NEUTRONIC BENCHMARKING OF SMALL GAS-COOLED SYSTEMS

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ABSTRACT

To demonstrate that nuclear reactors can be built faster and more economically than they have been in the past, the US Department of Energy Office of Nuclear Energy is sponsoring the development of a small nuclear reactor called the Transformational Challenge Reactor (TCR) \cite{1–2}. An important part of the design and licencing process of a new reactor is validation of the software used to analyze the reactor using established reactor physics benchmarks. This paper discusses validation of the neutronics software used to model four preliminary designs of the TCR core \cite{2}. Because the TCR core design uses innovative technology and methods, comparable established benchmarks are limited or do not exist. For this effort, established benchmarks from the International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP) \cite{3} were considered to be suitable for this design based on analysis using the SCALE/TSUNAMI-computed similarity indices to determine the amount of shared uncertainty between the design and each selected benchmark experiment. This paper addresses the challenges faced in benchmarking a unique reactor for licensing and construction, a task that will become more common as a new generation of innovative nuclear reactors are designed and built.

KEYWORDS: benchmark, validation, TSUNAMI, KENO, ICSBEP

1. INTRODUCTION

Neutronics modeling of the Transformational Challenge Reactor (TCR) is being performed in the SCALE module KENO-VI \cite{4}. To investigate the accuracy of KENO’s effective multiplication factor ($\text{k}_{\text{eff}}$) calculation for TCR designs, the TCR models (applications) were compared to models (benchmarks) that have been validated with physical experiments. The benchmarks for the comparison comprised 2,500 benchmarks from the International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP) \cite{3}.

This work is critical to the design process. The result of this study—the estimated error between computational and experimental $\text{k}_{\text{eff}}$—informs the process of designing the reactor core. Depending on the study’s results, the design must incorporate characteristics (e.g., reactivity adjustment mechanisms) to ensure that the reactor goes critical while still being safe. This process is especially important for advanced reactors, because significantly fewer advanced reactors have been built and operated than conventional light water reactors (LWRs). Therefore, there is less historical knowledge about the operation of advanced reactors than LWRs. Additionally, reactor designers and analysts have less experience with advanced reactor concepts \cite{5}.

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2. METHOD AND APPROACH

KENO is a three-dimensional Monte Carlo criticality computer code. KENO outputs each case’s effective multiplication factor (k\(_{\text{eff}}\)) and energy corresponding to the average lethargy causing fission (EALF). After each case has been run in KENO, it is run in the SCALE module TSUNAMI [6]. TSUNAMI (Tools for Sensitivity and Uncertainty Analysis Methodology Implementation) is used for sensitivity and uncertainty (S/U) analysis—it computes nuclear data sensitivity coefficients to establish similarity between benchmark experiments and design applications [7]. Then each case is compared to the benchmarks in the ICSBEP using the SCALE module TSUNAMI-IP.

For each comparison, TSUNAMI-IP returns an index for similarity assessment, c\(_k\). This index describes the shared uncertainty in k\(_{\text{eff}}\) values of the application and benchmark due to cross section uncertainties. The c\(_k\) varies from 0 to 1; a c\(_k\) value of 1 means that the uncertainties all come from the same reactions and nuclei at the same energies. This demonstrates that the experiment is a good fit for the application. A c\(_k\) value of 0 indicates that there is no similarity in the uncertainties [8]. A c\(_k\) value above 0.8 indicates that there is enough similarity to explore further. For cases in which none of the ICSBEP benchmarks were similar to the case being analyzed, the lower limit for the similarity index was dropped to 0.7.

Another important parameter in determining the similarity of the experiment to the application is the EALF, a single value used to describe the spectrum of the system. EALF is used to compare systems instead of relying on the average energy-causing fission, because “the logarithmic weighting of the neutron energy makes it easier to compare moderated systems” [9]. It is important to use continuous or very fine group cross sections when determining EALF to ensure its accuracy.

The benchmark cases used to compare to the applications in this work were run using KENO-VI ENDF/B-VII in 238 groups or continuous energy. The applications were run in SCALE 6.2.3/KENO-VI ENDF/B-VII using continuous energy.

3. RESULTS

Four candidate core designs exist consisting of different fuel and moderator forms. Case 1 has an intermediate spectrum and the fuel is TRISO particles. Case 2 has a thermal spectrum and the fuel is TRISO particles. Case 3 has a fast spectrum and the fuel is solid UO\(_2\) fuel. Case 4 has an intermediate energy spectrum and has solid UO\(_2\) fuel.

3.1 Case One

When Case 1 was compared to the ICSBEP benchmarks, 48 benchmarks had a c\(_k\) value above 0.8. Figure 1a shows that the spread of EALF values well encompasses Case 1’s EALF value: the experimental data are shown in blue, and the application is shown in red. The trend of the experimental data predicts a higher application EALF than is actual. This suggests that c\(_k\) and EALF will predict different biases.
**Figure 1a. EALF for the relevant experiments and Case 1.**

Figures 1b and 1c below show two different methods for estimating the error (delta k) between the application and a theoretical physical experiment of the application. Both figures show the error in $k_{\text{eff}}$ in per cent mille (pcm) for the 48 benchmarks with $c_k$ values above 0.8 when compared to Case 1. The dotted red lines are linear trend lines based on the benchmark values.

In Figure 1b, the trend line predicts that the $k_{\text{eff}}$ produced by KENO for Case 1 will be 1,410 pcm above its measured experimental value. In Figure 1c, the black line shows the EALF for Case 1, and the trend line predicts that the $k_{\text{eff}}$ produced by KENO for Case 1 will be 525 pcm below its measured experimental value. While these two methods produce different results neither of these methods is more correct than the other. Two results simply narrow down the range of possible answers.

**Figure 1b and 1c. The error between the model (left) and the corresponding experiment (right) as a function of $c_k$ and EALF.**

The charts in Figures 1b and 1c above show a cluster of experiments with suspiciously large error, as indicated with red ovals. These seven experiments belong to experiment IEU-MET-FAST-022. When they are removed, the figures change as shown below.
Figure 1d. Updated EALF for the relevant experiments and Case 1.

Figures 1e and 1f. The updated error between the model and the corresponding experiment as a function of $c_k$ and EALF.

After the previously referenced experiments were removed, the error in $k_{\text{eff}}$ in Figure 1e is 573 pcm, and the error in $k_{\text{eff}}$ in Figure 1f is 857 pcm. With this change, the estimation from the method in Figures 1b and 1e changed from -1410 to 573 pcm, and the estimation using the methods in Figures 1c and 1f changed from 525 to 857 pcm. The large change in the estimated value in the method used in Figures 1b and 1e shows that, in this case, this method is highly influenced by outliers.

3.2 Case Two

When Case 2 was compared to the ICSBEP models, no models were found with a $c_k$ value above 0.8. However, when the lower limit for $c_k$ was reduced to 0.7, 36 models were found with $c_k$ values between 0.7 and 0.8. Comparing the application to benchmarks that are not very similar is suboptimal; however, the analysis is limited to the experiments that have currently been evaluated. Figure 2a below shows that the spread of EALF values are lower than Case 2’s value. This is because all the benchmarks that matched with the application were classified as thermal, and the EALF of the application (0.7eV) is higher than in most thermal experiments.
**Figure 2a. EALF for the relevant experiments and Case 2**

Figures 2b and 2c below show two different ways of estimating the error (delta k) between the application and a theoretical physical experiment of the application. Both figures show the error in $k_{\text{eff}}$ in pcm for the 36 benchmarks that had $c_k$ values above 0.7 when compared to Case 2. The dotted red lines are linear trend lines based on the benchmark values.

The trend line in Figure 2b predicts that the $k_{\text{eff}}$ produced by KENO for Case 2 will be 3,608 pcm above its measured experimental value. In Figure 2c, the black line shows the EALF for Case 2. The trendline predicts that the $k_{\text{eff}}$ produced by KENO for Case 2 will be around 735 pcm above its measured experimental value.

**Figure 2b and 2c. The error between the model and the corresponding experiment as a function of $c_k$ and EALF.**

Figures 2b and 2c show a cluster of experiments with suspiciously large error, as indicated with red ovals. These five experiments belong to experiment LEU-COMP-THERM-045. An in-depth review of LEU-COMP-THERM-045 reveals several aspects of the experiment that call its validity as a benchmark into question. The fuel is $U_3O_8$ powder instead of $UO_2$, which could cause the differences. The fuel was made by putting powdered $U_3O_8$ in plastic bags and sealing them with small paper-covered twist wires and pressing the bag until the powder became solid. After this process, the plastic could not be removed from the fuel blocks, and it was found that “All of the cans were found to be slowly but steadily gaining weight.” [10] There are additional concerns regarding the accuracy of the concrete reflector composition in the cases in question, as well as the amount of filler used in the plexiglass reflected versions: “The exact dimensions and placement of all Plexiglas filler pieces were not provided.” [10] The filler used here is a material with the same composition as the reflector, and it was placed between the stacked oxide cans when they did not completely fill the available space inside the reflector shell. This experiment produced 21 critical experiments, and 14 out of 21 experiments had a difference in $k_{\text{eff}}$ greater than 1,000 pcm compared to the KENO ENDF V.II $k_{\text{eff}}$ values, with the error ranging between -767 and 2,159 pcm. Four of the five cases that are similar to the application described herein have errors above 1,000 pcm. When these cases are removed, the figures change as shown below.
Before the experiments were removed, the estimated error in $k_{\text{eff}}$ in Figure 2b was -3,608 pcm, and the estimated error in Figure 2c was -735 pcm. After the experiments were removed, the estimated error in Figure 2e is 1,119 pcm, and the error estimated in Figure 2f is 314 pcm. The large changes in each estimation of error when the experiments were removed suggest that for this case, both methods are influenced by outliers. Additionally, in the method shown in Figures 2c and 2f, the estimated error in $k_{\text{eff}}$ is conventionally found by interpolating between the experiments EALF values. However, if the previously referenced experiments are removed, this is no longer possible which adds uncertainty to the accuracy of Figure 2f.

### 3.3 Case Three

When Case 3 was compared to the ICSBEP benchmarks, 45 were found that had a $c_k$ value above 0.8. Figure 3a shows that the spread of EALF values well encompasses the model’s value. Unlike in Figure 1a, the trend of the benchmarks predicts an EALF close to the actual value of the application.
Figures 3b and 3c below show two different methods of estimating the error (delta k) between the application and a theoretical physical experiment of the application. Both figures show the error in $k_{\text{eff}}$ in pcm for the 45 benchmarks that had a $c_k$ value above 0.8 when compared to Case 3. The dotted red lines are linear trend lines based on the benchmark values.

The trend line in Figure 3b predicts that the $k_{\text{eff}}$ produced by KENO for Case 3 will be 2,517 pcm above its measured experimental value. In Figure 3c, the black line shows the EALF for Case 3. The trendline predicts that the $k_{\text{eff}}$ produced by KENO for Case 3 will be 102 pcm below its measured experimental value.

Figures 3b and 3c show a cluster of seven experiments with suspiciously large error, as indicated with red ovals. These experiments belong to experiments IEU-MET-FAST-022 and IEU-MET-INTER-001. When they are removed, the figures change as shown below.
3.4 Case Four

When Case 4 was compared to the ICSBEP models, 36 were found that had a $c_k$ value above 0.8. Figure 4a shows that the benchmark EALFs are higher than in the applications. This is because Case 4 is in the intermediate energy range, and the ICSBEP does not have many experiments in that range.
Figure 4b predicts that the $k_{\text{eff}}$ produced by KENO for Case 4 will be 3,062 pcm above its measured experimental value. Figure 4c predicts that the KENO value will be 24 pcm below experimental value. However, Figure 4c only has one experiment with a close EALF, making the uncertainty that comes with its predicted delta $k$ high.

![Figure 4b and 4c. The error between the model and the corresponding experiment as a function of $c_k$ and EALF.](image)

Figures 4b and 4c above show a cluster of seven experiments with suspiciously large error, as indicated with red ovals. These same experiments were suspicious in Case 3, as well. These experiments belong to experiments IEU-MET-FAST-022 and IEU-MET-INTER-001. When they are removed, the figures change, as shown below.

![Figure 4d. Updated EALF for the relevant experiments and Case 4.](image)

After the previously referenced experiments were removed, the error in $k_{\text{eff}}$ in Figure 4e is -2128 pcm, and the error in $k_{\text{eff}}$ in Figure 4f is 944 pcm. With this change, the estimation from the method in Figures 4b and 4e changed from -3,062 to -2128 pcm, and the estimation using the methods in Figures 4c and
4f changed from -24 to 944 pcm. In both methods, removal of these experiments led to an increase in the predicted $k_{\text{eff}}$ error by approximately the same amount.

4. CONCLUSIONS

In Case 1, the range of predicted $k_{\text{eff}}$ values is between 525 pcm and -1,410 pcm. The range of predicted $k_{\text{eff}}$ values in Case 2 is between 1,119 and -3,608 pcm. In Case 3, the range of predicted $k_{\text{eff}}$ values is between 660 pcm and -2,517 pcm. In Case 4, the range of predicted $k_{\text{eff}}$ values is between 944 pcm and -3,062 pcm.

These results show high predicted error. The experimental uncertainty in $k_{\text{eff}}$ is usually less than 100 pcm. Additionally, when comparing experimental and computational models, the error in $k_{\text{eff}}$ is below 1,000 pcm. The high predicted error and the uncertainties related to that error are caused by a lack of sufficiently similar experimental data. This is especially seen in Case 2, in which no experiments had an acceptably high $c_0$, and it is also evident in Cases 2 and 4, in which few experiments had similar EALF values. The lack of evaluated experiments for intermediate energy range and intermediate enrichment reactors is well known: currently only 268 out of 4,913 experiments in the ICSBEP have intermediate enrichment levels [11]. The ICSBEP is currently evaluating several of these experiments to determine if they are detailed and accurate enough to become evaluated benchmarks [12].

The future steps for this project are to downselect to one design and evaluate that design in more detail using additional methods. Additionally, the values that are the result of this work will be utilized by the TCR design team to ensure that reactor can go critical while still remaining safe.

ACKNOWLEDGEMENTS

This research is supported by the DOE-NE Transformational Challenger Reactor Program.

REFERENCES

1. V. Sobes, B. Hiscox, E. Popov, M. Delchini, R. Archibald, C. Hauck, P. Laiu, B. Betzler, and K. Terrani, “Artificial Intelligence Design of Nuclear Systems Empowered by Advanced Manufacturing,” forthcoming, Proceedings of PHYSOR 2020, Cambridge, UK, March 29–April 2, 2020.
2. B.J. Ade, A.J. Wysocki, B.R. Betzler, M.S. Greenwood, P.C. Chesser, J.J.W. Heineman, P.K. Jain, J.R. Burns, B.D. Hiscox, K.R. Smith, J.M. Risner, J.D. Rader, F. Heidet and A. Bergeron, “Candidate Core Designs of the Transformational Challenge Reactor,” forthcoming, Proceedings of PHYSOR 2020, Cambridge, UK, March 29–April 2, 2020.
3. International Handbook of Evaluated Criticality Safety Benchmark Experiments, NEA/NSC/DOK/95(93), OECD-NEA, Paris, France (2016).
4. S.M. Bowman. “KENO-VI Primer: A Primer for Criticality Calculations with SCALE/KENO-VI Using GeeWiz,” Oak Ridge National Laboratory (2008).
5. B.T. Rearden, “Nuclear Data and Benchmarking Program” SCALE Users’ Group Workshop, Oak Ridge National Laboratory, August 28, 2018
6. B.T. Rearden, D.E. Mueller, S.M. Bowman, R.D. Busch, and S.J. Emerson, “TSUNAMI Primer: A Primer for Sensitivity/Uncertainty Calculations with SCALE,” Oak Ridge National Laboratory (2009).
7. M.L. Williams and B.T. Rearden, “SCALE-6 Sensitivity/Uncertainty Methods and Covariance Data,” Nuclear Data Sheets, Volume 109, Issue 12, pp. 2796–2800 (2008).
8. B.T. Rearden and M.L. Williams, “Overview of the SCALE TSUNAMI Sensitivity and Uncertainty Analysis Tools,” Proceedings of the American Nuclear Society Annual Meeting 2007, Washington DC, USA, November 11–15, 2007.
9. D. Mennerdahl, W. Weber, Y. Naito, and J. Anno, “Reference Values for Nuclear Criticality Safety Appendix H: Similarities between Applications and Benchmarks,” OCED/NEA pp. 331–399.
10. Karla R. Elam, “LEU-COMP-THERM-045 : PLEXIGLAS OR CONCRETE-REFLECTED U(4.46)3O8 WITH H/U=0.77 AND INTERSTITIAL MODERATION,” NEA/NSC/DOC/(95)03/IV. Volume IV.

11. J.D. Bess, J.B. Briggs, T. Ivanova, I. Hill, and J. Gulliford, “Availability of Neutronics Benchmarks in the ICSBEP and IRPhEP Handbooks for Computational Tools Testing,” Proceedings of the International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering (M&C 2017).

12. C.M. Percher, A.J. Nelson, W.J. Zywiec, S.S. Kim, and D.P. Heinrichs, “Thermal Epithermal Experiments (TEX): Test Bed Assemblies for Efficient Generation of Integral Benchmarks,” Proceedings of ICNC 2019, 11th International Conference on Nuclear Criticality Safety, September 15–20, 2019, Paris, France.