

LA-UR-24-23779

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Title: Designing a Deimos-based Microreactor Criticality Experiment with MCNP and Whisper

Author(s): Maldonado, Alexis
Hoffman, Keenan Jeffrey
Stolte, Kristin Nichole
Perfetti, Christopher M.
Cutler, Theresa Elizabeth
Trellue, Holly Renee

Intended for: Physics of Reactors (PHYSOR), 2024-04-21/2024-04-24 (San Francisco, California, United States)

Issued: 2024-04-22



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ANS[®] PHYSOR 2024

International Conference on Physics of Reactors

Designing a Deimos- based Microreactor Criticality Experiment with MCNP and Whisper

Alexis Maldonado, Keenan J. Hoffman,
Kristin N. Stolte, Christopher Perfetti,
Theresa E. Cutler, Holly R. Trelue



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Overview

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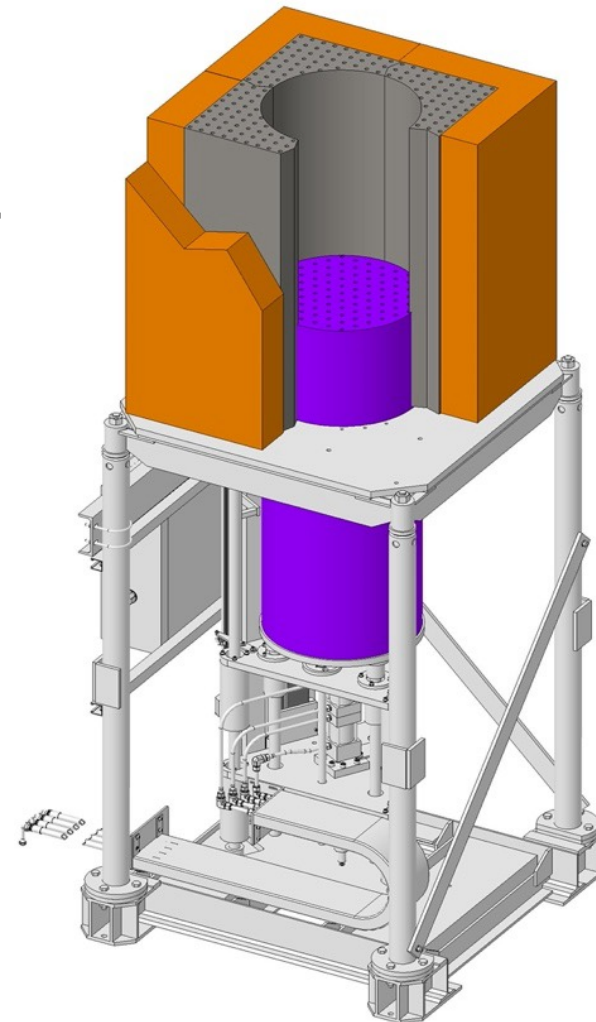
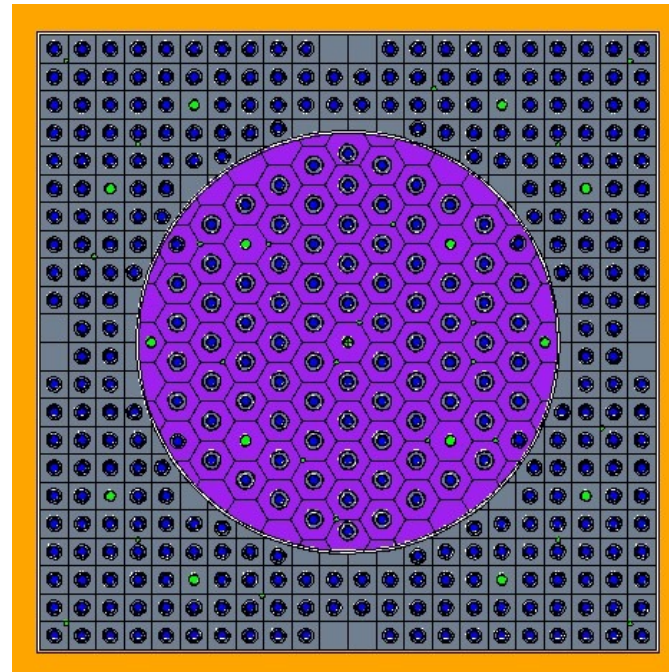
Introduction

- Experiments needed to better understand materials, reactivity, system behavior for advanced reactor concepts
 - Benchmark physics codes
 - Stepping-stone to full-scale prototype
 - Affordable and easier to execute
- **How do we know an experiment is representative of the full-scale system?**
 - For steady-state criticality simulations, correlation coefficients (C_k) are used
 - For transient simulations, work is underway to expand similarity coefficient framework with coupled multiphysics sensitivities

Deimos Experiment

- Graphite-moderated, beryllium-reflected, high assay low-enriched uranium (HALEU) tri-structural isotropic (TRISO) fueled experiment planned for summer 2024
- Will be executed at the National Criticality Experiment Research Center (NCERC)

- Orange, beryllium
- Gray, graphite, outer
- Purple, graphite, inner
- Blue, fuel
- Green, heater



Deimos Experiment

- Will be heated to 150°C to validate nuclear data at various temperatures
- Testbed for future advanced reactor experiments targeting +800 °C temperatures
- Potential benchmark for the International Criticality Safety Benchmark Evaluation Project (ICSBEP) and the International Handbook of Evaluated Reactor Physics Benchmark Experiments (IRPhE)

Theory - C_k Similarity Parameter

$$C_k(A, B) = \frac{S_A C_{xx} S_B^T}{\sqrt{S_A C_{xx} S_A^T} \sqrt{S_B C_{xx} S_B^T}}$$

Where:

- S_A and S_B^T are the sensitivity row vectors of systems A and B respectively
- C_{xx} is the nuclear data relative covariance matrix
- T is the transpose operator
- $C_k(A, B)$ is the correlation coefficient

Sensitivity coefficients are produced via Adjoint-based First-Order Perturbation Theory.

Theory - E_k Similarity Parameters

$$E_k(A, B) = \frac{S_A I_{xx} S_B^T}{\sqrt{S_A I_{xx} S_A^T} \sqrt{S_B I_{xx} S_B^T}}$$

Where:

- I_{xx} is the identity matrix in the same shape as the nuclear data covariance matrix

Unlike C_k , E_k does not fold in the nuclear data uncertainty, meaning it represents only the overlap between each system's sensitivity coefficients with respect to k for all nuclear data available

Methodology

- Monte Carlo N-Particle (MCNP6) code
 - Radiation Transport Code
 - Can generate sensitivity coefficients
- Whisper statistical code
 - Generates correlation coefficients, upper subcritical limits, and more with sensitivity coefficients
 - Whisper-tk is a Python version of Whisper that can be used to generate E_k similarity parameters and percentage of contributions to uncertainty

Similarity Coefficients for Deimos - ICSBEP

Table I. Top 10 C_k Benchmarks for the Deimos experiment and ICSBEP benchmarks

Benchmark	C_k	E_k
leu-comp-therm-028-017.i	69.06%	81.73%
ieu-comp-therm-002-003.i	69.06%	83.46%
leu-comp-therm-028-020.i	68.55%	81.54%
leu-comp-therm-028-018.i	68.40%	81.62%
leu-comp-therm-028-014.i	67.63%	83.28%
leu-comp-therm-028-019.i	67.59%	81.21%
leu-comp-therm-028-012.i	67.53%	83.27%
leu-comp-therm-028-016.i	67.32%	81.06%
leu-comp-therm-060-005.i	67.11%	87.22%
leu-comp-therm-060-006.i	66.88%	94.40%

Similarity Coefficients for Deimos – IRPhE and Others

Table II. Top C_k Benchmarks for the Deimos experiment and IRPhE benchmarks and select advanced reactor concepts

System	C_k	E_k
cnps_v58.i	84.42%	96.22%
snowflake_beo_300k_v0.i	78.83%	94.47%
htr10_gcr_resr_001_001.i	78.79%	92.68%
proteus_gcr_exp_001_001.i	77.58%	93.69%
vhtr_v0.i	76.34%	93.06%
snowflake_yh_300k_v0.i	72.94%	93.85%
rbmk_exp_001_001.i	63.23%	85.02%
agr_v0.i	57.43%	90.01%

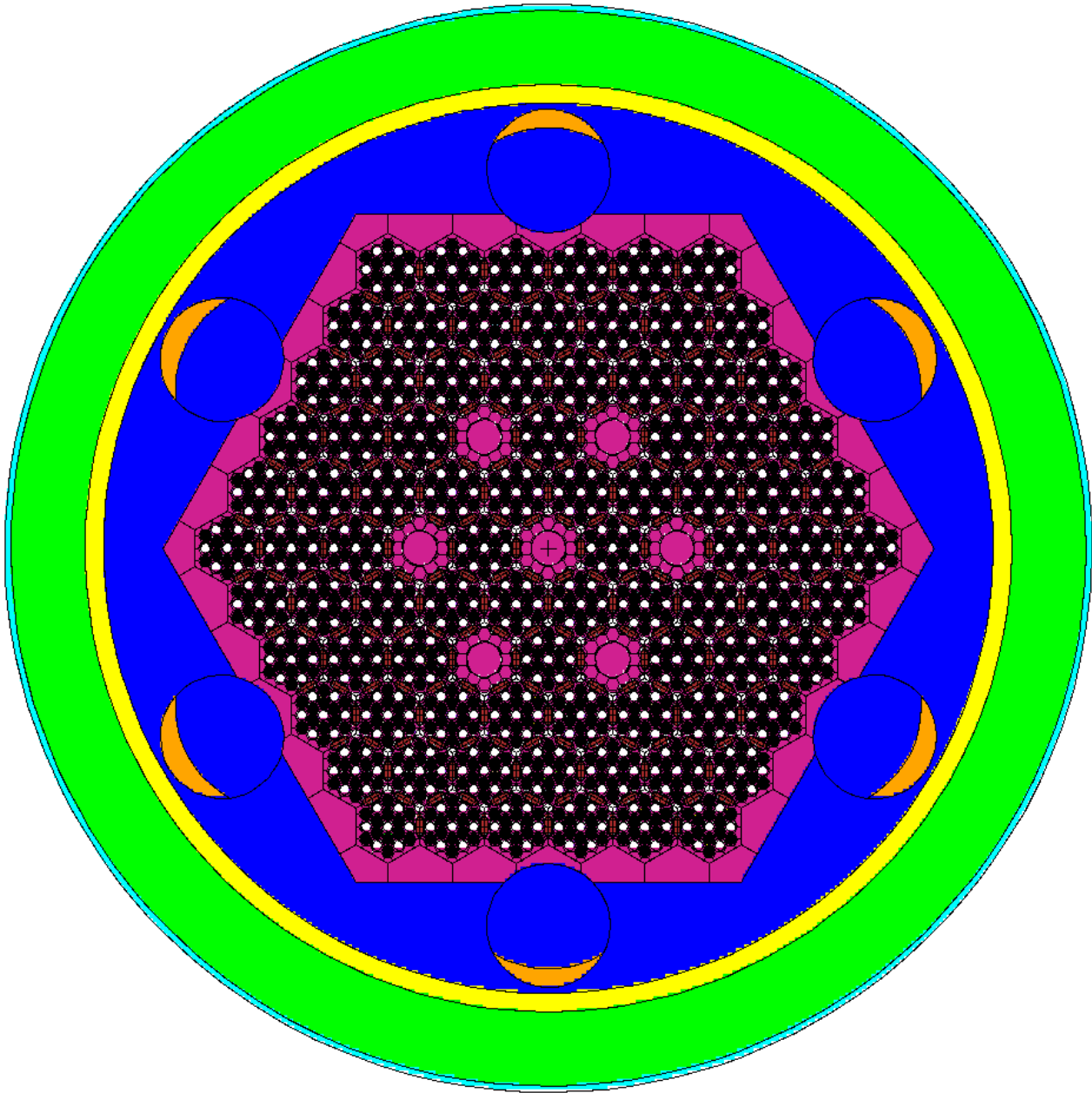
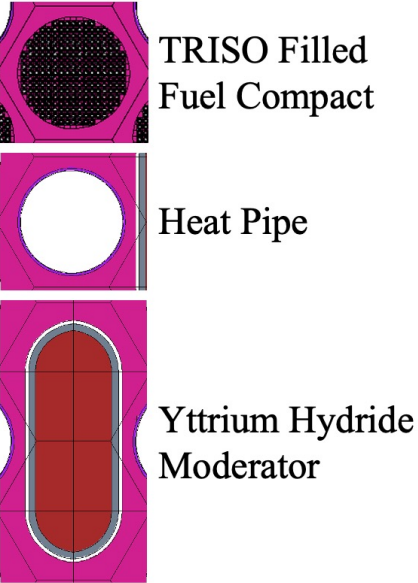
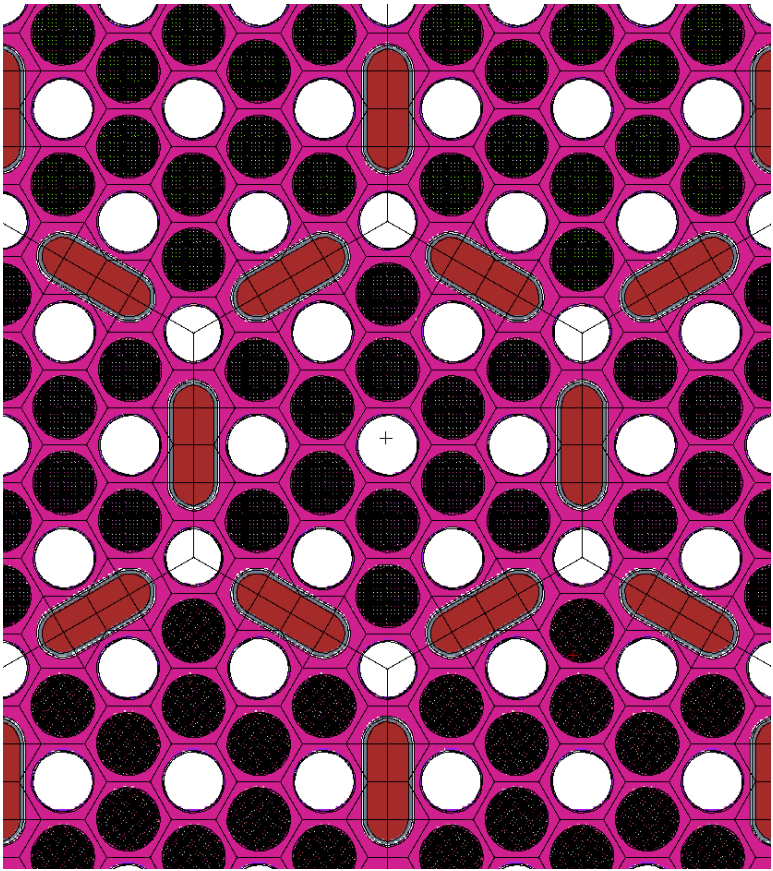
Takeaways

- Deimos is a unique experiment for both the ICSBEP and IRPhE benchmark suites
- Highest correlation coefficient is to the Compact Nuclear Power Source (CNPS) experiment, which uses the same fuel

Designing a Microreactor Criticality Experiment with over 95% C_k

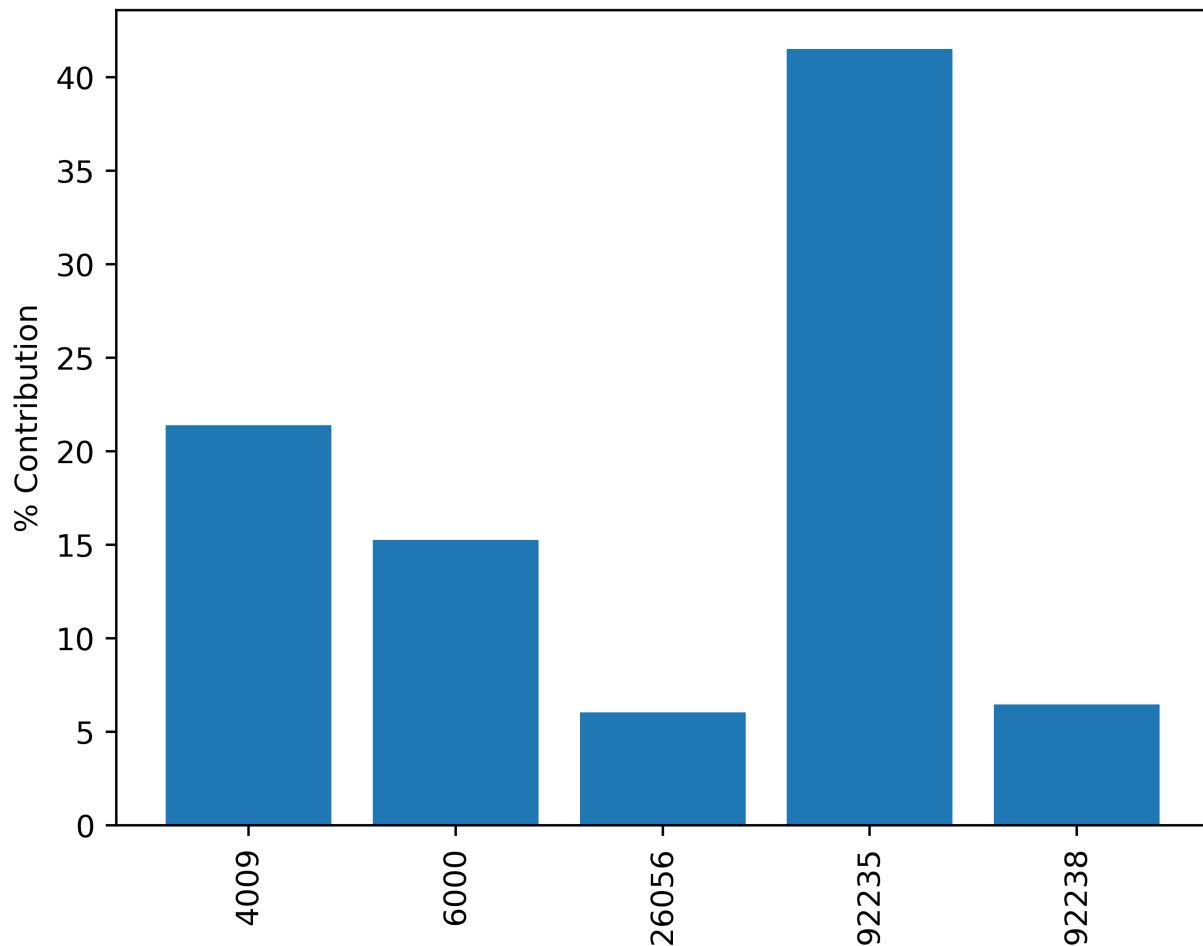
- The Nuclear Regulatory Commission (NRC) recommends a correlation coefficient of at least 90% for a demonstration of similarity for Nuclear Criticality Safety applications
- Designing such an experiment for an advanced reactor concept greatly improves confidence in nuclear data for conceptual design
- Experiments (\$10M) can act as a stepping-stone to a full-scale proptotype (\$100M+)

Snowflake Microreactor

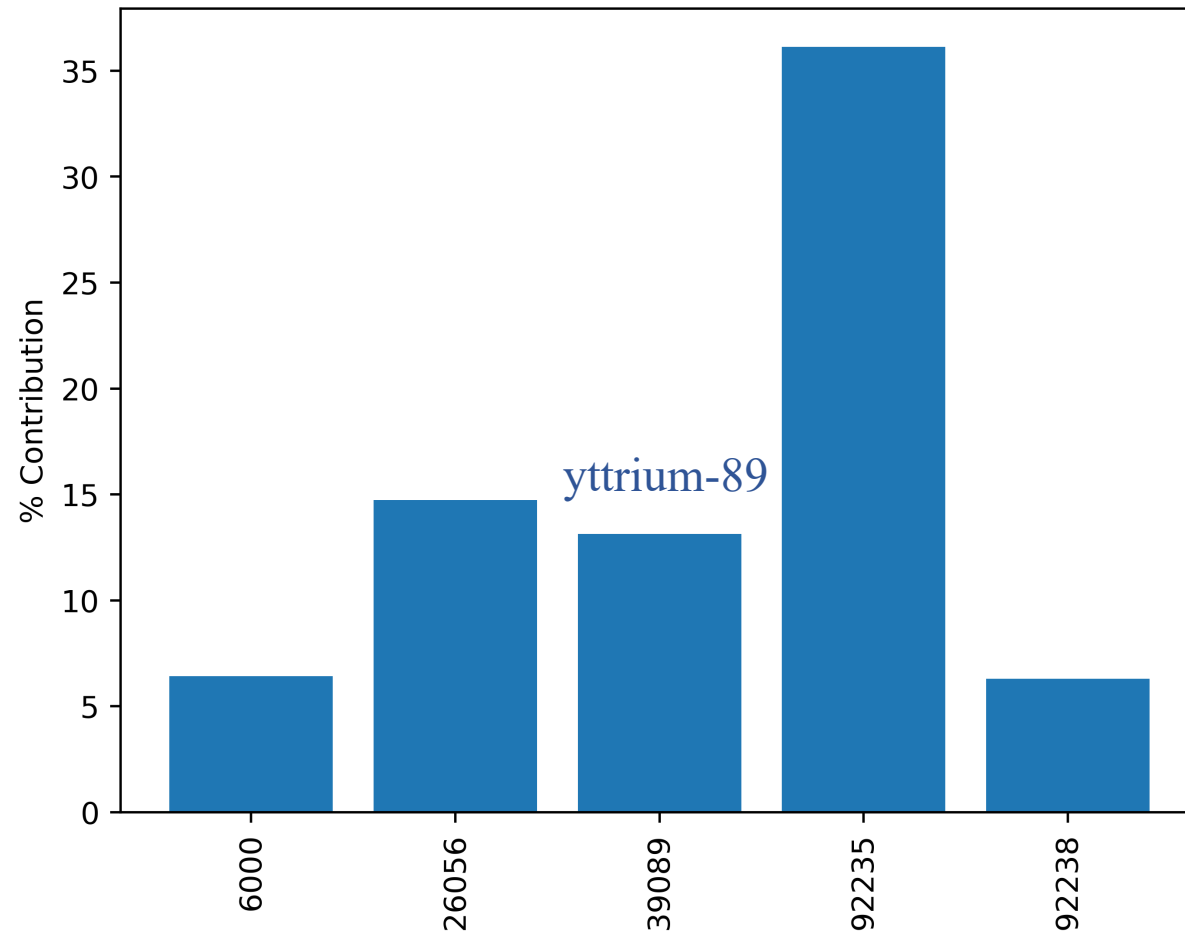


Nuclear Data Uncertainty Contributors

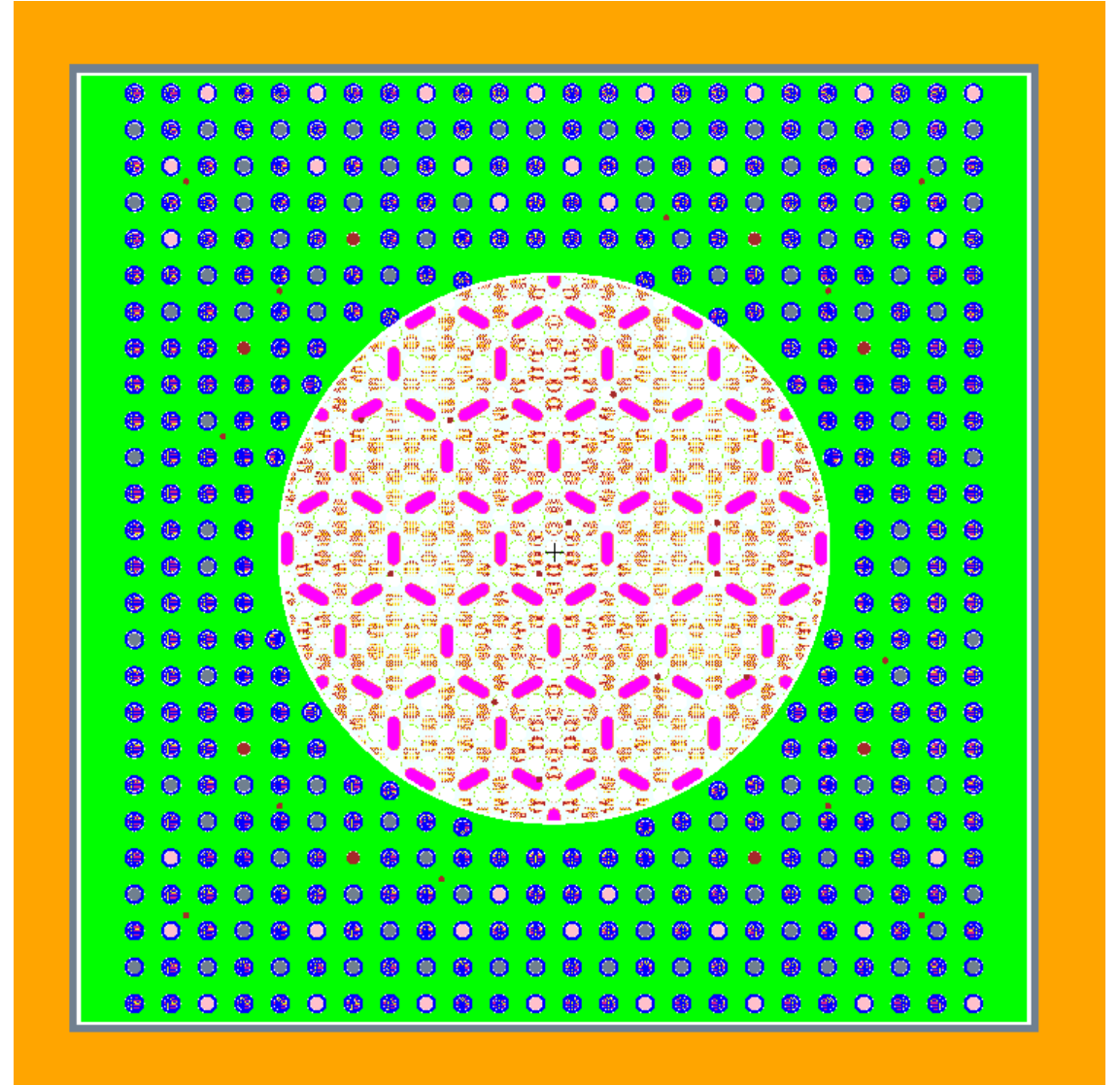
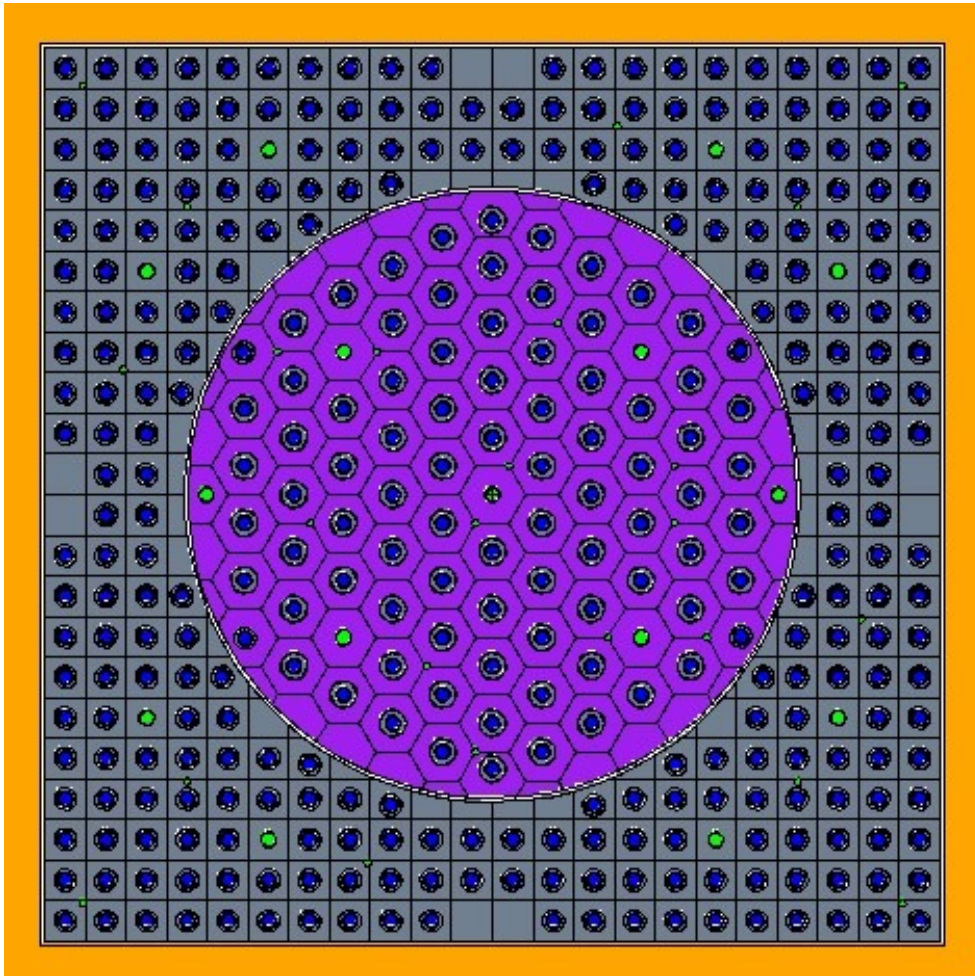
Benchmark [deimos_et_v1.i]
% contribution for each isotope



Application [snowflake_v0.i]
% contribution for each isotope



Deimos V0 and V32



Deimos Iterations

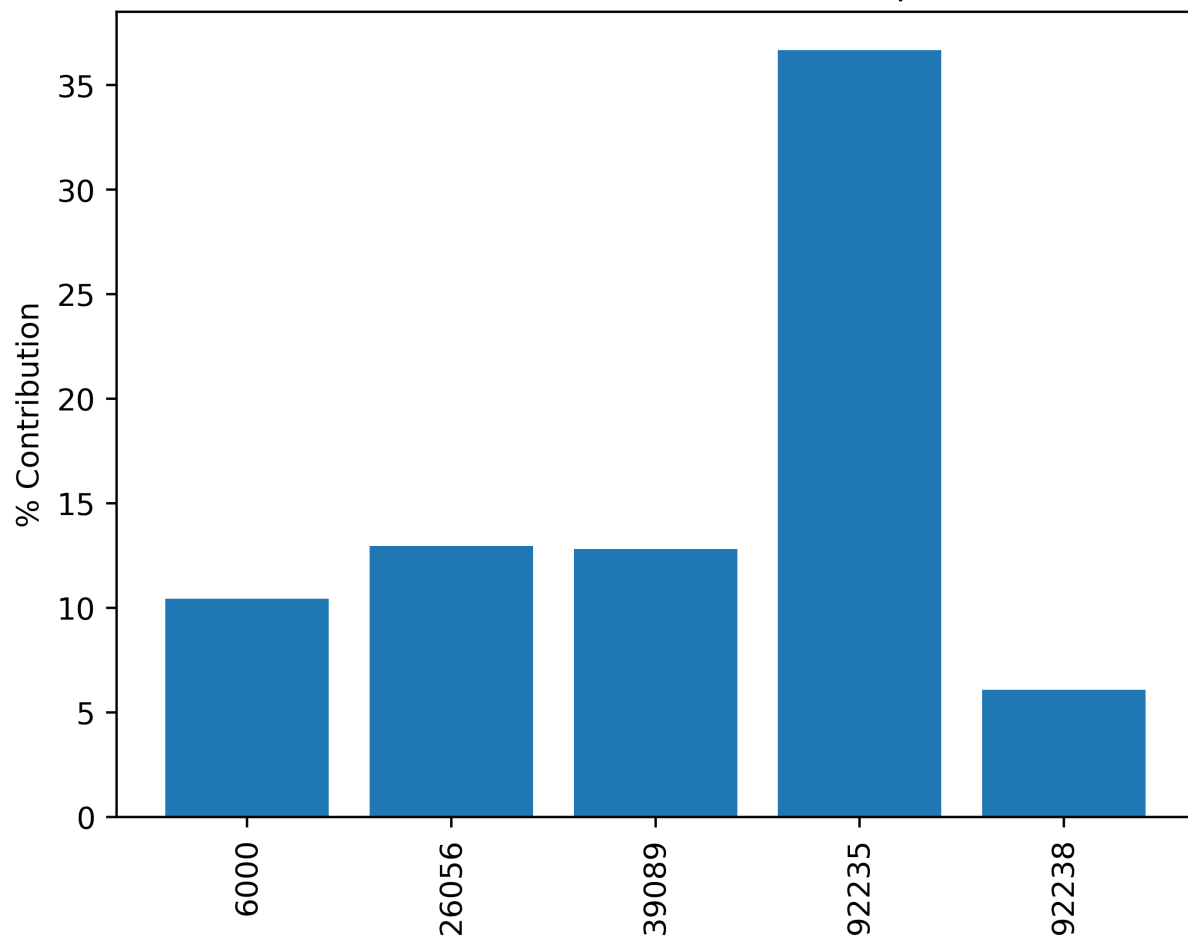
- Added fuel and heat pipes to the outer region
- Added Snowflake microreactor unit cells to the inner region

Table III. Deimos-like experiment similarity coefficients with Snowflake microreactor

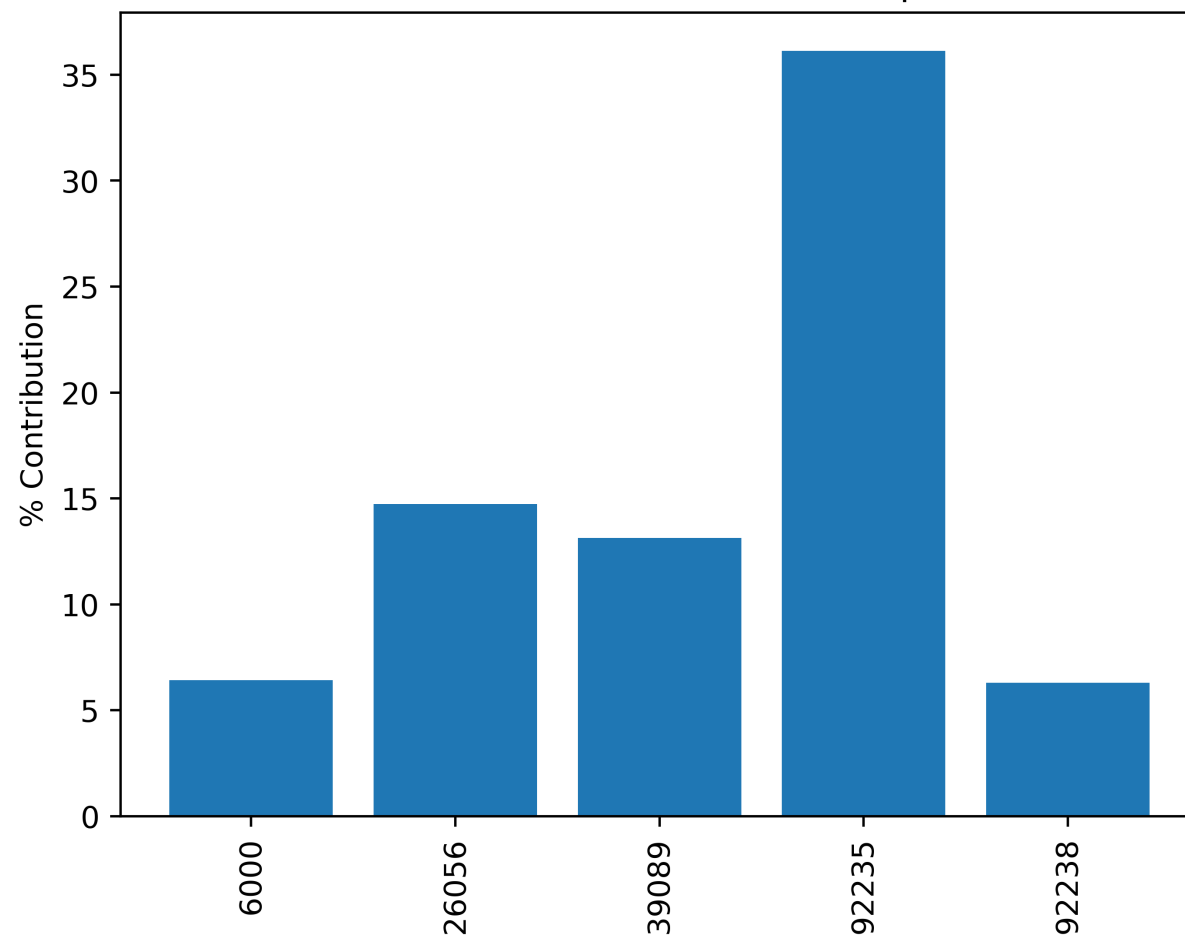
	Snowflake, 300 K C_k	Snowflake, 1200 K C_k	Snowflake, 300 K E_k
Deimos V32	96.26%	94.17%	98.78%

Nuclear Data Uncertainty Contributors

Benchmark [deimos_et_v32.i]
% contribution for each isotope



Application [snowflake_v0.i]
% contribution for each isotope



Conclusions

- Planned experiment for 2024
 - Will validate MCNP criticality, heat conduction, kinetics, and multiphysics simulations
 - Deimos will act as a testbed for future advanced reactor experiments
- Deimos would be a unique benchmark that covers a new region of nuclear data sensitivities and uncertainties in both the ICSBEP and the IRPhE
- Deimos can be modified to maximize similarity i.e. capture nuclear data uncertainties in experiment for advanced reactor concepts

Acknowledgements

This work was supported by the US Department of Energy through the Los Alamos National Laboratory and the Laboratory Directed Research & Development “Next Generation Small Nuclear Reactors”, 20220084DR. Los Alamos National Laboratory is operated by Triad National Security, LLC, for the National Nuclear Security Administration of U.S. Department of Energy (Contract No. 89233218CNA000001). Approved for unlimited release under LA-UR-23-32717.

Thank you to Jesson Hutchinson, who provided the Python scripts that generate nuclear-data induced uncertainty plots by utilizing the whisper-tk Python tools developed by Michael Rising. Thank you to Nick Wynne and Chris Romero for providing the Deimos Computer-Aided Design (CAD) drawing.

References

1. N. Thompson, A. Maldonado, T. Cutler, et. al., “The National Criticality Experiments Research Center and its role in support of advanced reactor design,” *Frontiers in Nuclear Energy*, LA-UR-22-31279 (2023).
2. T. Cutler, J. Lee, E. Luther, et. al., “The Deimos Experiment: Advanced Reactor Testbed,” *Transactions of the American Nuclear Society*, LA-UR-23-21742 (2023).
3. N. Wynne, C. D. Romero, “Deimos on Comet CAD,” (2023)
4. T. Adams, et. al. “MCNP® Code Version 6.3.0 Theory & User Manual,” Los Alamos National Laboratory, LA-UR-22-30006 (2022).
5. F. B. Brown, M. E. Rising, J. L. Alwin, “User Manual for Whisper-1.1”, Los Alamos National Laboratory, LA-UR-17-20567 (2017).
6. B. C. Kiedrowski, F. B. Brown, P. Wilson, “Adjoint-Weighted Tallies for k-Eigenvalue Calculations with Continuous-Energy Monte Carlo,” *Nucl. Sci. Eng.*, LA-UR-10-01824 (2010)
7. B. C. Kiedrowski, F. Brown, et al., “Whisper: Sensitivity/Uncertainty-Based Computational Methods and Software for Determining Baseline Upper Subcritical Limits,” *Nucl. Sci. Eng.* 181(1), pp.17-47 (2017).
8. M. L. Williams, B. L. Broadhead, M. A. Jessee, et. al., “TSURFER: An Adjustment Code to Determine Biases and Uncertainties in Nuclear System Responses by Consolidating Differential Data and Benchmark Integral Experiments,” Oak Ridge National Laboratory (2023).
9. D.A. Brown, M.B. Chadwick, R. Capote, et. al., “ENDF/B-VIII.0: The 8th Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data,” *Nucl. Data Sheets* (2018).
10. “International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook,” Nuclear Energy Agency (2023).
11. “International Handbook of Evaluated Reactor Physics Benchmark Experiments (IRPhE),” Nuclear Energy Agency (2023).

References

12. “ICSBEP participants” Nuclear Energy Agency (2023).
13. J. Fletcher, A. Maldonado, N. Thompson, “Towards a Benchmark with the Compact Nuclear Power Source”, LA-UR-22-26131 (2022)
14. G. E. Hansen, R. G. Palmer, “Compact Nuclear Power Source Critical Experiments and Analysis,” *Nucl. Eng. and Design* (1989).
15. “The High Temperature Gas Cooled Reactor Test Module Core Physics Benchmarks,” *International Atomic Energy Agency* (2003).
16. J. D. Bess, L. M. Montierth, O. Köberl, L. Snoj, “Benchmark Evaluation of HTR-PROTEUS Pebble Bed Experimental Program,” (2014).
17. K. J. Connolly, F. Rahnema, P. V. Tsvetkov, “Prismatic VHTR neutronic benchmark problems,” *Nucl. Eng. and Design* (2014).
18. E. Nobøl, “Description of the Advanced Gas Cooled Type of Reactor (AGR),” *Risø National Laboratory* (1996).
19. “Russian RBMK Reactor Design Information,” *Russian Academy of Science* (1993)
20. “Validation with Limited Benchmark Data,” *Nuclear Regulatory Committee* (2015)
21. A. Maldonado, C. Perfetti, “Utilizing Sensitivity and Correlation Coefficients from MCNP and Whisper to Guide Microreactor Experiment Design,” *Nucl. Eng. and Design* (2023).
22. H. R. Trellue, D.V. Rao, R. B. Wilkerson, et. al., “Simulation of Microreactor Design With Graphite Core Block, TRISO fuel, Heat Pipes, and Yttrium Hydride Moderator”, LANL, LA-CP-20-20306 (2020), U.S. Provisional Patent Application 1620.0121P, DOE Reference S-133,840.000.
23. K. Hoffman, A. Maldonado, T. Palmer, “Modeling Approaches for Depletion of a TRISO-Fueled Microreactor,” *PHYSOR* (2024).