multiple positions in test reactors available to NSUF users. MCNP models of test reactors were used to compute these flux profiles (F4 tallies).
2. Calculate displacement damage cross sections for multiple groups for chosen elements (Fig. 1). The standard tools for these calculations are SPECTER and the HEATR module of NJOY, which both use the Norgett-Robinson-Torrens (NRT) method for DPA calculations (Eq. 1 below). Both displacement energy (E_d) and available energy (E_a) were provided by SPECTER and NJOY.

Equation (1) $$DPA = \int_{E_{min}}^{E_{max}} \sigma_{disp}(E)\frac{d\Phi(E)}{dE}\,dE \text{ , where } \sigma_{disp} = \frac{0.8}{2E_d} * E_a$$

3. Calculate the capture cross-sections for the chosen elements. The RECONR module of NJOY was used for this, which uses a variety of methods described in the NJOY manual.
4. Calculate heat generation rates for each reactor position for the chosen elements. MCNP's F6 tally and NJOY's HEATR was used to compute heat generation rates for neutrons, prompt photon, and delayed photon.

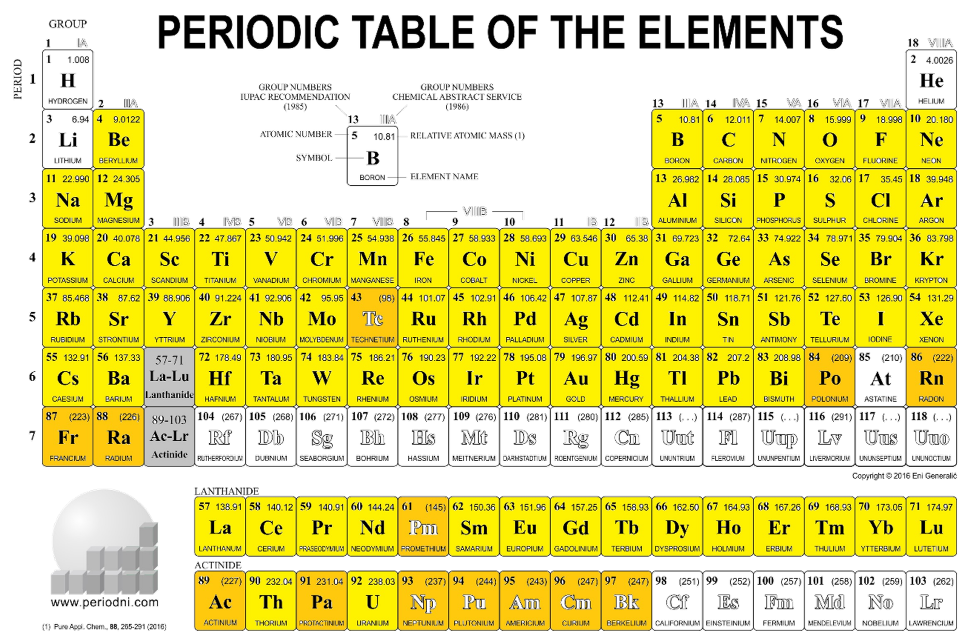

Figure 1: Elements included in the online calculator, totaling 92 elements and 760 nuclides.

Yellow: all naturally occurring isotopes plus isotopes required for activation-decay chains were included

Orange: Only those isotopes needed to complete activation-decay chains were included

White: element not included in the calculator

With data collected, the calculators can function. The process is as follows (outlined in Fig. 2):

1. The user inputs a composition and desired amount of damage (or irradiation time)
2. DPA/day was generated by Eq 1 above. Dividing the desired amount of damage by this value gives the number of days needed to reach that DPA in each reactor position.
3. Time from (2) is passed into the radioactivity calculator, which considers activation for 3 activity stages (daughter and granddaughter products, see Fig. 3). The number density for each isotope (N_x) is multiplied by decay constant (Eq. 2 below).

Equation (2) $$A_2 = \lambda_2 N_2\text{, where } N_2 = \frac{N_1\sigma_1\varphi}{\lambda_2+\sigma_2\varphi}\left[1-e^{-(\lambda_2+\sigma_2\varphi)t}\right] \text{ and } \frac{dN_2}{dt} = N_1\sigma_1\varphi - \lambda_2 N_2 - N_2\sigma_2\varphi$$

4. Heat rate/g of material was generated in step 4 above. That heat rate is multiplied by the weight fraction of each component.
5. The results are printed in a table for each reactor position available to NSUF users.

Validation

The DPA calculations were compared to accepted values in the SPECTER manual and previous work at INL. Activity was first compared to other online calculators. However, because those calculators consider only one activation stage, and due to variations in energy profile for different reactor positions, additional comparisons with previous INL work was necessary. ORIGEN and SCALE was also used to compare activation, and the decay trends match well between the new radioactivity calculator and ORIGEN (see Fig. 4 as an example). Validation for heat generation rates is currently being undertaken using experimental data from INL experiments. Generally, DPA and activity calculations compare and trend well compared to previous work and experimental data.

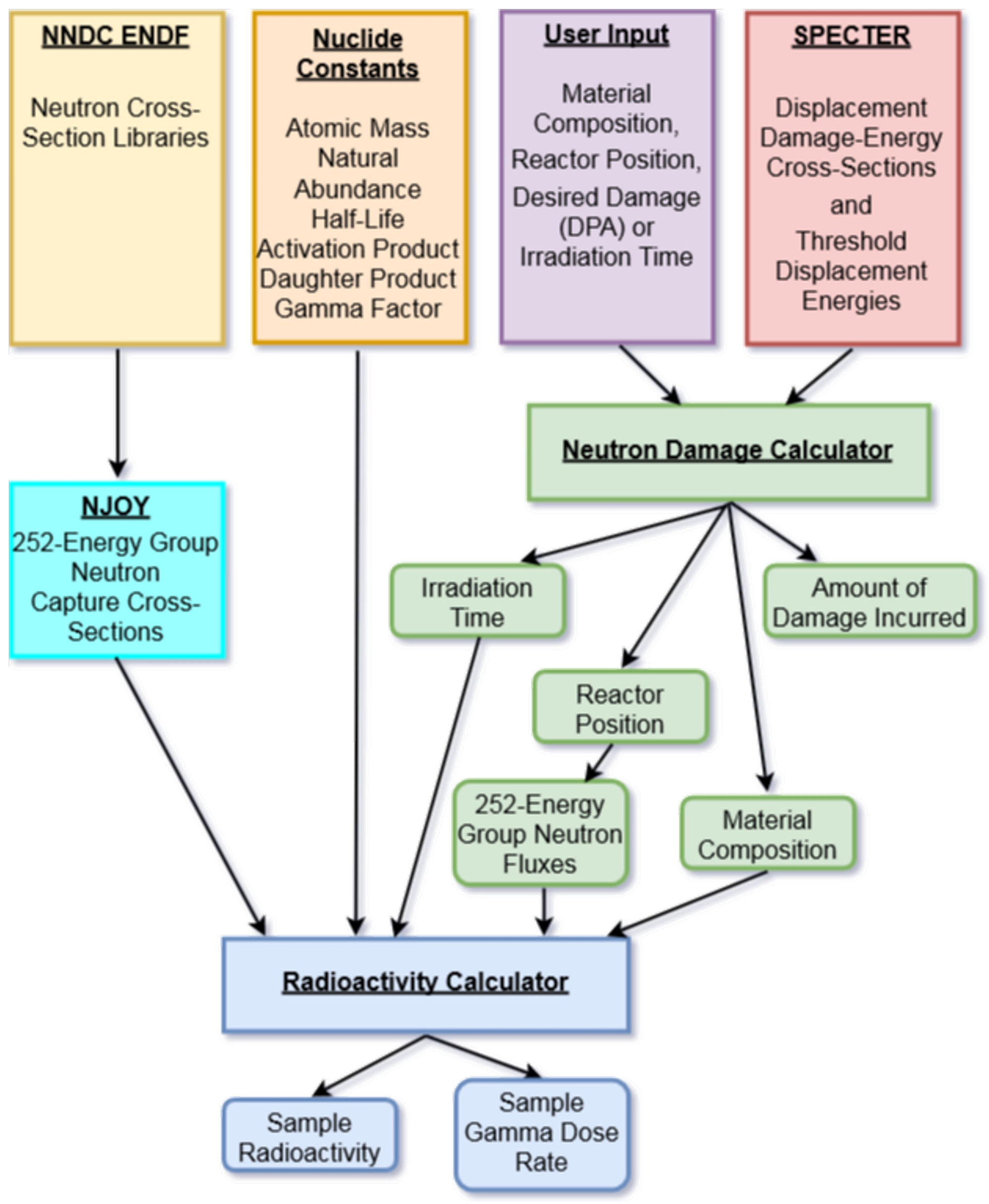

Figure 2: Data flow diagram of inputs required by and outputs from the Neutron Damage Calculator and the Radioactivity Calculator.

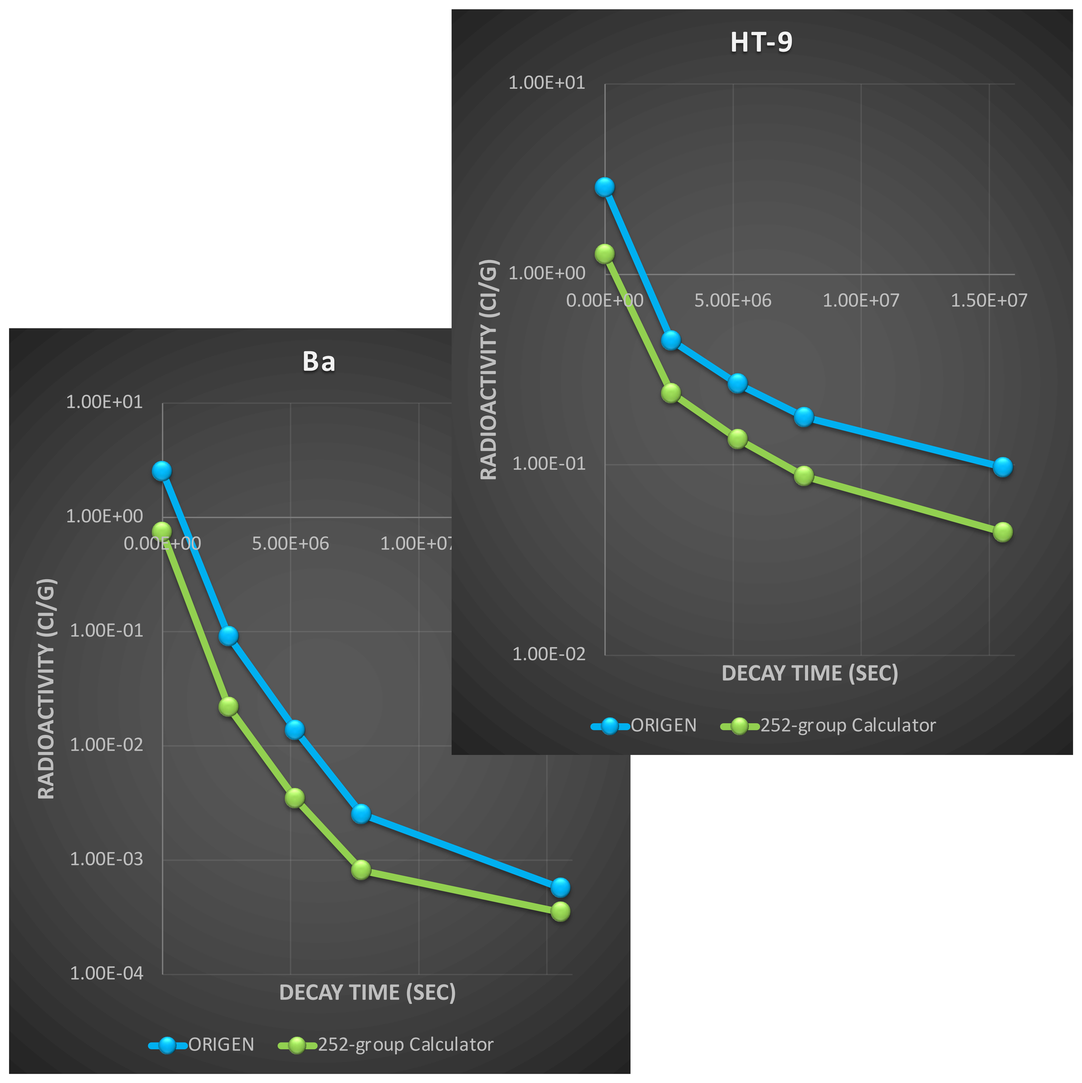

Figure 4: Decay trend comparison between ORIGEN and the 252-energy group calculator for the single element Barium and alloy HT-9.

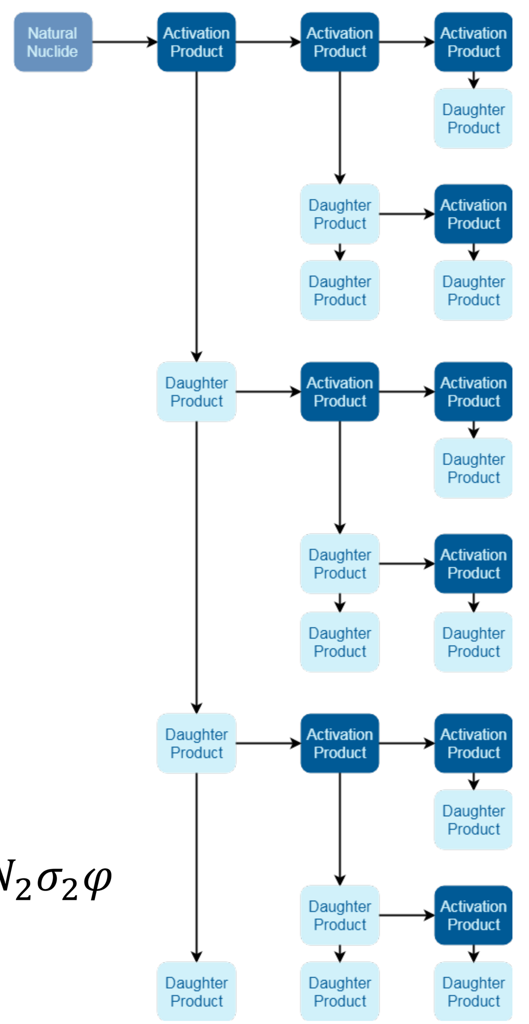

Figure 3: Activation-decay chain followed by the Radioactivity Calculator for naturally occurring nuclides.

Significance

The web-based radioactivity and neutron damage calculators provide an easily-accessible, user-friendly way for NSUF users and others to determine the feasibility of their experiments and obtain estimates for father calculations and experiment planning. Other web-based activation calculators do not have the specific flux profiles of user facility reactors, and only include one activation stage, which can miss a great deal. For example, ^{60}Co in stainless steel is a long-lived, powerful gamma emitter, and only considering the first activation stage misses four of the five activation paths (see below).

$^{59}Co \overset{\sigma}{\Rightarrow} {}^{60}Co$ - *Captured by other online calculators*

$^{58}Ni \overset{\sigma}{\Rightarrow} {}^{59}Ni \overset{\lambda}{\Rightarrow} {}^{59}Co \overset{\sigma}{\Rightarrow} {}^{60}Co$

$^{58}Fe \overset{\sigma}{\Rightarrow} {}^{59}Fe \overset{\lambda}{\Rightarrow} {}^{59}Co \overset{\sigma}{\Rightarrow} {}^{60}Co$

$^{58}Fe \overset{\sigma}{\Rightarrow} {}^{59}Fe \overset{\sigma}{\Rightarrow} {}^{60}Fe \overset{\lambda}{\Rightarrow} {}^{60}Co$

$^{57}Fe \overset{\sigma}{\Rightarrow} {}^{58}Fe \overset{\sigma}{\Rightarrow} {}^{59}Fe \overset{\sigma}{\Rightarrow} {}^{60}Fe \overset{\lambda}{\Rightarrow} {}^{60}Co$

These tools provide a considerable improvement over available online calculators, and provide reasonable estimates for data that would normally require expert analysis, empowering users and freeing up NSUF staff to provide further support to users in their proposal-writing process.