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Preliminary analysis of TREAT free-field experiments using OpenMC

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Abstract. This work analyses activation calculations for dosimetry materials during a steady-state irradiation in the Transient Reactor Test (TREAT) reactor core. Hence, we developed a workflow based on the Monte Carlo code OpenMC alongside a custom depletion solver. The irradiation-induced activity as a function of time is computed, and several sensitivity studies are performed to evaluate uncertainty. This study has shown activity computations are sensitive to flux amplitude, irradiation time, atoms quantity and microscopic cross sections. Stochastic uncertainties have been propagated to evaluate the activity uncertainty for each dosimetry material. Most uncertainties are below our target of 3%, which demonstrates OpenMC as a powerful predictive and analysis tool. The precise results obtained through this newly developed computation scheme will be used in future experiments to characterize quantities of interest when operating the TREAT reactor in new configurations.

1 Introduction

The Transient Reactor Test (TREAT) Facility is an air-cooled graphite-moderated test reactor. Since its restart in 2017, many programs have been successfully implemented (e.g., the Transient Heat-sink Overpower Response capsule (THOR) [1], the Transient Water Irradiation System for TREAT (TWIST) [2] and NASA's Sirius fuel material test series [3]). Ever-increasing ambitions led to the design and implementation of a more spacious experiment holder, the Big Broad Use Specimen Transient Experiment Rig (Big-BUSTER) [4], and therefore required a larger cavity within the reactor. Big-BUSTER has a volume four times greater than the previous experiment holder, BUSTER, allowing bigger experimental device tests in TREAT.

To install Big-BUSTER into the core, the core configuration had to be altered. Substantial core changes require many quantities to be re-established, such as control rod worths, temperature feedback tables, etc. Of particular interest is the energy-dependent neutron

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fluence in the new experimental cavity. A series of experiments, deemed the free-field characterization [5], were designed to measure the neutron fluence through the use of activation materials for TREAT reactor operations, including steady-state runs, temperature limited transients, and clipped transients, within the Big-BUSTER cavity. For each experiment in the campaign, a dosimeter tray that provides negligible perturbations in the neutron fluence is installed. Therefore, the reactor should behave as if there is no experiment present (i.e., with a free-field environment).

The dosimetry material activities must be precalculated to provide a conservative estimate for radiation protection purposes. This is usually done with conservative methods that provide a reliable overestimation of the activity of each material. Nevertheless, since the uncertainty associated with the experiment is low, simulating the free-field experiments is a good way to assess the accuracy of the state-of-the-art computational scheme that will be used in the future interpretation of TREAT experiments.

To perform the best-estimate calculations, methods are chosen to minimize the initial information required, even if this significantly increases the computational cost. Monte Carlo codes are suitable as experimental analysis tools because no spatial or energy mesh is required unlike deterministic codes.

OpenMC is a state-of-the-art, open-source Monte Carlo code [6]. OpenMC has been designed for research and development purposes and to be efficient with multi-CPU calculations. Its development community is very active. In addition, the Python user layer makes it easy to design a postprocessing workflow, chained calculations, and interactions with other codes.

In this paper, we design a workflow to calculate the activation of dosimetry materials during a constant power irradiation in a critical configuration. Our goal is to obtain the best estimate of each activity in the sample, where the stochastic uncertainty does not exceed 3%. Thus, experimental uncertainties are not taken into account.

2 Materials & Methods

This section gives an overview of the TREAT reactor and the experiment analysed followed by the computation scheme.

2.1 The TREAT reactor

The primary purpose of the TREAT facility is to irradiate experimental devices, typically a single item in the central cavity. The core is designed to provide prototypical reactivity and neutron fluence conditions that occur during reactivity injection accidents (see figure 1), but TREAT's versatility allows the experiments to be exposed to a variety of test conditions. TREAT is composed of a highly enriched UO_2 fuel diluted in a graphite matrix with air coolant. Reactivity is driven by sets of control rods, and transients are initiated by a rapid ejection of dedicated transient rods, resulting in a large reactivity injection and causing the power and fuel temperature to rapidly increase. Negative temperature feedback mechanisms decrease the reactivity as the transient progresses. Eventually, the negative reactivity overcomes the initial reactivity induced by the transient rod ejection and core power decreases, ending the transient. The reinsertion of the control rods (through mechanical and gravitational means) completely terminates the transient. The induced feedback effect

decreases the reactivity and power peaks before diminishing. The transient is stopped by dropping the control rods.

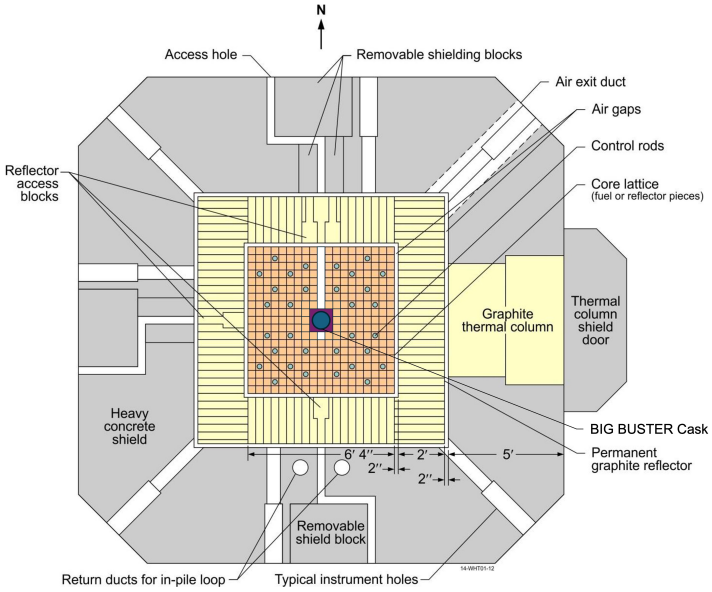

Figure 1. TREAT reactor with the Big-BUSTER cask. Adapted from [7].

2.2 Free-field experiment

For this paper, we will focus on the low power (80 kW), steady-state irradiation performed as part of the free-field characterization campaign. The target energy deposed is 576 MJ, which calculates to a duration of approximately 2 hours. The transient rods are moved at their maximum upper position and the remaining control rods are set to a position of 90.1 cm. This configuration is the same as that of the MCNP dataset used as a reference in the development of our openmc model of TREAT. The experimental critical configuration is not yet known and will be determined after the experiment is performed.

The dosimeter tray holds several activation materials at the center of the experimental zone. The tray is divided into three holders, oriented south, northeast, and northwest (see figure 2). The materials listed in table 1 were designed for different purposes:

- Foils, tabs, and fission dots are chosen to obtain activated materials of a wide range of half-life and uncorrelated cross sections to measure the flux at the center of the core for a given core power level.
- A wire (modeled in 11 sections) running from the center to the top of the core is used to characterize the axial flux distribution in the experimental zone.

The detailed location of each material is displayed in figure 3.

As activation material volumes are very low compared to the volume of our model, a

significant amount of computational power is needed to achieve proper convergence. For the OpenMC simulations, we used High-Performance Computing resources (see Acknowledgements).

Table 1. Dosimetry material characteristics

Name	Main element	Quantity	Volume
foil1	Nickel	3	$9.63 \times 10^{-3} cm^3$
foil2	Iron	3	$1.61 \times 10^{-2} cm^3$
foil3	Titanium	3	$3.22 \times 10^{-2} cm^3$
foil4	Zirconium	3	$1.61 \times 10^{-2} cm^3$
foil5	Gold - Aluminium	3	$1.61 \times 10^{-2} cm^3$
foil6	Cobalt - Aluminium	3	$1.61 \times 10^{-2} cm^3$
tab	Sulfur	6	$1.21 \times 10^{-1} cm^3$
dot	Zirconium - Uranium	6	$4.32 \times 10^{-3} cm^3$
wire	Iron	11	$2.69 \times 10^{-1} cm^3$

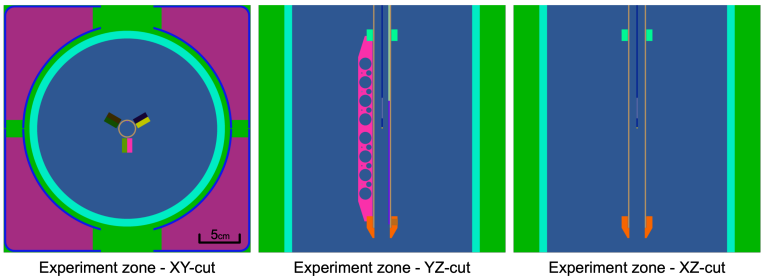

Figure 2. Dosimeter tray in the Big-BUSTER cavity.

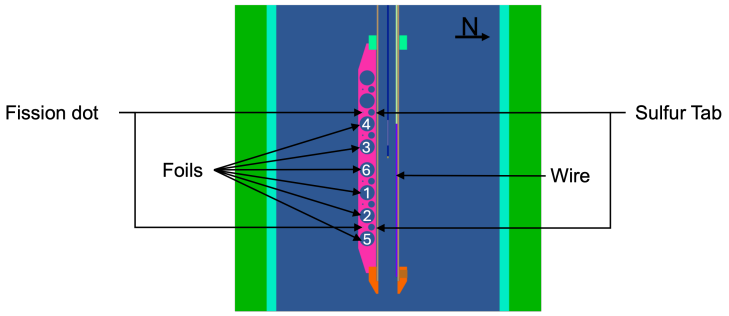

Figure 3. Location of activation materials.

2.3 Computation scheme

The computation scheme developed to compute activation is detailed in figure 4.

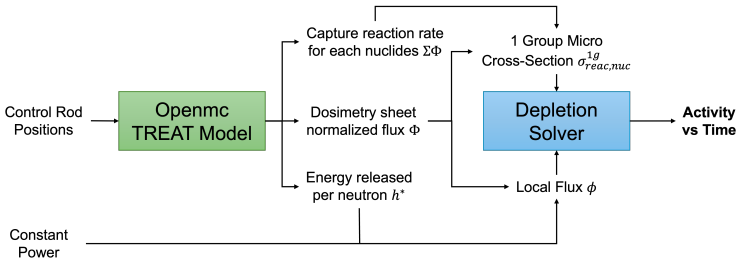

Figure 4. Activation computation scheme.

OpenMC computation

The experiment critical configuration is modeled in OpenMC, and an eigenvalue calculation is performed. Since the modeled experiment is an irradiation at steady-state power, we assume that computed quantities can be considered constant. The normalized flux per neutron and reaction rate for each nuclide and each reaction are tallied for each of the activation materials. The energy released per neutron is tallied over the whole core. These scores are needed to compute the local fluxes and one-group microscopic cross sections used in the depletion computation.

Point quantities definition

The depletion solver is based on a point model. Therefore, the one-group microscopic cross section is defined by the equation:

$$\sigma^{1g}_{reac,nuc} = \frac{\int \Sigma(r,E)_{reac,nuc}\Phi(r,\Omega,E)\ \mathrm{dr}\ \mathrm{d}\Omega\ \mathrm{dE}}{\int N(r)_{nuc}\Phi(r,\Omega,E)\ \mathrm{dr}\ \mathrm{d}\Omega\ \mathrm{dE}}, \tag{1}$$

where Σ is the macroscopic cross section for a given reaction and a given nuclide, Φ is the normalized flux per neutron obtained from an OpenMC eigenvalue calculation, and N is the atom density. The integration is performed on the whole energy and angular spectrum but is limited to the material volume. The relation between the core power level P, the energy deposited in the core per neutron h^*, and the local flux in the material ϕ is given by the equation:

$$\phi = \frac{P}{h^*}\int \Phi(r,\Omega,E)\ \mathrm{dr}\ \mathrm{d}\Omega\ \mathrm{dE}. \tag{2}$$

Depletion solver

When this study was carried out, OpenMC capabilities regarding depletion solving didn't match our needs. Therefore, we developed our own simple depletion solver based on the OpenMC framework to recover reactions and decay chains. The evaluation library used was ENDF/B-VII.1. It solves the evolution of nuclide quantity vector X over time:

$$\dot{X} = \mathbf{A}X. \tag{3}$$

In this equation, $\mathbf{A}$ is the mass-transfer matrix. Each component takes the following form:

$$i \neq j \Rightarrow \mathbf{A}_{i,j} = +\lambda_{j\to i} + \sigma^{1g}_{j\to i}\phi, \tag{4}$$

$$i = j \Rightarrow \mathbf{A}_{i,i} = -\lambda_i - \sum_k \sigma^{1g}_{i\to k}\phi, \tag{5}$$

with i and j the i^{th} and j^{th} component of the quantity vector X, respectively. A reaction or decay transferring a given quantity from the X_i to the X_j component is symbolised by $i \rightarrow j$.

Therefore, as coefficients are constant over time, the system of equation is linear and can be easily solved. The depletion solver we developed is based on the *SciPy* Python library and uses a *Radau* method. Once the quantity vector is obtained for every time step, each component is weighted by the nuclide associated decay constant to get each nuclide contribution to activity.

3 Results & Discussion

This section evaluates the computed activity curves, then performs a sensitivity analysis, and finally, propagates uncertainties to compute the activation uncertainty.

3.1 Activity curves

The activity of dominant nuclides from iron and nickel activation foils are displayed in figure 5 over 90 days of decay time following irradiation. The variety of activation products created during irradiation provides various activity "periods" after the reactor operation. Nuclides with smaller half-lives contribute to the activity early in the decay time, while long-term behavior is dominated by nuclides with longer half-lives. In the case of nickel foil, the long-term behavior in the sample activity is dominated by ^{58}Co ($t_{1/2}$ = 70.86 days) produced from the reaction ^{58}Ni(n,p)^{58}Co. For iron foils, the long-term activity is dominated by ^{55}Fe and ^{59}Fe ($t_{1/2}$ = 1002 and 44.5 days, respectively). Both ^{55}Fe and ^{59}Fe are produced by thermal neutron absorption in the reactions ^{54}Fe(n,γ)^{55}Fe and ^{58}Fe(n,γ)^{59}Fe, respectively.

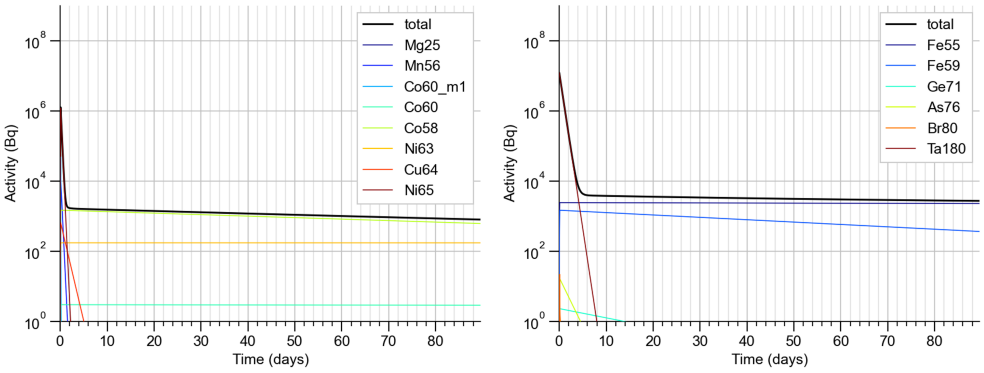

Figure 5. Activity vs. time for a nickel foil (left) and an iron foil (right).

3.2 Sensitivity computations

For each variable, sensitivity is calculated by increasing the value of the variable by 1% and recalculating the activity. Next, we calculate the mean of the relative difference between the recalculated activity and the reference activity (with no change in the variables). Four parameters had an important impact on sensitivity (see table 2). Uncertainties caused by

irradiation and atom quantity can be reduced by correcting the computed activity by the measured irradiation time and mass of the sample to irradiate. Therefore, this pre-analysis provides no evaluation of these uncertainties. Nevertheless, uncertainty on flux and cross sections must be evaluated with precision to estimate activity uncertainty.

Table 2. Sensitivity of mean activity to different parameters.

Quantity	Computed sensitivity
Flux	1.0%/%
Irradiation Time	1.0%/%
Atoms Quantity	1.0%/%
Cross sections	1.0%/%

Uncertainty of the flux as defined in Eq.2 can be easily propagated as it is directly output by OpenMC. However, the microscopic cross-section uncertainty can only be evaluated if a sensitivity analysis for each nuclide and each reaction is performed. An example of sensitivity analysis is displayed in figure 6 accounting for every reaction per nuclide.

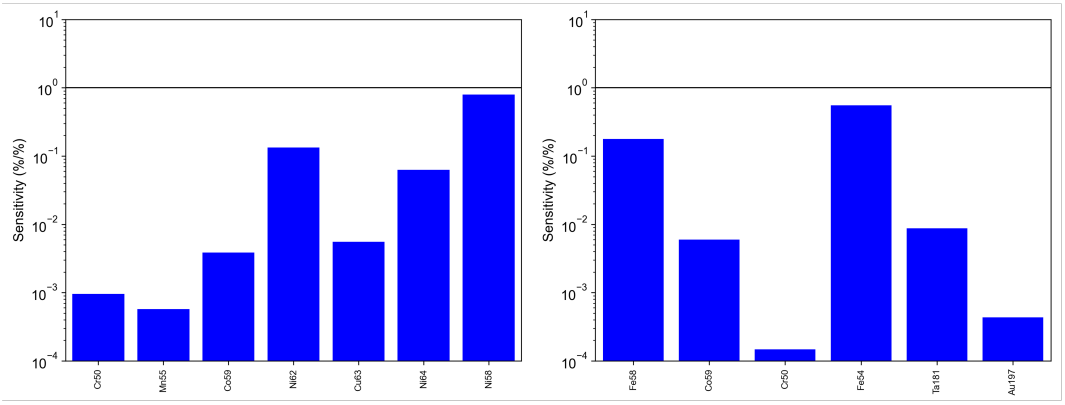

Figure 6. Highest sensitivity to nuclide cross sections for nickel foils (left) & iron foils (right).

3.3 Contribution to uncertainty

As we computed the activity sensitivity to the microscopic cross section for each reaction and nuclide, we can propagate the uncertainty computed by OpenMC. The results are displayed in table 3. Uncertainties have been propagated neglecting correlations.

The computational cost of our simulation is $50,000\,\text{CPU} - \text{h}$. For most activation materials, the uncertainty respects the 3% uncertainty criterion set in the introduction. Convergence still needs to be improved for foils 3, 4, and 5 and fission dots. Most of the wire sections respect the 3% uncertainty criterion. Our pre-analysis demonstrates that microscopic cross-section evaluation has the highest contribution to uncertainty compared to flux uncertainty. However, it should be noted that the uncertainty associated with the nuclear data evaluation is not negligible, and can sometimes be greater than the stochastic

Table 3. Sensitivity of mean activity to different parameters.

Material name	Cross-section uncertainty	Flux uncertainty	Total (2σ)
foil1 - 0	1.8%	0.3%	1.8%
foil1 - 1	2.3%	0.3%	2.3%
foil1 - 2	1.9%	0.3%	2.0%
foil2 - 0	0.3%	0.4%	0.5%
foil2 - 1	0.4%	0.3%	0.5%
foil2 - 2	0.4%	0.3%	0.5%
foil3 - 0	2.3%	0.3%	2.3%
foil3 - 1	4.0%	0.3%	4.0%
foil3 - 2	3.9%	0.3%	3.9%
foil4 - 0	5.0%	0.3%	5.0%
foil4 - 1	6.7%	0.4%	6.7%
foil4 - 2	6.2%	0.4%	6.3%
foil5 - 0	4.3%	0.3%	4.3%
foil5 - 1	5.7%	0.5%	5.7%
foil5 - 2	5.4%	0.3%	5.4%
foil6 - 0	1.9%	0.4%	1.9%
foil6 - 1	1.7%	0.3%	1.7%
foil6 - 2	1.8%	0.4%	1.8%
dot - 0	9.4%	1.1%	9.5%
dot - 1	8.3%	0.9%	8.4%
dot - 2	8.9%	1.0%	8.9%
dot - 3	9.8%	0.9%	9.8%
dot - 4	10.7%	0.8%	10.7%
dot - 5	9.6%	0.9%	9.6%
tab - 0	2.4%	0.3%	2.4%
tab - 1	2.7%	0.4%	2.7%
tab - 2	1.9%	0.4%	2.0%
tab - 3	2.1%	0.4%	2.1%
tab - 4	1.8%	0.4%	1.8%
tab - 5	1.7%	0.4%	1.8%
wire - 0	0.3%	0.2%	0.3%
wire - 1	0.3%	0.2%	0.4%
wire - 2	0.3%	0.1%	0.3%
wire - 3	0.3%	0.2%	0.4%
wire - 4	0.4%	0.2%	0.5%
wire - 5	0.4%	0.3%	0.5%
wire - 6	0.5%	0.3%	0.6%
wire - 7	0.5%	0.4%	0.6%
wire - 8	0.9%	0.5%	1.0%
wire - 9	1.6%	0.9%	1.8%
wire - 10	3.7%	1.6%	4.1%

uncertainty. The materials used in the experiment have been chosen to minimize this uncertainty, but further investigation during the future experimental analysis might be necessary.

Other sources can cause errors in activity evaluations, such as the P/h^* ratio. Indeed,

TREAT power is measured towards the thermal balance sheet, which lacks precision. However, this induces the same bias for every activity measurement, which can be corrected with a post-experiment analysis. Correcting this bias will be crucial to analyze more complex experiments involving temperature-limited or clipped transients. Once this and the other experimental biases are corrected, we expect measurements to remain in the range of uncertainty computed in this analysis.

4 Conclusion

This work presents a pre-analysis of a TREAT experiment where dosimetry materials are activated under a steady-state flux. The OpenMC Monte Carlo code is employed along other custom tools. Our goal is to keep model statistical uncertainty below 3%, which is overall respected regarding dosimetry materials activity. Therefore, we have demonstrated the capabilities of OpenMC as a powerful experiment analysis tool. Experimental results of the free-field characterization campaign in TREAT are expected soon. Hence, our future work is a complete experiment interpretation based on our computation scheme. This future work will provide valuable data and quantity of interest for operating the TREAT reactor in its new configuration.

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