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Evaluation of the NSUF Reactor Activation and Damage (RAD) Calculator's Damage Component

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ABSTRACT

As part of the Combined Materials and Experiment Toolkit (CoMET) project, the Nuclear Science User Facilities (NSUF) developed the Reactor Activation and Damage (RAD) Calculator to be used as a general scoping tool to estimate radiation damage in terms of displacements per atom (DPA) and the resulting radioactivity of materials post-neutron irradiation. The calculator is intended to estimate experimental feasibility and be a helpful tool to scope out irradiation proposals. The damage component of the calculator estimates the DPA produced in a reactor irradiation for a limited set of known materials and guides researchers to potential irradiation facilities from the available NSUF research and test reactors. The calculator is not intended as a replacement for in-depth experimental design and dose calculations represented in the physics Engineering Calculations and Analysis Reports (ECAR). Internal validation studies were performed to compare the damage component of the calculator and a series of INL "as-run" physics ECARs for existing Advanced Test Reactor (ATR) experiments. The accuracy of the calculator was within ±50% of the DPA values in the ECARs with more than 85% of the tests being within ±20%. Based on these results, the damage component of the RAD Calculator can be deployed and expected to competently perform. Future modifications to improve the RAD calculator are recommended:

- It is recommended that, prior to the calculator being launched, a cautionary statement be created to make users aware of materials with known challenges that the calculator will not handle (e.g., fissile and fertile material are not considered).
- It is recommended for a displacement threshold energy (E_d) correction bias to be considered. (FY 2021)
- It is recommended to include aspects of thermal transmutations (e.g., Ni transmutation and the production of helium and hydrogen from the ^{58}Ni (n,α) and (n,p) reactions). (FY2021)

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TABLES

ACRONYMS

ARC-DPA	Athermal recombination corrected displacements per atom
ATR	Advanced Test Reactor
CoMET	Combined Materials and Experiment Toolkit
DPA	Displacements per atom
ECAR	Engineering Calculations and Analysis Report
EFPD	Effective full power days
ENDF	Evaluated Nuclear Data File
GENDF	Group Evaluated Nuclear Data File
INL	Idaho National Laboratory
NSUF	Nuclear Science User Facilities
PKA	Primary knock-on atom
RAD	Reactor Activation and Damage

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1. Introduction

The Nuclear Science User Facilities (NSUF) provide researchers access to nuclear research facilities and expertise all over the United States and at the Belgian Center for Nuclear Research (SCK/CEN). One special capability of the NSUF is providing access to nuclear research and test reactors often used for conducting material testing experiments. These services are provided at no cost to the researcher through a competitive, peer-reviewed process. With so many proposals being submitted simultaneously, an NSUF information management resource called the Combined Materials Experiment Toolkit (CoMET) was implemented to speed up the review process and give users access to the information and tools necessary for designing meaningful experiments and writing the best proposals possible. One of CoMET's tools is the Reactor Activation and Damage (RAD) Calculator.

For those with little or no background in it, neutron irradiation in research and test reactors can be a challenging subject to include in a proposal. That is why the RAD Calculator was created to assist users with providing estimates of irradiation and post-irradiation conditions, enabling them to select the best neutron irradiation and post-irradiation examination facilities for reaching their experiment goals. The RAD Calculator is a general scoping tool that estimates radiation damage in terms of DPA, in addition to the resulting radioactivity of the material post-irradiation. This report evaluates the neutron damage component of the RAD Calculator. The evaluation of the activation component of the calculator is covered in report INL/EXT-20-58080.

2. Background

2.1 Displacement Damage

DPA is a simple calculation when all the variables are known. Equations 1,2, and 3 show the general equation used [1]:

$$\text{DPA} = \int_0^t R_d(t`)dt` \tag{1}$$

$$R_d(t) = \int_0^\infty \sigma_d(E,t)\phi(E,t)dE \tag{2}$$

Equation 2 can be approximated as [1]:

$$R_d = \sum_{i=1}^{G} \sigma_{d,i}\phi_i \tag{3}$$

Where:

- t is the irradiation time.
- R_d is the displacement reaction rate for the material.
- σ_d is the damage pseudo-cross-section created by Norgett, Robinson, and Torrens [2].

- ϕ is the scalar flux.

2.1.1 Kinchin-Pease (K-P) Model

The above equations are derived from a method created by Norgett, Robinson, and Torrens [2] based on the Kinchin-Pease (K-P) model [3]. The K-P model is used to calculate the number of displacements that occur during the reaction of a material to an incoming particle. The equations used are as follows:

$$N_{d,x}(E) = \begin{cases} 0, & 0 < E_{R,x} < E_d \\ 1, & E_d < E_{R,x} < 2E_d \\ \dfrac{E_{R,x}}{2E_d}, & 2E_d < E_{R,x} < E_I \\ \dfrac{E_I}{2E_d}, & E_I < E_{R,x} \end{cases} \quad (4)$$

Where:

- N_d is the number of displacements caused by the primary knock-on atom (PKA).
- Index x denotes the specific nuclear reaction that occurred. This does matter, as it impacts the recoil energy of the nucleus.
- E_R is the recoil energy of the PKA.
- E is the energy of the incident neutron.
- E_I is the energy level above which the ions lose their energy solely through ionization, and below which energy loss can be modeled by plastic hard-sphere scattering.
- E_d is the average displacement threshold energy.

2.1.2 Norgett-Robinson-Torrens(NRT) Model

The Norgett-Robinson-Torrens (NRT) method proposes the use of a variable called "displacement efficiency", which is calculated to be 0.8 [2]. Equation 5 shows the NRT equation for determining the number of displacements, where κ is the 0.8 displacement efficiency:

$$N_{d,x}(E) = \frac{\kappa \widehat{E_x}(E)}{2E_d} \quad (5)$$

The energy of an incoming particle is a critical aspect of material damage since it must have enough energy to permanently displace an atom. This threshold, which the energy the incoming particle transfers to the displaced atom must exceed, is called "average displacement threshold energy" and is denoted as E_d. $\hat{E}$ is the available energy for an elastic collision to cause displacements. It is calculated via the NRT method, as seen in Equations 6–10 [2]:

$$\widehat{E_x} = \frac{E_{R,x}}{1 + kg(\epsilon)} \quad (6)$$

$$g(\epsilon) = 3.4008\epsilon^{\frac{1}{6}} + 0.40244\epsilon^{\frac{3}{4}} + \epsilon \quad (7)$$

$$k = 0.1337 Z_1^{\frac{1}{6}} \left(\frac{Z_1}{A_1}\right)^{\frac{1}{2}} \quad (8)$$

$$\epsilon = \left(\frac{A_2 E}{A_1 + A_2}\right)\left(\frac{a}{Z_1 Z_2 e^2}\right) \quad (9)$$

$$a = \left(\frac{9\pi^2}{128}\right)^{\frac{1}{3}} a_0 \left(Z_1^{\frac{2}{3}} + Z_2^{\frac{2}{3}}\right)^{-\frac{1}{2}} \quad (10)$$

Where:

- $\hat{E}$ is the damage energy: the energy available to cause displacements. It factors in things such as energy lost to ionizations without causing a displacement.
- A is the atomic mass of the PKA or target atom.
- Z is the atomic number of the PKA or target atom.
- Index 1 is for the PKA, and Index 2 is for the target atom.
- a_0 is the Bohr radius.
- e is the fundamental charge unit.

However, Jung et al. found that using the average displacement threshold energy (E_d) created inaccurate results, and so proposed to compensate for this by using effective displacement threshold energy ($E_{d,eff}$) instead. These new values are higher, on the order of 120eV versus 40eV [4]. Idaho National Laboratory (INL) currently does not use $E_{d,eff}$ values. The debate over which values to use highlights the high uncertainty in calculating DPA.

2.1.2.1 Calculating σ_d

The damage pseudo-cross-section is simply the number of caused displacements multiplied by the specific nuclear reaction cross-section, as shown in the following equation:

$$\sigma_{d,x}(E) = N_{d,x}(E)\sigma_x(E) = \frac{\sigma_x(E)\kappa\widehat{E_x}(E)}{2E_d} \quad (11)$$

However, it is more common to calculate the damage-energy-cross-section, $D_x(E)$ [eV-barns]:

$$D_x(E) = \sigma_x(E)\widehat{E_x}(E) \quad (12)$$

Combining Equations 11 and 12 is rather intuitive:

$$\sigma_{d,x}(E) = \frac{\kappa D_x(E)}{2E_d} \quad (13)$$

The total damage pseudo-cross-section is a simple sum over all reactions for Equation 13:

$$\sigma_d(E) = \sum^{\forall x \in X} \frac{\kappa D_x(E)}{2E_d}$$

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2.1.2.2 Calculating Recoil Energy

The only information now needed is the recoil energy of the PKA. This is calculated by NJOY, a nuclear data processing code, using the following [5]:

$$E_{R,x}(E,\mu) = \frac{AE}{(A+1)^2}(1 - 2R_x\mu + R_x^2)$$

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$$R_x = \sqrt{1 - \frac{(A+1)(-Q_x)}{AE}}$$

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Where:

- E is the energy of the incident neutron.
- μ is the cosine of the angle between the recoiled nucleus and the incident neutron.
- Q_x is the mass difference for the specific nuclear reaction occurring.

Using this, the average recoil energy can be calculated as:

$$\widehat{E_x}(E) = \int_{-1}^{1} f(E,\mu)\hat{E}_x\big(E_R(E,\mu)\big)d\mu$$

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Where the f function is the angular distribution of the impacted nucleus. By combining Equations 12 and 17, the damage-energy-cross-section $D_x(E)$ may be calculated as:

$$D_x(E) = \sigma_x(E) \int_{-1}^{1} f(E,\mu)\hat{E}_x\big(E_R(E,\mu)\big)d\mu$$

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2.2 Nuclear Data Discretization

Ideally, all nuclear calculations should be conducted in a continuous energy space; however, the amount of data that must be stored and operated on makes these methods cumbersome and inefficient. Therefore, the RAD Calculator uses a discrete group structure for conducting these nuclear calculations. The goal of collapsing a cross-section is ultimately to find a given reaction rate via the following equations:

$$R_{X,Y} = \int_{0}^{\infty} N_Y \sigma_{X,Y}(E)\phi(\mathrm{E})\mathrm{dE}$$

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Or:

$$R_{X,Y} = N_Y \sum_{g=1}^{G} \sigma_{X,Y,g} \phi_g$$

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Where:

- $\sigma_{X,Y}(E)$ is the continuous cross-section of interest for reaction X and isotope Y.
- $\sigma_{X,Y,g}$ is the group cross-section for reaction X, isotope Y, and group g.
- N_Y is the number density of isotope Y.

Having equal weighting for the cross-sections will mis-predict the reaction rate. This is because it will treat all dE slices equally, whether or not there is neutron flux to induce the reaction in that energy slice. Instead, the cross-section must be collapsed to preserve the reaction rate. Therefore, the following must hold:

$$\int_0^{\infty} N_Y \sigma_{X,Y}(E) \phi(E) dE = N_Y \sum_{g=1}^{G} \sigma_{X,Y,g} \phi_g$$

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An argument can then be made that, for this to hold for all energies, it must hold for all discrete groups:

$$N_Y \int_{E_{g+1}}^{E_g} \sigma_{X,Y}(E) \phi(E) dE = N_Y \sigma_{X,Y,g} \phi_g$$

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Where the group flux is defined as:

$$\phi_g \triangleq \int_{E_{g+1}}^{E_g} \phi(E) dE$$

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It then follows that the proper way to collapse a group cross-section is given in Equation 24:

$$\sigma_{X,Y,g} = \frac{\int_{E_{g+1}}^{E_g} \sigma_{X,Y}(E) \phi(E) dE}{\int_{E_{g+1}}^{E_g} \phi(E) dE}$$

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It is now apparent that, problematically enough, the flux of the system must first be known to collapse the cross-section. A simplifying assumption can be made of the flux:

$$\phi_g = c_g \int_{E_{g+1}}^{E_g} \psi_g(E) dE$$

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Where:

c_g is a constant.

ψ_g is a flux shape function that is known.

This is to say that we assume each group is a constant multiplied by a flux shape. This assumption breaks down with coarse energy groups, as the flux shape cannot be known and will be altered by the various reactions occurring. However, when the group structure is sufficiently fine enough, effects such as resonance self-shielding will not affect the flux shape for a single group, but simply that groups' amplitude. This is valid for groups roughly the size of a major resonance. The common flux shapes are a Maxwellian thermal distribution, a $\frac{1}{E}$ distribution, and a fission $[\chi(E)]$ distribution.

2.2.1 Calculating Inverse Damage Rates

With the flux and σ_D data, it is now possible to calculate inverse damage rates, i.e. the time it takes to accumulate 1 DPA of damage. For convenience, the following vectors are used:

$$\overrightarrow{\sigma_{X,Y}} \triangleq < \sigma_{X,Y,1}, \sigma_{X,Y,2}, \dots, \sigma_{X,Y,G} > \vec{\phi} \triangleq < \phi_1, \phi_2, \dots, \phi_G > \quad (26)$$

The volumetric reaction rate for an arbitrary reaction, X, is then given by:

$$R_{X,Y} = N_Y \overrightarrow{\sigma_{X,Y}} \cdot \vec{\phi} \quad (27)$$

Even though the calculator is 0-dimensional and does not consider density, dimensional analysis shows that density is unnecessary. The units are shown in brackets.

$$\overrightarrow{\sigma_{X,Y}}[L^2] \cdot \vec{\phi}\left[\frac{\#}{L^2 T}\right] = \left[\frac{\#}{T}\right] \quad (28)$$

Where:

- L represents units of length.
- T represents units of time.
- # represents a quantity.

Damage is measured in DPA. Since DPA is a dimensionless unit, the desired quantity will be in $\left[\frac{T}{\#}\right]$. Therefore, the damage inverse rate can be found by the following equation:

$$R_{D,Y}^{-1} = \frac{d}{\overrightarrow{\sigma_{D,Y}} \cdot \vec{\phi}} \quad (29)$$

Where:

- d is the unit conversion factor. It converts from barns to cm^2 and from seconds to days. This is: $1.157\overline{407} \times 10^{18}$.

3. Calculator Methodology

3.1 Calculating Displacements per Atom (DPA)

The inverse damage rate $\left[\frac{\text{days}}{\text{DPA}}\right]$ for mixed materials such as alloys is found through a weighted average. This average is weighted by the atomic ratio and not the weight ratio of the constituent elements. The atomic ratio must be calculated, as the user specifies a weight fraction for the material. Due to the DPA rate's reliance on the crystal's displacement energy, atomic number, and atomic mass, this

approximation is only valid in certain situations. For it to hold, the atomic weights and displacement threshold energies must be similar [6]. It would then break down in compounds where the bonds are different than in elemental form. For example, the displacement threshold energy for O_2 and UO_2 are quite different.

The user can either specify an irradiation length in days in the reactor, or a radiation damage target. The calculator then uses the inverse damage rate to find either the radiation damage achieved, or the time required to meet the goal radiation damage level. The inverse damage rate is found through the following weighted average:

$$\overline{R_d^{-1}} = \frac{1}{\sum_{i=1}^{I}\left(\frac{c_i}{A_i}\right)} \sum_{i=1}^{I} \frac{c_i R_{d,i}^{-1}}{A_i} \tag{30}$$

Where:

- c_i is the weight composition ratio for element/isotope i.
- A_i is the atomic mass.
- $R_{d,i}^{-1}$ is the DPA inverse rate.
- I is the total number of constituents for the material.

It then follows that:

$$DPA = \frac{t}{\overline{R_d^{-1}}} \tag{31}$$

$$t = \text{DPA} \cdot \overline{R_d^{-1}} \tag{32}$$

Where t is the irradiation time in days.

3.2 Pre-processing of Nuclear Data

The calculator stores data for the damage calculations as an inverse damage rate in $\frac{\text{days}}{\text{DPA}}$ for each element and each reactor position. To calculate this inverse rate, the following must be completed:

1. Calculate the group flux for the reactor position using the group structure given in Appendix A: 252-group structure.
2. Calculate the damage pseudo-cross-section (σ_d) using the same group structure.
3. Take the dot-product of the flux and σ_d vectors to retrieve the displacement rate.
4. Invert the rate and convert from seconds into days.

3.2.1 Calculation of Flux Distributions

Fluxes for each reactor position were calculated through MCNP6 [7] using models created by the responsible institution.

3.2.2 Calculation of the Damage Pseudo-cross-section (σ_D)

NOTE: A microscopic cross-section measures the effective cross-sectional area of the nucleus seen by a neutron or other projectile. It is not a probability, though it does impact the probability of interaction. Therefore, cross-sections are measured in barns, a unit of area. A damage pseudo-cross-section has units of displacement-barns, but since displacements are a quantity, they are really in units of barns. However, that does not mean it is a cross-section. The damage pseudo-cross-section does not

measure the surface area of a nucleus and has no direct physical correlation, like the Reynold's number, or how newton-meters-work and newton-meters-torque are not comparable. For simplicity's sake, the damage pseudo-cross-section may be referred to as sigma-D or σ_d.

The sigma-D values were calculated using NJOY21 [8], a modern nuclear data processing code. This was done automatically using the python3 script, NJOY_DPA. The sigma-D value must be calculated for each isotope separately. Therefore, the sigma-D value for an element must be calculated as the weighted average of the naturally occurring isotopes. The natural isotopic concentrations were taken from pyENDF6's implementation of Meija's report [9]. pyENDF6 is a derivate of OpenMC [10], but with all the code unrelated to reading evaluated nuclear data files (ENDFs) removed. An example input file is given in Appendix B: NJOY21 Input.

For each isotope, NJOY completes the following calculations:

1. Convert the input ENDF data from ASCII [11] (text) into binary format.
2. Reconstruct the pointwise continuous cross-sections to allow interpolation with an error tolerance of 0.1%.
3. Doppler broaden the cross-sections from 0 K to 600 K, with an error tolerance of 0.01%.
4. The total damage-energy-cross-section $[D(E)]$ is calculated in eV-barns and stored as material file (MF) = 3, and material table (MT) = 444. NJOY_DPA overrides NJOY21's internal value for displacement threshold energy (E_d) with E_d (not $E_{d,eff}$) values from Konobeyev et al. [12]
5. A copy of all the continuum data is stored to an ASCII ENDF.
6. The total damage-energy-cross-section value is then collapsed into the 252-group structure in Appendix A: 252-group structure, with a lower energy bound of 10 neV. The σ_0 value was set to 1E+10 to simulate infinite dilution. The Legendre order was set to 1, under the assumption that no strong heterogeneities are present in the sample. The collapsing flux is a combination of a Maxwellian thermal distribution, a 1/E epithermal distribution, and a fission fast distribution. The parameters are:
    a. Thermal break (transition from thermal to epithermal): 0.1eV
    b. Thermal temperature: kT, where "k" is the Boltzmann constant and "T" is the temperature in Kelvin
    c. Fission break: 820keV
    d. Fission temperature: 1.4MeV.
7. The collapsed σ_d was then written to a special ENDF called a "Group ENDF" (GENDF) in ASCII form.

NJOY_DPA then uses pyENDF6 to read in the group structure and data from the GENDF. The file contains both the damage-energy-cross-section data, and the flux data used to collapse that data. Note that this is in eV-barns. Equation 14 must then be used to calculate σ_d. NJOY_DPA does this calculation to achieve σ_d.

3.2.3 NJOY HEATR Damage Energy Calculation

NJOY21 calculates the damage-energy-cross-section [D(E)] by a modified form of the NRT model, as shown below [5]:

$$\hat{E}(E_R) = \frac{E_R}{1 + kg(\epsilon)}$$

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$$g(\epsilon) = 3.4008\epsilon^{\frac{1}{6}} + 0.40244\epsilon^{\frac{3}{4}} + \epsilon$$

$$\epsilon = \frac{E_R}{E_L}$$

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$$E_L = \frac{30.724 Z_1 Z_2 \left(Z_1^{\frac{2}{3}} + Z_2^{\frac{2}{3}}\right)^{\frac{1}{2}} (A_1 + A_2)}{A_L}$$

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$$k = \frac{0.0793 Z_1^{\frac{2}{3}} Z_2^{\frac{1}{2}} (A_1 + A_2)^{\frac{3}{2}}}{\left(Z_1^{\frac{2}{3}} + Z_2^{\frac{2}{3}}\right)^{\frac{3}{4}} A_1^{\frac{3}{2}} A_2^{\frac{1}{2}}}$$

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Where:

- E_R is the recoil energy of the PKA.
- Z is the atomic number of the PKA and the target atom.
- A is the atomic mass of the PKA and the target atom.
- Index 1 for Z and A is for the recoil atom, and Index 2 is for the target atom in the crystal lattice.

As can be seen, the $g(\epsilon)$ functions of the NRT model and NJOY's implementation are identical. Also, it is easy to become convinced that ϵ is the same for both models. However, the k function for NJOY differs from NRT, though the reason for this difference is not readily clear.

Using this information, the damage energy-cross-section $D(E)$ may be calculated by Equation 18 (reproduced here):

$$D_x(E) = \sigma_x(E) \int_{-1}^{1} f(E,\mu) \widehat{E_x}\big(E_R(E,\mu)\big) d\mu$$

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The f function is the angular distribution of the impacted nucleus. This data is provided in the ENDF/B library in (MF) = 4. NJOY21 uses a 20-point Gauss-Legendre quadrature to perform this integration [5].

3.2.4 Calculating Inverse Damage Rates

The NJOY_DPA python module is then run again, reading in flux and σ_d data from office-open XML workbooks (.xlsx) and performing the calculations in Equation 3 for every material and reactor position given. The results are then stored in a third workbook.

3.2.5 Assumptions

It is important for the user to know that the values the RAD Calculator provides are based on assumptions that may not match the exact parameters of their experiment. It is assumed that:

- The fluxes are time invariant and will not change during the whole irradiation process. This ignores the effects of depletion and control element shimming.
- The material composition will not vary over time and will not undergo any form of activation. This ignores the impact of ^{59}Ni on neutron damage in nickel. This impact is generally considered non-negligible.
- All inserted materials contain their naturally occurring isotopic concentrations.
- All materials are positioned at the axial center line of the reactor (±10cm). Fluxes were simulated in MCNP for a target right circular cylinder of 1cm diameter × 20cm long of pure iron.
- Reactors operate at the following powers:
    - ATR: 110 MW (22 MW lobe power)
    - High Flux Isotope Reactor: 85 MW
    - Massachusetts Institute of Technology Reactor: 6 MW
    - PULSTAR: 1 MW
- All experiments operate at 600 K.
- The group structure is fine enough to not need iterative flux solutions in order to preserve reaction rates.
- The materials are, effectively, infinitely dilute and do not impact the flux of the reactor.
- The materials are not fissile and do not fission. This calculator will not handle fissile or fertile materials.

3.2.6 Data Libraries and Calculator Versions

Table 1. Citations for data sources used for the pre-processing of the data.

Data	**Source**
Natural isotope abundance	Meija [9] via pyENDF6, a derivative of OpenMC [10]
Nuclear data	ENDF-B/VIII.0 [13]
Boltzmann constant	SI [14]
Displacement threshold energy (E_d)	Konobeyev et al. [12]
Efficiency (κ)	NRT [2]
Avogadro's number (N_a)	SI [14]

Table 2. Versions of python scripts used to pre-process the current version of the nuclear data in the calculator.

Code Repository	**git SHA1 of Library**
NJOY_DPA	a2de012f9eddfdfbffefefc61b9e863aed6f4141
pyENDF6	692f7a13d63aa107ac6e5d0cf5fc2d887a168161

4. Validation

4.1 Methodology

The RAD Calculator is a general scoping tool and is not intended to replace calculations performed by professional analysts as part of the experiment design process. However, for the RAD Calculator to be useful, it must be reasonably accurate in the results it produces. In order to validate the damage component of the RAD Calculator, a series of as-run physics ECARs for ATR experiments were used as a benchmark to check the overall accuracy of the DPA results. A variety of configurations based on the sample and its position with respect to the core centerline were selected from each of the ECARs listed below in Table 3. INL analysts use Monte Carlo N-Particle (MCNP) [7] code and follow INL's internal guide (GDE-594) in order to perform DPA calculations.

Table 3. Benchmark As-Run Physics ECARs for ATR experiments.

ECAR No.	Project No.	Title
4341	31418	BSU-8242 1 DPA As-run Physics Analysis
3028	31091	As-run Physics Analysis for the Drexel University EFT Project in the ATR
3029	31091	As run Physics Analysis for the Drexel University A-3 Project in the ATR
2978	29609	As-run Physics Analysis for the University of Illinois A-11 Drop-In Project in the ATR
4320	31226	ATR As-run Physics Evaluation of the UCF-3 Experiment
3219	30946	As-run Physics Analysis for the UCSB-2 Leadout Experiment in I-22
3050	31039	As-run Physics Analysis for the Utah State University Project in the ATR
3338	29584	As-run Physics Analysis for the EPRI-3 Experiment for Cycles 155B and 158B

For each configuration, the sample's elemental composition in weight percent (wt.%) and EFPD were taken from the ECARs and entered into the RAD Calculator to calculate DPA. A series of adjustments and corrections were then applied to the calculator's DPA output to account for the difference between the ECARs' parameters and the calculator's reference parameters listed in section 3.2.5. The calculator DPA was adjusted for axial flux shape by multiplying it by the ratio of the fluence at each configuration to the maximum fluence of all the selected configurations. To adjust for power, the calculator DPA was also multiplied by the ratio of the lobe power used in the ECAR to the calculator's assumed lobe power of 22 MW for ATR. The calculator uses updated E_d values from Konobeyev et al. which may differ from those used in each ECAR, so adjustments based on the displacement threshold energy (E_d) values were made as well. This was done by multiplying the calculator DPA results by the ratio of the calculator's E_d to the E_d used in the ECARs. After all the adjustments and corrections were made, the final calculation of DPA was compared to the ECAR DPA values, and a deviation was calculated. Appendix C shows the results.

4.2 Results

Because the RAD Calculator is intended to be a scoping tool, an acceptability threshold of ±50% deviation was established for the DPA calculations. After adjusting the results for the difference in assumptions between the ECARs and the calculator, the calculator's final corrected DPA values fall within ±50% of the DPA values in the ECARs. In fact, more than 85% of the tests are within ±20%. These results imply that the damage component of the RAD Calculator serves as an excellent scoping tool for NSUF users and can be expected to competently perform. However, being a scoping tool, the limitations associated with the RAD Calculator must be addressed.

4.2.1 E_d Values and Mixed Materials

One limitation of the RAD Calculator, and really of any DPA calculation being performed, relates to the E_d values. There is no standard set of E_d values used to calculate DPA. This is because various sources have different values for the same element. For example, updated values from Konobeyev et al. use 37 eV for Si [12], Greenwood and Smither use 25 eV [6], and Heinisch et al. use 35 eV [15]. The variation in E_d values of the same element among various sources makes DPA a challenging parameter to compare. Furthermore, the calculator uses an average E_d value for mixed materials such as alloys, composites, and compounds, weighted by the atomic ratio of the elements in the material. This method is also used by INL analysts and so represents a standard if potentially flawed approach.

Originally, DPA calculations were considered for pure elements only. Consequently, the problem with using an E_d weighted average for mixed materials is that it does not take into account either the secondary displaced atoms that are dependent on all possible combinations of recoiling atoms and matrix atoms or the difference in binding energies between compounds and pure elements [16]. For example, the calculations for the displacement threshold energies of materials such as Li_2O must consider the probabilities of the projectile/target combinations, where Li atoms can displace both O atoms and Li atoms, and where O atoms can do so as well. Heinisch et al. have addressed this problem for SiC using molecular dynamics and computer simulations. They were able to calculate the following displacement energies of the four projectile/target combinations in SiC: 41 eV for C/Si, 35 eV for Si/Si, 24 eV for Si/C, and 20 eV for C/C. That is, for the C/Si combination, the C atom must have a minimum energy of 41 eV to provide the 35 eV to displace the Si atom. From these displacement threshold energies, Heinisch et al. were able to come up with total damage pseudo-cross-sections as a function of energy for SiC [15]. The problem is that this type of computational analysis has only been completed for a few mixed materials and, with the development of advanced nuclear material technology, there is a large quantity of mixed materials for which displacement threshold energies, and thus damage pseudo-cross-sections, have not been calculated.

4.2.2 Transmutations

Another limitation of the RAD Calculator is that it does not account for damage caused by neutron irradiation-induced transmutations and the associated recoil atom displacement cascades. For example, the transmutations of nickel — particularly the $^{58}Ni(n,\gamma)^{59}Ni(n,\alpha)$ and the $^{58}Ni(n,\gamma)^{59}Ni(n,p)$ reactions — are not considered. Thus, the production of hydrogen and helium are not tracked and the damage they produce in a material is not accounted for. Not only are helium and hydrogen a problem, but the $^{59}Ni(n,\alpha)$ and $^{59}Ni(n,p)$ reactions are very exoergic, where charged particles and heavy atomic recoils are produced, also causing radiation damage [19]. Consequently, if users have nickel in their material, the calculator will give a conservative irradiation time estimate by underestimating the actual radiation damage. Currently, INL analysts performing DPA calculations in the ECARs used in this evaluation also do not have a methodology to account for damage caused by transmutation reactions. So, the results of the RAD Calculator and the ECARs should still be similar. There have been studies on the damage caused by hydrogen and helium concentrations using the code SPECTER. These studies found that 548 appm of helium generation in nickel is accompanied by 1 DPA of radiation damage [17].

However, the RAD Calculator does not use SPECTER, and it would need to be incorporated into the calculator to determine hydrogen and helium concentrations. A significant challenge with using SPECTER is that it currently has data for only 41 elements.

4.2.3 Materials Not Handled by the RAD Calculator

The final limitation of the RAD Calculator is that it does not calculate damage for all known elements. The damage pseudo-cross-sections for the elements listed below are not generated in the calculator for the following reasons and the application will output an error rather than calculate a damage value:

1. H, He, N, O, F, Ne, Cl, Ar, Kr, Xe, Hg, and Br due to being a gas or liquid at room temperature. Even if these elements were in a compound, the E_d value would be incorrect.
2. Tc, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr, Rf, Db, Sg, Bh, Hs, Mt, Ds, Rg, Cn, Nh, Fl, Mc, Lv, Ts, Og, Po, Pm, At, Rn, Fr, Ra, and Ac due to being synthetic or rare. This would impede the calculator from performing the DPA calculations because the natural isotopic compositions would be unclear.
3. Damage to fissile or fissionable material caused by fissions is not calculated and so DPA values for uranium and thorium would be significantly low.

5. Summary

Validation results indicate that this new tool meets the acceptance criterion by providing DPA approximations that fall well within the original target of ±50% of the reference values. However, the RAD Calculator is a general scoping tool and it is not intended to replace calculations performed by professional analysts that require more in-depth analysis. This new tool will provide users the capability to estimate radiation damage based on their conceptual experiment design so they can select appropriate facilities for their potential irradiation proposals. It is recommended that modifications to the RAD calculator be implemented to improve DPA calculations. These recommended modifications are outlined in section 6.

6. Recommendations

6.1 Changes Outside the Scope of CoMET

Some limitations are associated with the RAD Calculator, and the changes needed to mitigate these limitations, fall outside the scope of this project. For example, finding the E_d values for mixed materials that consider secondary displaced atoms is a project in and of itself, and can only be completed through molecular dynamics and extensive computational analyses. However, efforts to create more accurate methods have not culminated in a standard method to perform such analyses. Nonetheless, the DPA component of the RAD Calculator is sufficient for its intended purpose as a scoping tool for NSUF experiments as long as both the calculator and the analysts use the same methods to calculate DPA. Consistency is vital since the RAD Calculator is intended to be the first step in the experimental analysis process and is therefore bound to the INL analysis process.

Therefore, it is recommended that a consistent practice be incorporated, so the same E_d values for each element are used, as well as the same method for calculating the E_d values of mixed materials. One way of doing this internally throughout INL is by developing a consensus methodology and then updating GDE-594 to prescribe which E_d values should be used for each element, how they should be calculated for mixed materials, and where any deviations from these methods were made.

6.2 Changes Before Deployment

Prior to deployment, caution statements were added to the calculator to inform users who input irradiation conditions falling outside the calculator's limitations of the potentially inaccurate results.

These caution statements inform users whenever irradiation conditions include elements not capable of being handled by the calculator, such as those listed in Section 4.2.3. Users will also be informed that transmutations for materials such as nickel are not currently handled by the calculator. All other assumptions mentioned in section 3.2.5 are also made known to the user.

6.3 Future Developments

Although the RAD Calculator is an excellent scoping tool, knowing how the neutron energy spectrum between different facilities affects radiation damage would also help users identify the appropriate facility for meeting their experiment-related needs. Damage caused by nuclear transmutations are a critical component of any future release, but transmutation calculations can be difficult to perform, especially for long chains of transmutations that may exist in extended irradiation campaigns [18]. In the future, the calculator can be improved in order to account for damage caused by nuclear transmutations. However, this cannot be done until a standard methodology is developed in collaboration with neutronics analysts and material scientists. One potential methodology is by using helium measurements compared to predictions from SPECTER to verify results. This would include updating SPECTER to incorporate more elements.

6.3.1 State of the Art: Athermal Recombination Corrected DPA (arc-dpa)

It has long been widely known that DPA does not correlate with the number of stable Frenkel-pairs produced in irradiated material. Currently, the field has been working on updating DPA models to accurately represent the number of Frenkel-pairs and other defects remaining in the material post-irradiation. A major development on this front was the creation of the athermal recombination-corrected dpa (arc-dpa) model, which compensates for the inefficiencies of causing displacements that occur at high recoil energies. The updated model is [19]:

$$N_{d,arcdpa} = \begin{cases} 0, & E_R < E_d \\ 1, & E_d < E_R < \dfrac{2E_d}{0.8} \\ \dfrac{0.8E_R}{2E_d}\xi(E_R), & \dfrac{2E_d}{0.8} < E < \infty \end{cases} \quad (37)$$

This has an energy dependent efficiency of:

$$\xi(E_R) = \frac{1 - c_{arcdpa}}{\dfrac{2E_d}{0.8}} E_R^{b_{arcdpa}} + c_{arcdpa} \quad (38)$$

Where c and b are tunable parameters adjusted to match the experimental data.

Although arc-dpa is state of the art, it is not yet the standard. In large part, this is because there is no clear path forward as to how it can be correlated with the large amounts of historical data available. Due to industry not yet adapting arc-dpa, the RAD Calculator does not use it. However, the RAD Calculator could be updated to use the arc-dpa model. NSUF should monitor this field and consider adoption once the legacy data issue is solved, and industry begins to adopt the model.

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Appendix A: 252-group structure

Group Number	Upper Energy Bound (eV)
1	1.00E-04
2	5.00E-04
3	7.50E-04
4	1.00E-03
5	1.20E-03
6	1.50E-03
7	2.00E-03
8	2.50E-03
9	3.00E-03
10	4.00E-03
11	5.00E-03
12	7.50E-03
13	1.00E-02
14	2.53E-02
15	3.00E-02
16	4.00E-02
17	5.00E-02
18	6.00E-02
19	7.00E-02
20	8.00E-02
21	9.00E-02
22	1.00E-01
23	1.25E-01
24	1.50E-01
25	1.75E-01
26	2.00E-01
27	2.25E-01
28	2.50E-01
29	2.75E-01
30	3.00E-01
31	3.25E-01
32	3.50E-01
33	3.75E-01
34	4.00E-01
35	4.50E-01
36	5.00E-01
37	5.50E-01
38	6.00E-01
39	6.25E-01
40	6.50E-01
41	7.00E-01
42	7.50E-01
43	8.00E-01
44	8.50E-01
45	9.00E-01
46	9.25E-01
47	9.50E-01
48	9.75E-01
49	1.00E+00
50	1.01E+00
51	1.02E+00
52	1.03E+00
53	1.04E+00
54	1.05E+00
55	1.06E+00
56	1.07E+00
57	1.08E+00
58	1.09E+00
59	1.10E+00
60	1.11E+00
61	1.12E+00
62	1.13E+00
63	1.14E+00
64	1.15E+00
65	1.18E+00
66	1.20E+00
67	1.23E+00
68	1.25E+00
69	1.30E+00
70	1.35E+00
71	1.40E+00
72	1.45E+00
73	1.50E+00
74	1.59E+00
75	1.68E+00
76	1.77E+00
77	1.86E+00
78	1.94E+00
79	2.00E+00
80	2.12E+00
81	2.21E+00
82	2.30E+00
83	2.38E+00
84	2.47E+00
85	2.57E+00
86	2.67E+00
87	2.77E+00
88	2.87E+00
89	2.97E+00
90	3.00E+00
91	3.10E+00
92	3.20E+00
93	3.50E+00
94	3.73E+00
95	4.10E+00
96	4.70E+00
97	5.00E+00
98	5.40E+00
99	6.00E+00
100	6.25E+00
101	6.50E+00
102	6.75E+00
103	6.88E+00
104	7.00E+00
105	7.15E+00
106	8.10E+00
107	9.10E+00
108	1.00E+01
109	1.15E+01
110	1.19E+01
111	1.29E+01
112	1.44E+01
113	1.60E+01
114	1.70E+01
115	1.85E+01
116	1.94E+01
117	2.00E+01
118	2.05E+01
119	2.12E+01
120	2.18E+01
121	2.25E+01
122	2.50E+01
123	2.75E+01
124	3.00E+01
125	3.13E+01
126	3.18E+01
127	3.33E+01
128	3.38E+01
129	3.50E+01

Group Number	Upper Energy Bound (eV)
130	3.55E+01
131	3.60E+01
132	3.70E+01
133	3.71E+01
134	3.73E+01
135	3.76E+01
136	3.80E+01
137	3.91E+01
138	3.96E+01
139	4.10E+01
140	4.24E+01
141	4.40E+01
142	4.52E+01
143	4.83E+01
144	5.06E+01
145	5.34E+01
146	5.80E+01
147	6.10E+01
148	6.30E+01
149	6.50E+01
150	6.75E+01
151	7.20E+01
152	7.60E+01
153	8.00E+01
154	8.17E+01
155	9.00E+01
156	9.70E+01
157	1.01E+02
158	1.05E+02
159	1.08E+02
160	1.13E+02
161	1.16E+02
162	1.18E+02
163	1.19E+02
164	1.22E+02
165	1.43E+02
166	1.70E+02
167	1.80E+02
168	1.88E+02
169	1.89E+02
170	1.92E+02
171	1.93E+02

Group Number	Upper Energy Bound (eV)
172	2.02E+02
173	2.07E+02
174	2.10E+02
175	2.20E+02
176	2.40E+02
177	2.85E+02
178	3.05E+02
179	5.50E+02
180	6.70E+02
181	6.83E+02
182	9.50E+02
183	1.15E+03
184	1.50E+03
185	1.55E+03
186	1.80E+03
187	2.20E+03
188	2.25E+03
189	2.50E+03
190	3.00E+03
191	3.74E+03
192	3.90E+03
193	5.70E+03
194	8.03E+03
195	9.50E+03
196	1.30E+04
197	1.70E+04
198	2.00E+04
199	3.00E+04
200	4.50E+04
201	5.00E+04
202	5.20E+04
203	6.00E+04
204	7.30E+04
205	7.50E+04
206	8.20E+04
207	8.50E+04
208	1.00E+05
209	1.28E+05
210	1.49E+05
211	2.00E+05
212	2.70E+05
213	3.30E+05

Group Number	Upper Energy Bound (eV)
214	4.00E+05
215	4.20E+05
216	4.40E+05
217	4.70E+05
218	4.92E+05
219	5.50E+05
220	5.73E+05
221	6.00E+05
222	6.70E+05
223	6.79E+05
224	7.50E+05
225	8.20E+05
226	8.61E+05
227	8.75E+05
228	9.00E+05
229	9.20E+05
230	1.01E+06
231	1.10E+06
232	1.20E+06
233	1.25E+06
234	1.32E+06
235	1.36E+06
236	1.40E+06
237	1.50E+06
238	1.85E+06
239	2.35E+06
240	2.48E+06
241	3.00E+06
242	4.30E+06
243	4.80E+06
244	6.43E+06
245	8.19E+06
246	1.00E+07
247	1.28E+07
248	1.38E+07
249	1.46E+07
250	1.57E+07
251	1.73E+07
252	2.00E+07

Appendix B: NJOY21 Input

Note: items inside {} are the relevant data replaced by the Python script

```
--------- Tapes ----------------
-- 20: Input endf
-- 21: Binary input
-- 22: PENDF of reconstruction
-- 23: PENDF of doppler broadened
-- 25: PENDF of total sigma_d
-- 27: Plot of total sigma_d
-- 26: Binary GENDF of 252-group xs
-- 40: ascii output of PENDF of HEATR
-- 41: ascii output of GENDF ^

--Convert to Binary
moder
20 -21
--Convert to a PENDF and reconstruct the structure
reconr
-21 -22/
'Base PENDF for all {matName}'/
{material}/
0.001/
0/
--Doppler broaden
broadr
-21 -22 -23/
{material} 1/
0.001/
{temperature}/
0/
-- calculate sigma_d
heatr
-21 -23 -25 27/
{material}  1 0 0 0 2 {ed}/
444 /
-- write out the continuous cross-section
moder
-25 40/
-- Group into 252 group
groupr
-21 -25 0 -26/
{material} 1 0 4 1 1/
```

```
'JEFF 252-group structure for {matName}'/
{temperature}/
1.0e10/
252/ number of groups
1e-8
1.00E-04 5.00E-04 7.50E-04 1.00E-03 1.20E-03 1.50E-03 2.00E-03 2.50E-03 3.00E-03
4.00E-03 5.00E-03 7.50E-03 1.00E-02 2.53E-02 3.00E-02 4.00E-02 5.00E-02 6.00E-02
7.00E-02 8.00E-02 9.00E-02 1.00E-01 1.25E-01 1.50E-01 1.75E-01 2.00E-01 2.25E-01
2.50E-01 2.75E-01 3.00E-01 3.25E-01 3.50E-01 3.75E-01 4.00E-01 4.50E-01 5.00E-01
5.50E-01 6.00E-01 6.25E-01 6.50E-01 7.00E-01 7.50E-01 8.00E-01 8.50E-01 9.00E-01
9.25E-01 9.50E-01 9.75E-01 1.00E+00 1.01E+00 1.02E+00 1.03E+00 1.04E+00 1.05E+00
1.06E+00 1.07E+00 1.08E+00 1.09E+00 1.10E+00 1.11E+00 1.12E+00 1.13E+00 1.14E+00
1.15E+00 1.18E+00 1.20E+00 1.23E+00 1.25E+00 1.30E+00 1.35E+00 1.40E+00 1.45E+00
1.50E+00 1.59E+00 1.68E+00 1.77E+00 1.86E+00 1.94E+00 2.00E+00 2.12E+00 2.21E+00
2.30E+00 2.38E+00 2.47E+00 2.57E+00 2.67E+00 2.77E+00 2.87E+00 2.97E+00 3.00E+00
3.10E+00 3.20E+00 3.50E+00 3.73E+00 4.10E+00 4.70E+00 5.00E+00 5.40E+00 6.00E+00
6.25E+00 6.50E+00 6.75E+00 6.88E+00 7.00E+00 7.15E+00 8.10E+00 9.10E+00 1.00E+01
1.15E+01 1.19E+01 1.29E+01 1.44E+01 1.60E+01 1.70E+01 1.85E+01 1.94E+01 2.00E+01
2.05E+01 2.12E+01 2.18E+01 2.25E+01 2.50E+01 2.75E+01 3.00E+01 3.13E+01 3.18E+01
3.33E+01 3.38E+01 3.50E+01 3.55E+01 3.60E+01 3.70E+01 3.71E+01 3.73E+01 3.76E+01
3.80E+01 3.91E+01 3.96E+01 4.10E+01 4.24E+01 4.40E+01 4.52E+01 4.83E+01 5.06E+01
5.34E+01 5.80E+01 6.10E+01 6.30E+01 6.50E+01 6.75E+01 7.20E+01 7.60E+01 8.00E+01
8.17E+01 9.00E+01 9.70E+01 1.01E+02 1.05E+02 1.08E+02 1.13E+02 1.16E+02 1.18E+02
1.19E+02 1.22E+02 1.43E+02 1.70E+02 1.80E+02 1.88E+02 1.89E+02 1.92E+02 1.93E+02
2.02E+02 2.07E+02 2.10E+02 2.20E+02 2.40E+02 2.85E+02 3.05E+02 5.50E+02 6.70E+02
6.83E+02 9.50E+02 1.15E+03 1.50E+03 1.55E+03 1.80E+03 2.20E+03 2.25E+03 2.50E+03
3.00E+03 3.74E+03 3.90E+03 5.70E+03 8.03E+03 9.50E+03 1.30E+04 1.70E+04 2.00E+04
3.00E+04 4.50E+04 5.00E+04 5.20E+04 6.00E+04 7.30E+04 7.50E+04 8.20E+04 8.50E+04
1.00E+05 1.28E+05 1.49E+05 2.00E+05 2.70E+05 3.30E+05 4.00E+05 4.20E+05 4.40E+05
4.70E+05 4.92E+05 5.50E+05 5.73E+05 6.00E+05 6.70E+05 6.79E+05 7.50E+05 8.20E+05
8.61E+05 8.75E+05 9.00E+05 9.20E+05 1.01E+06 1.10E+06 1.20E+06 1.25E+06 1.32E+06
1.36E+06 1.40E+06 1.50E+06 1.85E+06 2.35E+06 2.48E+06 3.00E+06 4.30E+06 4.80E+06
6.43E+06 8.19E+06 1.00E+07 1.28E+07 1.38E+07 1.46E+07 1.57E+07 1.73E+07 2.00E+07
0.1 {boltzmannTemp} 820e3 1.4e6 /
3 444 'damage pseudo-cross-section for {matName}'/
0/
0/
-- write back into ASCII endf
moder
-26 41/
stop
```

Appendix C: ECAR vs RAD Calculator Data

Experiment	Material	EFPD*	ATR Position*	Distance from Core CL* [cm]	ECAR DPA	Initial Calculator DPA[a]	Adjusted DPA[b]	Deviation[c]
BSU-8242	Al-22.7Hf	54.5	A7	-39.15	0.97	2.403	1.14	17%
BSU-8242	Fe-0.75Ni-0.75Mn-0.63Mo-0.35Cr-0.275Si-0.27C-0.05V-0.025P-0.025S	54.5	A7	15.13	1.00	1.428	1.28	28%
BSU-8242	Fe-0.75Ni-0.75Mn-0.63Mo-0.35Cr-0.275Si-0.27C-0.05V-0.025P-0.025S	54.5	A7	-42.26	0.69	1.428	0.88	28%
BSU-8242	Ni-21.42Cr-9Mo-5Fe-3.65Nb-1.0Co-0.5Mn-0.5Si-0.4Al-0.4Ti-0.1C-0.05Ta-0.015P-0.015S	54.5	A7	17.89	1.07	1.613	1.27	18%
BSU-8242	Ni-21.42Cr-9Mo-5Fe-3.65Nb-1.0Co-0.5Mn-0.5Si-0.4Al-0.4Ti-0.1C-0.05Ta-0.015P-0.015S	54.5	A7	17.82	1.04	1.613	1.28	23%
Drexel-A3	Si-30C	53.6	A3	10.55	2.11	1.027	1.91	9%
Drexel-A3	Si-30C	53.6	A3	0.70	2.20	1.027	1.95	11%
Drexel-A3	Ti-14.5Si-12C	53.6	A3	10.70	1.56	1.257	1.72	11%
Drexel-A3	Ti-14.5Si-12C	53.6	A3	0.85	1.61	1.257	1.77	10%
Drexel-A3	Ti-14Al-12C	53.6	A3	10.40	1.55	1.298	1.67	8%
Drexel-A3	Ti-14Al-12C	53.6	A3	0.55	1.58	1.298	1.73	9%
Drexel-EFT	Si-30C	183.8	EFT	10.55	4.72	2.033	3.39	28%
Drexel-EFT	Si-30C	183.8	EFT	0.70	4.83	2.033	3.48	28%
Drexel-EFT	Ti-14.5Si-12C	183.8	EFT	10.70	3.40	2.497	3.01	11%
Drexel-EFT	Ti-14.5Si-12C	183.8	EFT	0.85	3.45	2.500	3.13	9%
Drexel-EFT	Ti-14Al-12C	183.8	EFT	10.40	3.34	2.580	2.96	11%
Drexel-EFT	Ti-14Al-12C	183.8	EFT	0.55	3.29	2.580	3.00	9%
EPRI-3	Ni-15.5Cr-7Fe-2.5Ti-1Co-0.95Nb-1Mn	54.9	CFT	0.50	1.55	2.005	1.59	3%
EPRI-3	Fe-22Cr-12.5Ni-5Mn-2.25Mo-1Si	51.4	CFT	0.50	1.46	1.720	1.61	10%
Illinois	Fe	351	A11	-0.64	8.75	8.234	8.76	0%
Illinois	Fe	162.5	A11	-14.71	4.02	3.812	4.19	4%
Illinois	Fe	57.3	A11	-36.59	1.11	1.344	1.19	7%

Experiment	Material	EFPD*	ATR Position*	Distance from Core CL* [cm]	ECAR DPA	Initial Calculator DPA[a]	Adjusted DPA[b]	Deviation[c]
Illinois	Fe-12.14Cr-0.5C	351	A11	-0.64	8.78	8.120	8.81	0%
Illinois	Fe-12.14Cr-0.5C	162.5	A11	-14.16	4.16	3.759	4.32	4%
Illinois	Fe-12.14Cr-0.5C	57.3	A11	-36.31	1.14	1.326	1.20	6%
UCF-3	Al	215.38	B8	0.00	4.09	4.941	4.31	5%
UCF-3	Fe	215.38	B8	0.00	2.00	2.464	2.15	7%
UCF-3	Mo	215.38	B8	0.00	1.53	1.526	1.44	6%
UCF-3	U	215.38	B8	0.00	1.03	2.017	1.23	20%
UCF-3	Zr	215.38	B8	0.00	2.25	2.614	2.28	1%
UCSB-2	Fe-3.63Ni-2.24Cr-2.06Mn-0.86Cu-0.1Co-0.01V	427.1	I22	-55.40	0.08	0.167	0.08	9%
UCSB-2	Fe-3.63Ni-2.24Cr-2.06Mn-0.86Cu-0.1Co-0.01V	427.1	I22	-29.29	0.18	0.167	0.16	11%
UCSB-2	Fe-3.63Ni-2.24Cr-2.06Mn-0.86Cu-0.1Co-0.01V	427.1	I22	21.97	0.19	0.167	0.17	11%
UCSB-2	Fe-3.63Ni-2.24Cr-2.06Mn-0.86Cu-0.1Co-0.01V	427.1	I22	1.56	0.20	0.170	0.19	9%
UCSB-2	Fe-3.63Ni-2.24Cr-2.06Mn-0.86Cu-0.1Co-0.01V	427.1	I22	53.24	0.08	0.167	0.07	12%
Utah State	Al-1Mg-0.6Si-0.25Cu-0.2Cr	188.4	B2	-16.68	3.97	4.324	3.98	0%
Utah State	Al-22.7Hf	188.4	B2	12.99	3.50	3.728	3.31	5%
Utah State	Al-22.7Hf	188.4	B2	5.40	3.93	3.728	3.67	7%
Utah State	Al-22.7Hf	188.4	B2	1.54	3.97	3.728	3.59	10%
Utah State	Al-22.7Hf	188.4	B2	-1.51	3.97	3.728	3.59	10%
Utah State	Hf-37.8Al	188.4	B2	-11.91	2.57	2.475	2.27	12%

* ECAR parameters.
a. The initial DPA value the calculator provides.
b. The DPA value after adjusting the Initial Calculator DPA to account for the difference between the ECARs' parameters and the calculator's assumed parameters.
c. The deviation of the Adjusted DPA value from the ECAR DPA value.