Sensitivity Studies, Gap Analysis, and Benchmark Experiment Optimization for Reactor Physics and Criticality Safety Applications

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INTRODUCTION

Many new reactor designs, such as advanced reactors and micro reactors, have materials that lack nuclear data validation. This is also true for many other applications in criticality safety and global security. Both differential and integral experiments are needed to validate cross-section data. Without this, a user cannot have confidence in the predicted results of a radiation-transport code. This work describes an approach called ARCHIMEDES (Application Relevant Critical/Subcritical HEU/Pu-based Integral Measurements for Enhancing Data and Evaluating Sensitivities) to design new criticality experiments that have similar k_{eff} cross-section sensitivities to an application of interest. This process involves simulations to generate cross-section sensitivities to a parameter of interest (such as k_{eff}), a gap analysis to determine which existing benchmarks are most similar to the application, and an experiment optimization.

Recently, there has been a great deal of interest in the reactor physics community on advanced reactors, micro reactors, and accelerator driven systems (ADS). This work will apply the described method to specific examples in this area. The focus of this work will be on the sensitivity study and gap analysis, while future work will include experiment design.

BACKGROUND

Evaluators use nuclear data from high-quality differential measurements combined with sophisticated theoretical model calculations to create nuclear data libraries such as ENDF/B-VIII.0 [1]. Comparisons of simulated and measured data from benchmark-quality integral measurements are then used to validate the nuclear data and computational methods. LANL has designed and executed integral experiments (critical and subcritical benchmarks) since 1946 [2]. Starting in 1992, these experiments have been documented in the International Criticality Safety Benchmark Evaluation Project (ICSBEP) [3], which contains thousands of critical and subcritical configurations. The ICSBEP benchmark models are used to test both nuclear data and computational methods. Testing with these benchmarks is performed for every cross-section library release (such as in Section XII of the ENDF/B-VIII.0 release [1]) as well as for releases of radiation transport codes (such as MCNP®[1] [4]).

When designing criticality experiments, Monte Carlo codes have often been used and generally involve a perturbation technique. With adjoint-based methods, a single model can be used to determine k_{eff} cross-section sensitivities to every nuclide and reaction present in the model. The sensitivity coefficient ($S_{k,x}$) with respect to k_{eff} for a nuclear data item x is the ratio of the relative differential change in k_{eff} to the relative differential change in x as seen in Eq. 1. Note that "k" is used to represent k_{eff} in the equations used in this work. A review of the history of perturbation and sensitivity techniques for Monte Carlo codes has been published [5].

$$S_{k,x} = \frac{\partial k_{eff}/k_{eff}}{\partial x/x} \quad (1)$$

The Whisper [6] code was developed for criticality safety applications and compares the k_{eff} cross-section sensitivities of an application model to a suite of criticality benchmarks. The sensitivity coefficients from Eq. 1 are organized into a sensitivity row vector S. This is done both for the application model (A) and each benchmark model (B). The cross-section library (such as ENDF) is used to obtain the nuclear data covariance matrix C_{xx}. The covariance in k_{eff} for systems A and B is found using Eq. 2.

$$Cov_k(A,B) = S_A C_{xx} S_B^T \quad (2)$$

The variance is the special case when two models are the same as shown in Eq. 3.

$$Var_k(A) = Cov_k(A,A) = S_A C_{xx} S_A^T \quad (3)$$

The similarity coefficient (c_k) for models A and B is given in Eq. 4.

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$$c_k(A,B) = \frac{Cov_k(A,B)}{\sqrt{Var_k(A)}\sqrt{Var_k(B)}} \quad (4)$$

A c_k of 1 means that the systems have identical sensitivities. For ARCHIMEDES the main use of Whisper is to determine similarities between the application model and benchmark models. We will also use proposed experiments instead of existing benchmark models.

As mentioned above, criticality experiments are designed either to help validate a nuclear data need or to match a specific application. When designing an experiment for a nuclear data need, the sensitivity coefficient ($S_{k,x}$) is typically maximized for the nuclear data item x in the energy range of interest. Even after adjoint-based capabilities were introduced, this was typically done using brute force perturbations. For this type of approach, one first determines their constraints (often based on available nuclear material), then performs perturbations on a large number of variables (moderator material, moderator thickness, reflector material, etc.) and finally runs Monte Carlo simulations before selecting the best design(s). In recent years, this approach has been performed with a mathematical optimization. To date, this has included Bayesian optimization [7], genetic algorithm [8], and Powell's method [9].

METHOD

An example of the process flow for ARCHIMEDES is shown in Fig. 1. This process has been previously described [10]. The first step in the process is to generate a model of the application (shown at the top in Fig. 1). The second step is to use the radiation-transport code(s) to determine cross-section sensitivities. These sensitivities are determined for the application model as well as ~1300 ICSBEP and IRPhEP [11] benchmark models. For this work MCNP6.2 [12] has been used to generate the models and perform the radiation-transport.

The third step is to perform a gap analysis, which compares the application to existing criticality benchmarks. Two methods are utilized for the gap analysis. The first method uses the Whisper [5] code to compare the application to a library of criticality benchmarks based on k_{eff} cross-section sensitivities as described in the background section. In addition, a second method distills sensitivity data into a readable form through the use of heatmaps as shown in Fig. 2. The heatmap tool [13] was developed to identify gaps in integral benchmarks. It first reads in the k_{eff} cross-section sensitivities of ICSBEP benchmarks. The user then provides a sensitivity cutoff (10^{-3} was used for this work). The tool creates plots that show the number of benchmarks that exceed that cutoff for that energy bin.

The last step in the process is perform an experiment optimization (bottom of Fig. 1). The goal of the optimization in this work is to design a new critical experiment that has a higher similarity coefficient to the application than the existing ICSBEP benchmarks. Given that, it is desirable for the similarity coefficient (c_k) to be as high as possible for the experiment design. For this work, Bayesian optimization is used in which c_k is maximized using a Gaussian Process (GP) [14]. The bottom of Fig. 1 shows a contour plot for an example problem; the contour lines are for various c_k values. This optimization has been previously described in detail [15-16]. The impact of this specific PF-4 casting problem has been shown in other work [17].

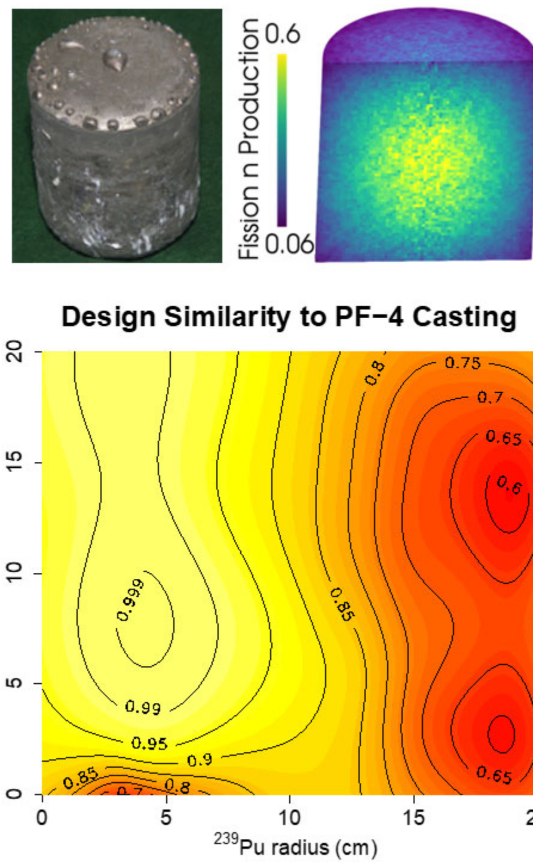

Figure 1. ARCHIMEDES Process. A Pu ingot is shown at top and an experiment optimization for Pu casting is shown at the bottom.

RESULTS

This work investigates the cross-section sensitivities and gap analysis for three examples. The first is based upon the Travelling Wave Reactor (TWR) [18]. It should be noted that cross-section sensitivities have been previously investigated for the TWR [19]. The second example is Kilopower, which is a design for a compact fission nuclear power system to enable long-duration stays on planetary surfaces [20]. The Kilopower Reactor Using Stirling Technology (KRUSTY) [21] experiment, built at the

National Criticality Experiments Research Center (NCERC) [22], was designed as a demonstration for Kilopower. The third example is a lead-bismuth eutectic cooled accelerator-driven system (ADS) to transmute minor actinides (MAs) designed by the Japan Atomic Energy Agency (JAEA) [23].

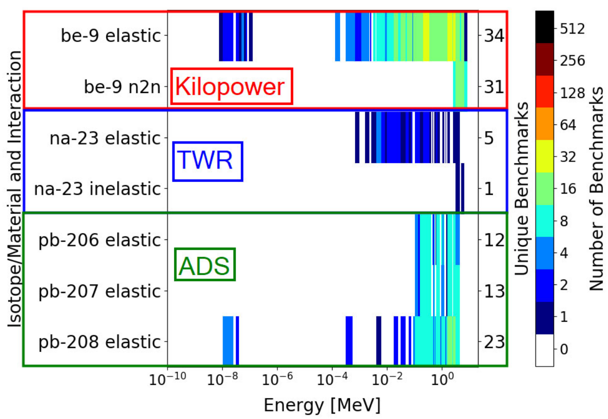

Figure 2. Heatmap showing the number of benchmarks similar to several reactions of interest for the three examples.

The most important reactions (ranked by $|S_{k,x}|$ when the sensitivities are integrated over all energies) will be shown in the presentation. For the TWR, the expected fissionable material reaction cross-sections (^{235}U ν and fission) have the highest sensitivities. It can also be seen that ^{23}Na elastic scattering plays a role, which is important since it likely has higher cross-section uncertainties. Very few experiments exist as shown in Fig. 2. For Kilopower it is not surprising that ^{235}U and ^{9}Be reactions are the most important. For the ADS system many actinides are important (Np, Pu, and Am). In addition, the ADS system is somewhat sensitive to both elastic and inelastic scattering for the nuclides that make up the majority of Pb abundance (206, 207, and 208). Elastic scattering for these nuclides are shown in Fig. 2; inelastic is not shown as there are no benchmarks that exceed the sensitivity threshold for these reactions.

Table I shows the benchmarks that are most similar (highest c_k) for the TWR example, as calculated by Whisper (the other applications will be shown in the presentation). For the TWR example it can be seen that ICSBEP and IRPhEP benchmarks with high c_k values exist. Also high on this list are two Zeus-based HEU/NU configurations (labelled “Zeus LEU” in Table I) which are being prepared for submission to ICSBEP [24]. These experiments were actually performed to provide lead data associated with the ADS application. It should be noted, however that none of these top benchmarks are among those sensitive to ^{23}Na scattering in Fig. 2. This shows the need to look at a similarity coefficient for specific reactions only. This subject is further explored in [16], which is also presented at this conference.

For Kilopower, many HEU-MET-FAST series benchmarks exist which have high c_k values. Note that the KRUSTY experiment has a c_k value of 0.9975, even higher than the top benchmark in the current suite; this is not surprising, since KRUSTY was designed using the same fuel and reflectors as Kilopower. For the ADS system all benchmarks have very low c_k values. This is due to the importance of minor actinides in the ADS system. This, combined with the general lack of benchmarks with other actinides, shows the importance of future experiments to study these isotopes and the need to look at similarity coefficients for specific reactions.

Table I. Benchmarks with the highest similarity coefficient (c_k) for the TWR application.

TWR	
benchmark	c_k
ZPR-FUND-EXP-003-001	0.9924
BFS2-FUND-EXP-001-001	0.9847
ZPR-FUND-EXP-005-001	0.9782
ZPR-FUND-EXP-001-001	0.9513
ZPR-FUND-EXP-004-001	0.9497
Zeus LEU	0.9382
Zeus LEU	0.9376
ieu-met-fast-005-001	0.9267

CONCLUSIONS

Advanced reactors, micro reactors, and ADS systems have new nuclear data needs. This work applied a process to investigate the cross-section sensitivities and perform a gap analysis on three examples relevant to the reactor community. Results show the importance of new critical experiments for Na, Pb, and actinides (such as Np and Am). Future work includes performing an experiment optimization to design potential critical experiments for these applications. This will include investigations of contributions of specific reactions to the similarity coefficient as described in a separate talk at this conference [16].

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