

# Recent applications of Serpent related to nuclear technology research and development

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Thanks to collaborators on these projects:  
B. Betzler, A. Wysocki, J. Gorton, C. Lu, K. A. Terrani,  
J. W. McMurray, G. Singh, B. D. Wirth, and others

# Outline

Discussion of recent applications of Serpent in support of nuclear technology research and development

- FHR DR design, including cross section generation with Serpent and core calculations with PARCS
- Informing thermodynamic simulation of TRISO particle constituents in HTGR with Serpent burnup calculations
- Impact of FCM fuel form on HTGR core design
- SiC-f/SiC-m channel box deformation analysis

# ADTR Study: Background

- A 2017 U.S. DOE study of advanced reactor technology options, capabilities, and requirements within the context of national needs and public policy to support innovation in nuclear energy.

## A Summary of the Department of Energy's Advanced Demonstration and Test Reactor Options Study

Nuclear Technology

D. Petti,<sup>a\*</sup> R. Hill,<sup>b</sup> J. Gehin,<sup>c</sup> H. Gougar,<sup>a</sup> G. Strydom,<sup>a</sup> T. O'Connor,<sup>d</sup> F. Heidet,<sup>b</sup> J. Kinsey,<sup>b</sup> C. Grandy,<sup>b</sup> A. Qualls,<sup>c</sup> N. Brown,<sup>c</sup> J. Powers,<sup>c</sup> E. Hoffman,<sup>b</sup> and D. Croson<sup>ip,a</sup>

Preconceptual design of a fluoride high temperature salt-cooled engineering demonstration reactor: Motivation and overview <sup>☆</sup>

Annals of Nuclear Energy

A. Louis Qualls, Benjamin R. Betzler, Nicholas R. Brown <sup>\*</sup>, Juan J. Carbajo, M. Scott Greenwood, Richard Hale, Thomas J. Harrison, Jeffrey J. Powers, Kevin R. Robb, Jerry Terrell, Aaron J. Wysocki, Jess C. Gehin, Andrew Worrall

Annals of Nuclear Energy

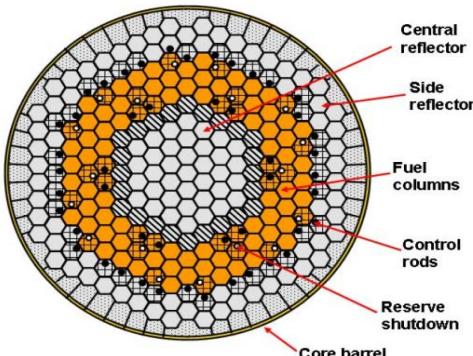
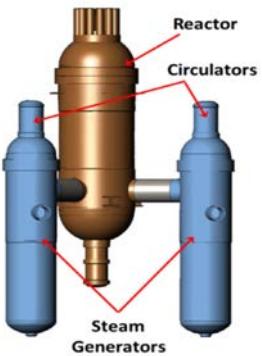
Preconceptual design of a fluoride high temperature salt-cooled engineering demonstration reactor: Core design and safety analysis <sup>☆</sup>



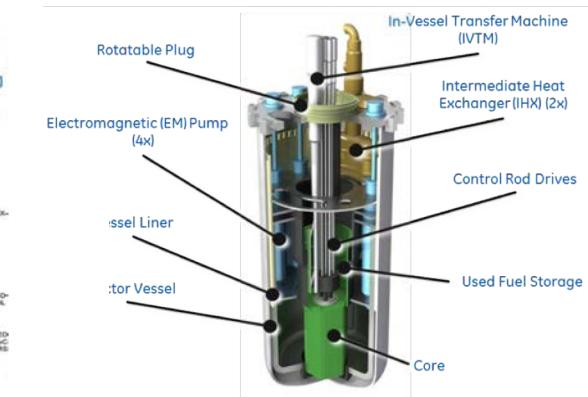
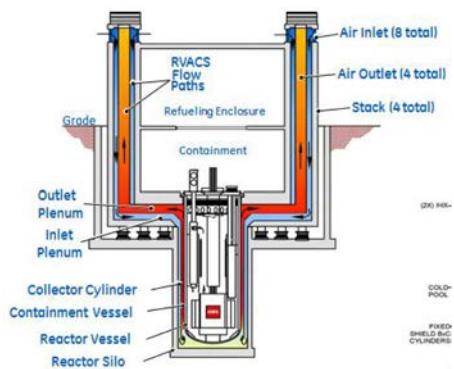
Nicholas R. Brown <sup>a,b,\*</sup>, Benjamin R. Betzler <sup>a</sup>, Juan J. Carbajo <sup>a</sup>, Aaron J. Wysocki <sup>a</sup>, M. Scott Greenwood <sup>a</sup>, Cole Gentry <sup>a</sup>, A. Louis Qualls <sup>a</sup>

# Resultant Top Options

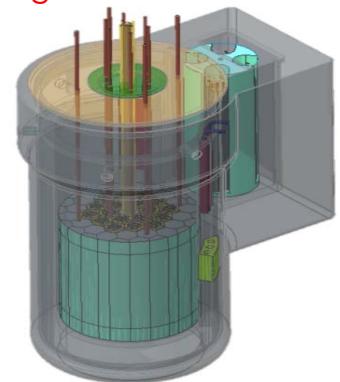
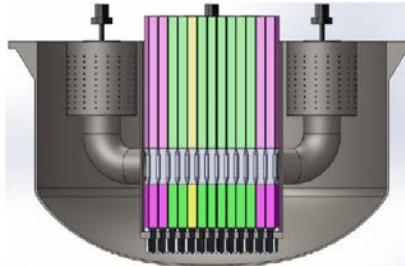
Strategic Objective 1: Process heat demonstration – modular HTGR **commercial demonstration**



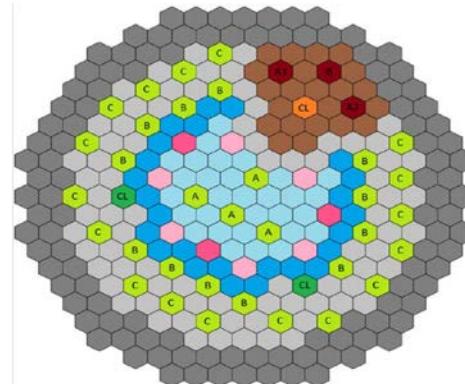
Strategic Objective 2: Resource Utilization and Waste Management – SFR **commercial demonstration**



Strategic Objective 3: Demonstrating a Less Mature Technology – FHR or LFR **engineering demonstration**



Strategic Objective 4: Test Reactor to Provide Fast Neutrons – Sodium-cooled Fast Test Reactor

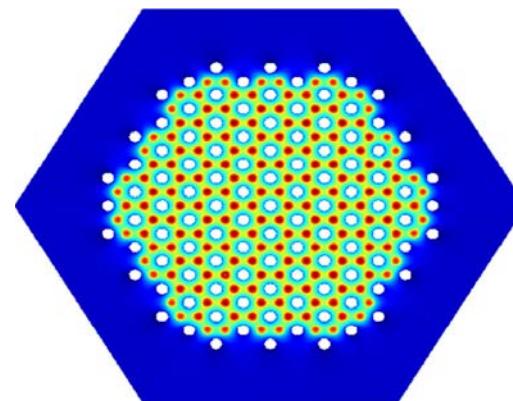


Inner core (30)
Outer core (25)
Prim. control (6)
Sec. control (3)
Reflector (77)
Shield (111)
Fast test location (33)
Fast closed loop (2)
Moderator (22)
Thermal test location (3)
Thermal closed loop (1)

# Need: Design Toolkit for FHRs

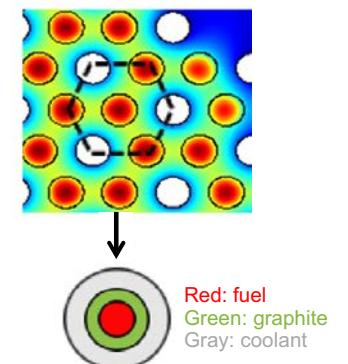
- One challenge the FHR DR team faced is the lack of a set of comprehensive core design and licensing tools for FHRs
- PARCS-FHR (with Serpent for few-group cross sections) was developed
  - Contributors: Aaron Wysocki, Ben Betzler, and Nicholas Brown
- FHR-relevant thermal feedback capability into PARCS
  - FLiBe hydraulic properties
  - Compact and graphite properties

Detailed Temperature Calculation  
(e.g. from COMSOL)



Simplified Temperature Calculation  
in PARCS (similar to RELAP5-3D)

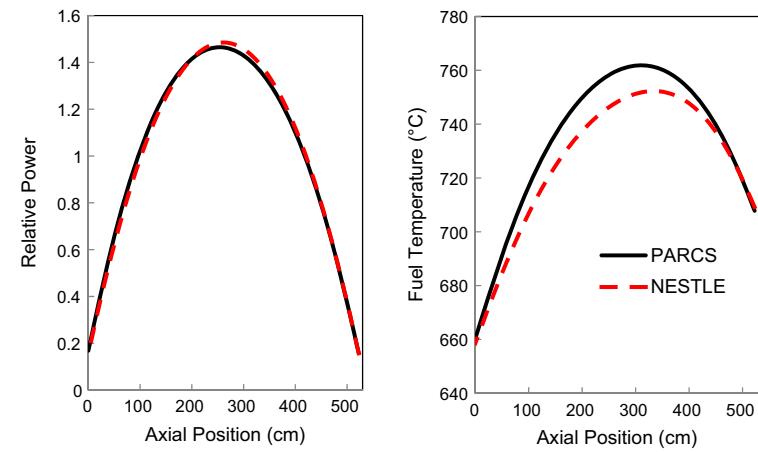
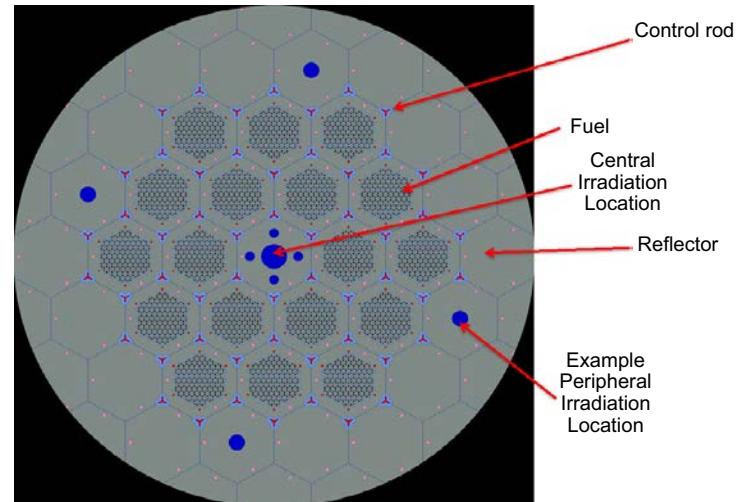
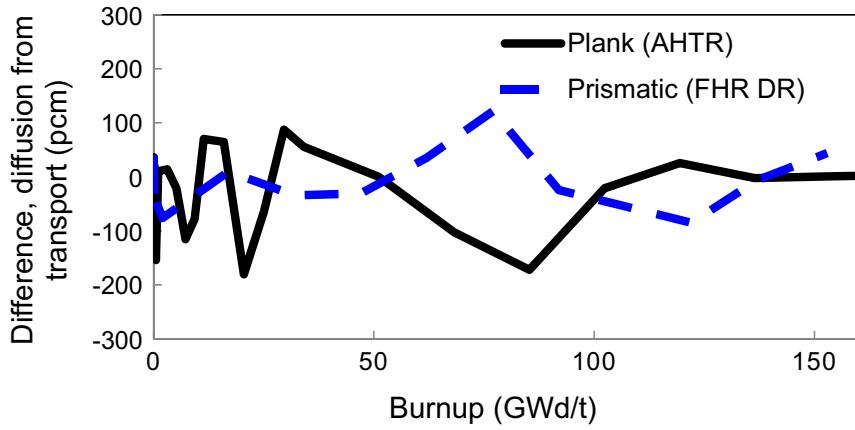
→ Reduce the detailed geometry to an equivalent sub-assembly (preserving total flow area and fuel volume)  
→ Scale the thermal conductivity to give the appropriate fuel temperatures



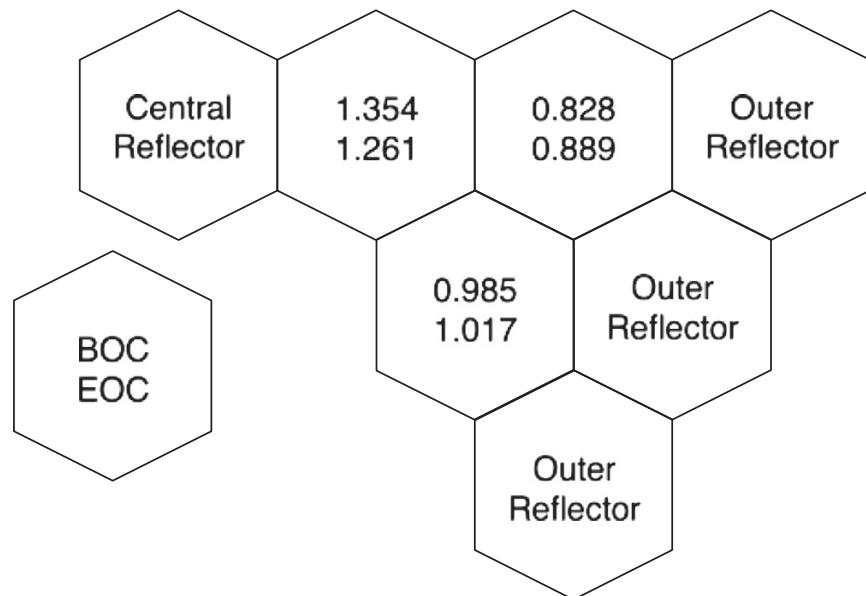
In a separate effort, Cole Gentry (UTK) demonstrated nodal core analysis for FHRs with Serpent-NESTLE and a 4-group structure  
For the FHR DR, the 4-group structure worked as well as the more complicated structures

# Serpent Cross Section Generation

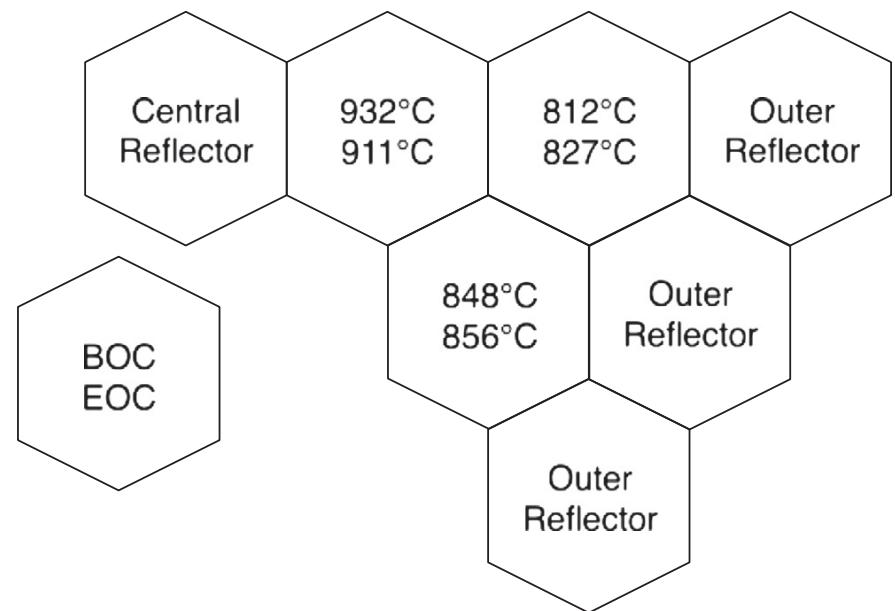
- Full-core models in Serpent that account for region dependent variations in spectrum/leakage were needed to correctly collapse cross sections and discontinuity factors for the small FHR DR
- For the FHR-DR, region dependent cross sections are easy, because it is a prismatic, single-batch core



# PARCS-FHR: Example Results

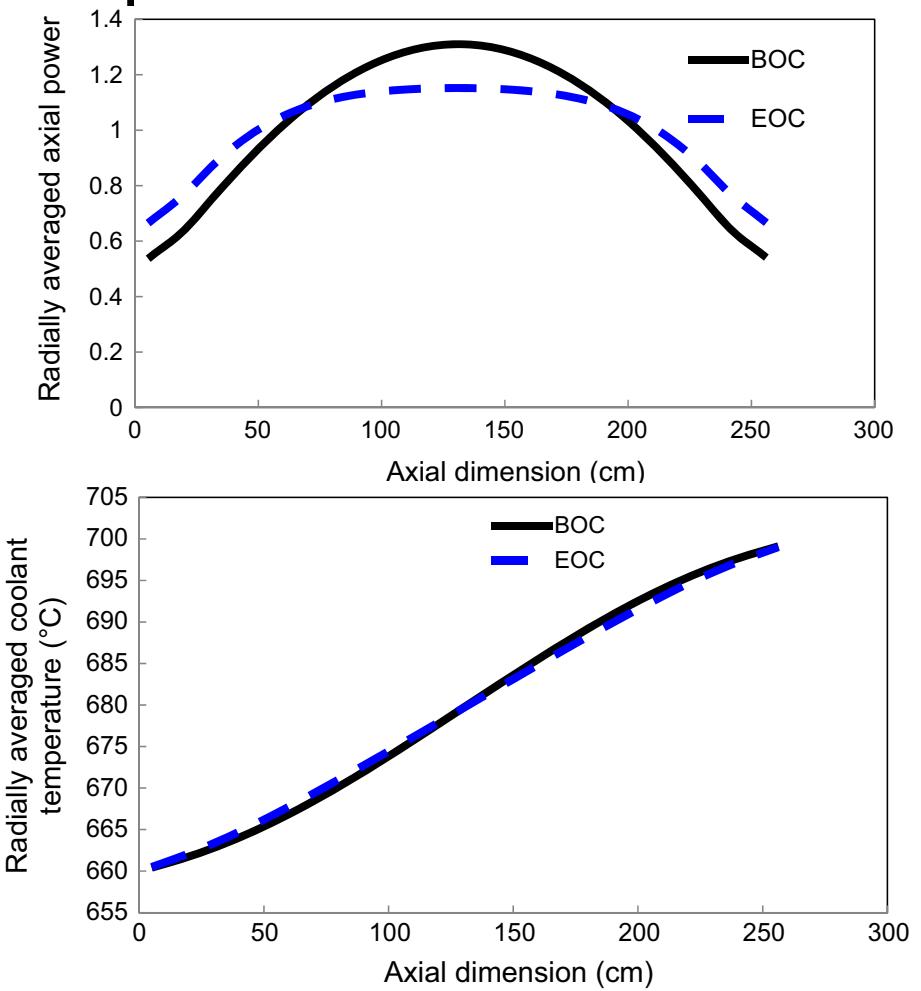
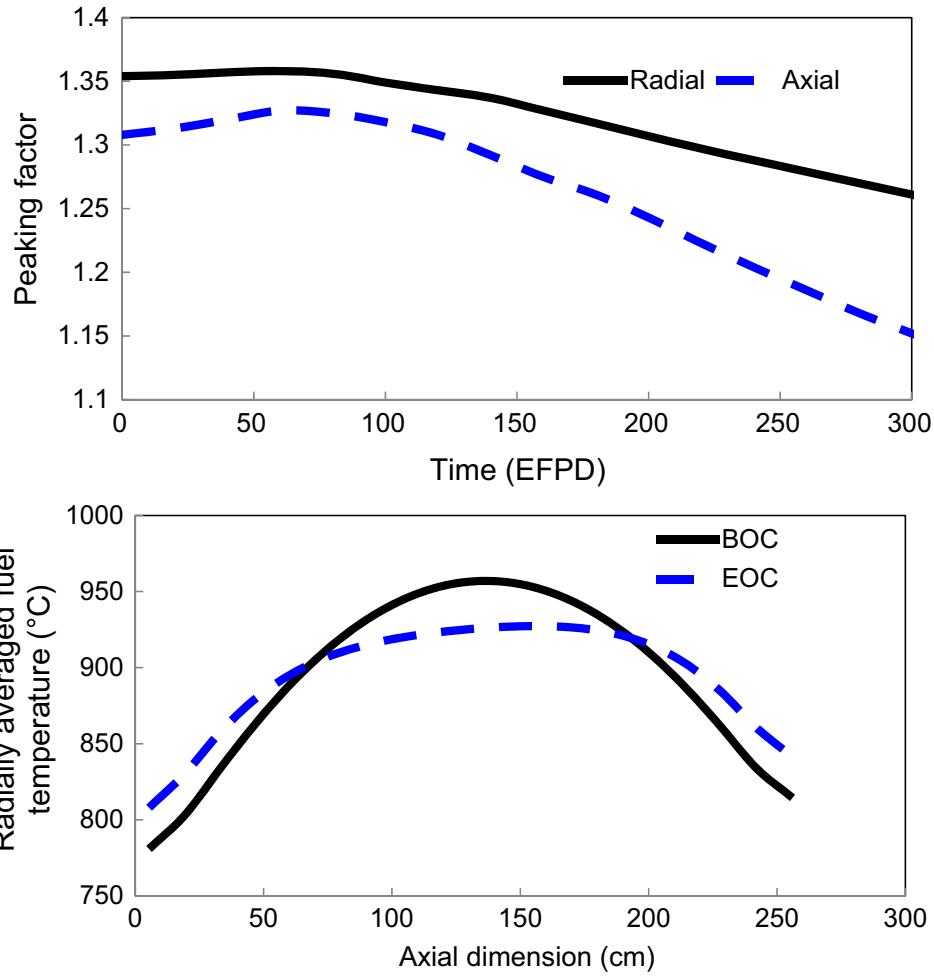


1/6-th Core Power Distribution



1/6-th Core Temperature Distribution

# PARCS-FHR: More Example Results



# Serpent and PARCS-FHR: Conclusions

- Conventional two-step method applied to FHRs
- We found the four-group structure Cole Gentry developed for plank-based FHRs is also relevant for prismatic FHRs (actually, it works even better for these systems)
- Capability was quickly ramped up and used for scoping calculations for this point design
- Additional work is needed to further develop and refine the two-step core analysis capability for other FHR concepts, such as the Kairos PB FHR

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# Informing thermodynamic simulations of HTGR TRISO fuel behavior with Serpent

- Three important failure mechanisms in HTGR fuel for high burnup are:
  - SiC layer rupture
  - SiC corrosion by CO
  - coating compromise from kernel migration
- All are related to high CO pressures from O release when uranium present as UO<sub>2</sub> fissions and the O is not bound by other elements
- CO buildup from excess O is controlled with additional uranium in the form of a carbide, UCx, and this fuel form is designated UCO

Determining the minimum required uranium carbide content for HTGR UCO fuel kernels<sup>☆</sup>



Jacob W. McMurray <sup>a,\*</sup>, Terrence B. Lindemer <sup>b</sup>, Nicholas R. Brown <sup>c,1</sup>, Tyler J. Reif <sup>d</sup>, Robert N. Morris <sup>e</sup>, John D. Hunn <sup>e</sup>

<sup>a</sup> Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6063, United States

<sup>b</sup> MPi Business Solutions, Inc., Knoxville TN 37915, United States

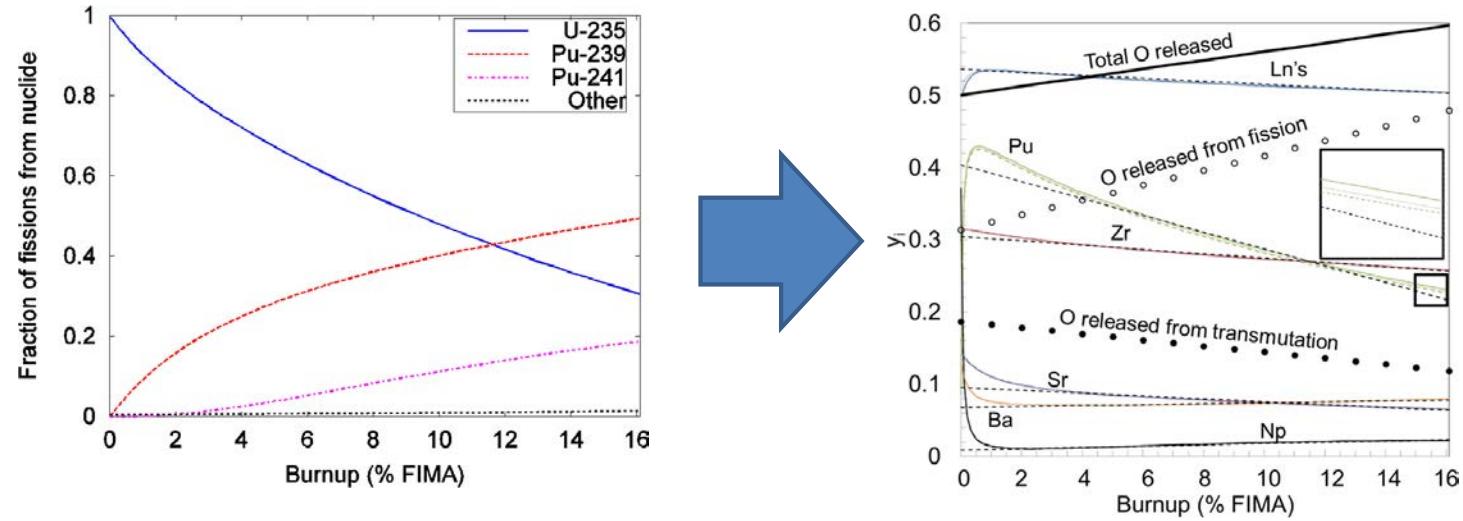
<sup>c</sup> Reactor and Nuclear Systems Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6165, United States

<sup>d</sup> X-Energy, LLC, 7701 Greenbelt, MD 20770, United States

<sup>e</sup> Fusion and Materials for Nuclear Systems Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6093, United States

# Feeding CALPHAD with Serpent: Conclusions

- CALPHAD calculates thermodynamic composition of a chemical mixture
- Serpent depletion results were fed to CALPHAD to determine the optimal uranium carbide content in UCO TRISO fuel
- This was compared with previous reduced order models
- Optimal UCx content for example case is about ~5%



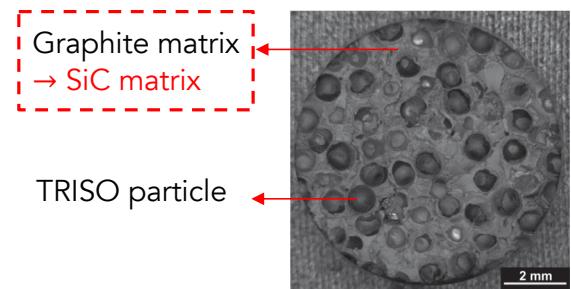
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# HTGR Core Design with FCM Fuel

- Fully Ceramic Microencapsulated (FCM) fuel consists of TRISO fuel particles embedded in a matrix of silicon carbide (SiC).
  - Higher stability under irradiation
  - Better fission product retention ability
  - Less sensitive to physical disturbances
  - Higher oxidation resistance



Fully ceramic microencapsulated fuel in prismatic high temperature gas-cooled reactors: Analysis of reactor performance and safety characteristics

Cihang Lu<sup>a</sup>, Briana D. Hiscox<sup>b,1</sup>, Kurt A. Terrani<sup>c</sup>, Nicholas R. Brown<sup>a,\*</sup>

<sup>a</sup> Pennsylvania State University, University Park, PA 16802, USA

<sup>b</sup> Massachusetts Institute of Technology, Cambridge, MA 02139, USA

<sup>c</sup> Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

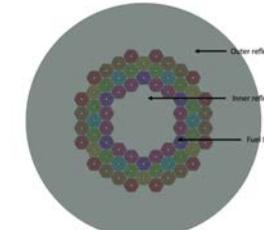
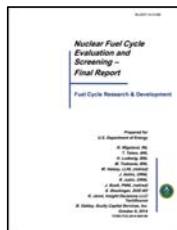
What are the key changes in fuel cycle performance of an mHTGR with the FCM fuel form?

- Fuel cycle length
  - Natural resource requirement
- 2-D neutronics model
- 
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graph LR; A["➤ Fuel cycle length<br/>➤ Natural resource requirement"] --> B["2-D neutronics model"]
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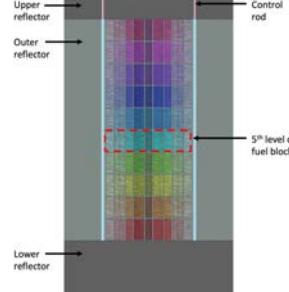
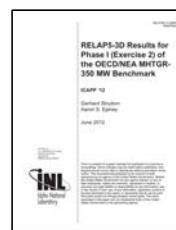
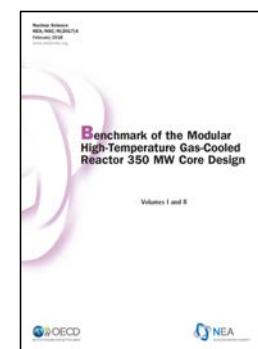
What is the potential impact of the FCM fuel form on reactor performance and safety characteristics of mHTGRs?

(10 CFR 50 Appendix A)

- Reactivity temperature coefficients (RTC)
  - Decay power
  - Control rod worth
  - Steady-state power distribution
  - Steady-state temperature distribution
- 3-D neutronics model
- Thermal-Hydraulics ring model
- 
- ```
graph TD; A["➤ Reactivity temperature coefficients (RTC)<br/>➤ Decay power<br/>➤ Control rod worth<br/>➤ Steady-state power distribution<br/>➤ Steady-state temperature distribution"] --> B["3-D neutronics model"]; A --> C["Thermal-Hydraulics ring model"]
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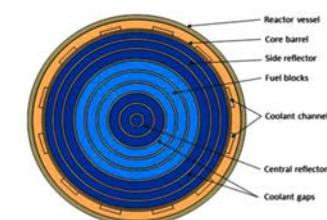
2-D neutronics model



3-D neutronics model

International Benchmark Definition  
of the MHTGR-350 MW core design

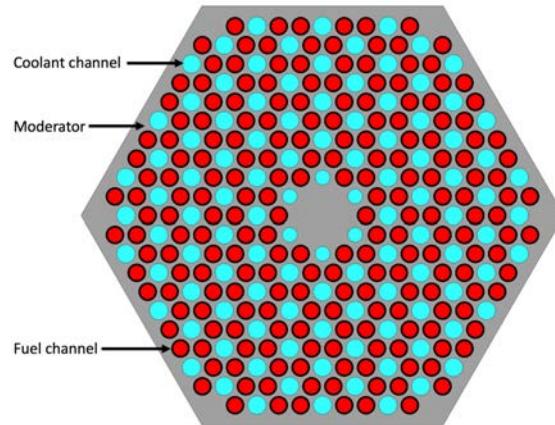
(Strydom and Epiney, 2012)



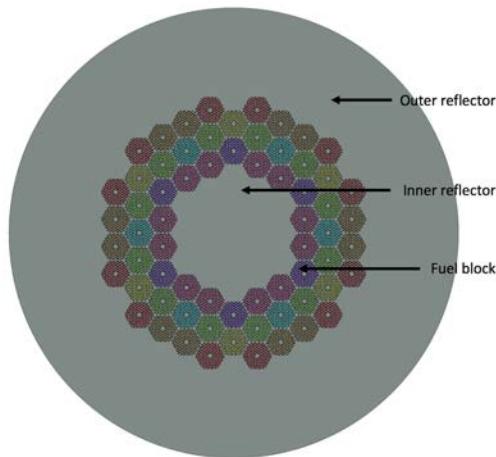
Thermal-Hydraulics ring model

The U. S. Department of Energy,  
Office of Nuclear Energy (DOE-  
NE) chartered Nuclear Fuel Cycle  
Evaluation and Screening Study

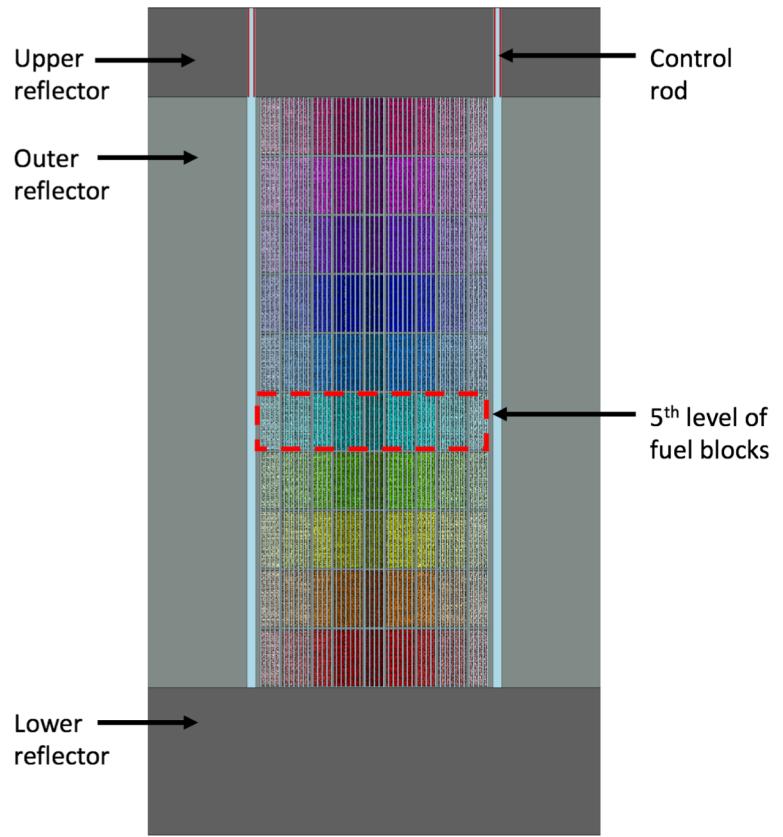
(Pope, 2012)



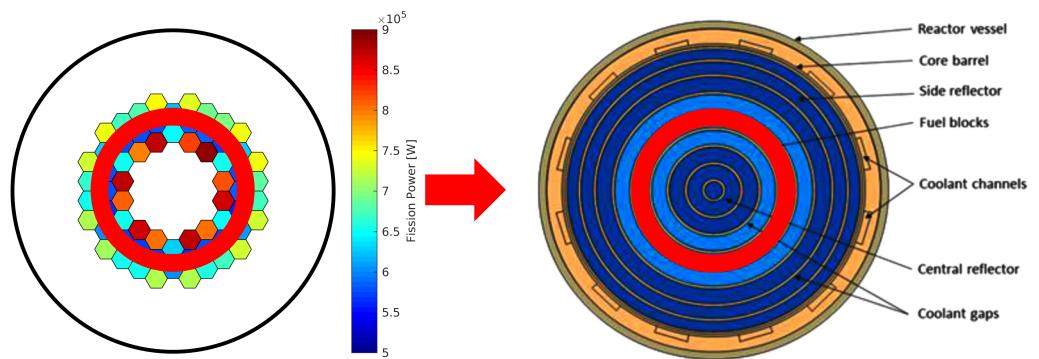
Fuel cycle length	Maintained
Natural resource requirement	75%↑
Reactivity temperature coefficients	Similar
Decay power	3%↑



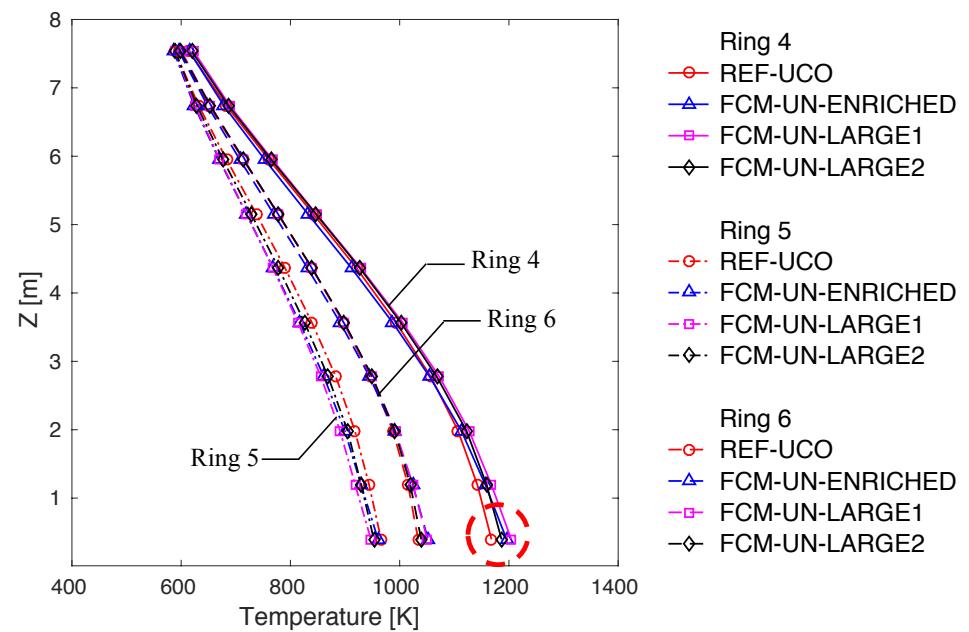
Case	$^{235}\text{U}$ Mass [kg]	Enrichment [%]	Kernel Volume [cm <sup>3</sup> ]
REF-UCO	-	-	-
FCM-UN-ENRICHED	48%↑	9%↑	-
FCM-UN-LARGE1	75%↑	-	30%↑
FCM-UN-LARGE2	44%↑	-	6%↑



<b>Control rod worth</b>	<b>15.5%↓</b>
<b>Power distribution</b>	<b>Similar</b>

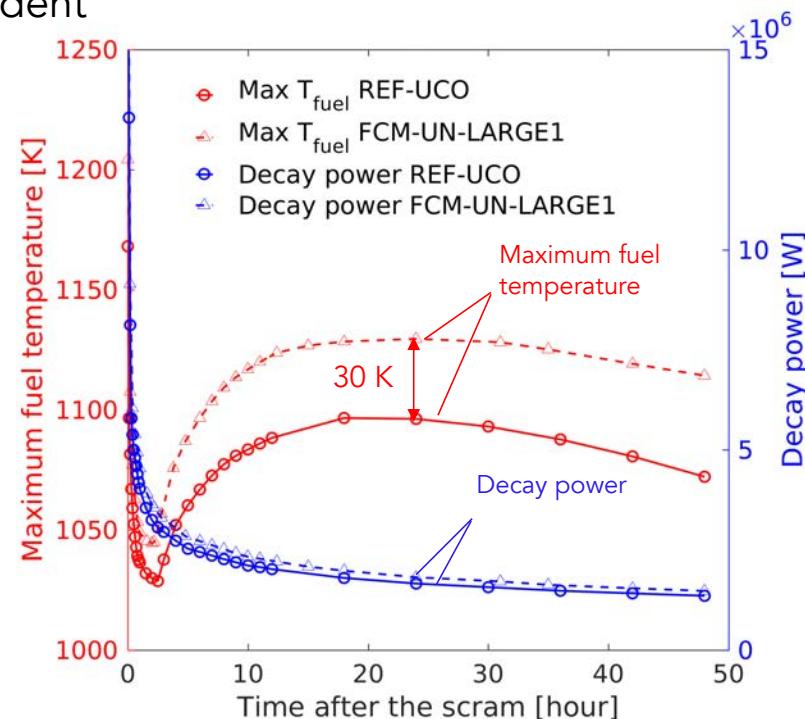
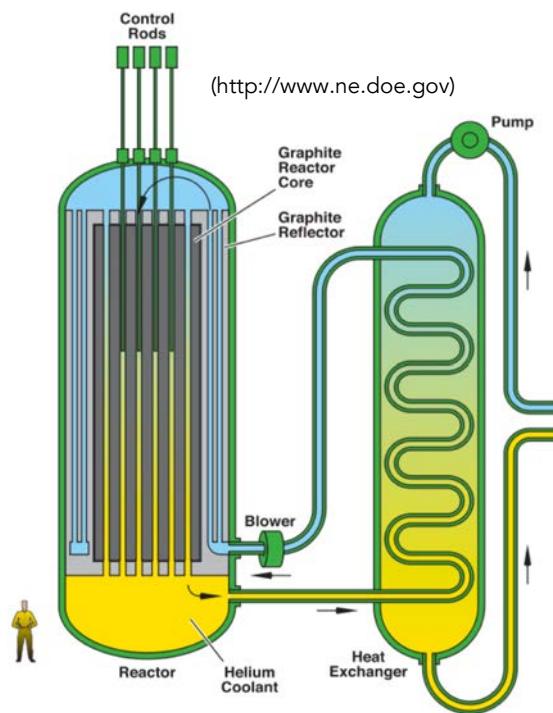


(Strydom and Epiney, 2012)



How does the FCM fuel form impact infrequent and limiting design basis fault conditions?

- Pressurized and Depressurized Loss Of Forced Circulation Accidents (P- and D-LOFC)
- Control Rod Withdrawal Accident



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# Analysis of SiC-f/SiC-m BWR Channel Box with CASL CTF and Serpent

The 2011 accident at the Fukushima-Daiichi nuclear power plant led to an increased focus on Accident Tolerant Fuel (ATF) materials.

Silicon carbide fiber-reinforced, silicon carbide ceramic matrix composites (SiC/SiC) are a top ATF candidate.

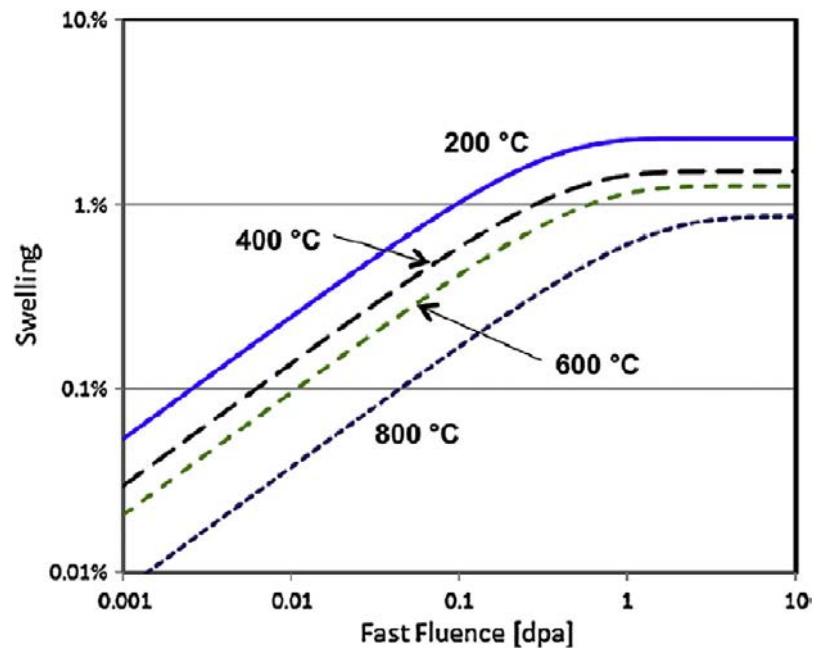
This presentation focuses on the predicted thermal hydraulic and neutronic characteristics of a SiC/SiC channel box in a boiling water reactor (BWR) fuel assembly.

These characteristics impact the viability of deploying SiC/SiC channel boxes.

# Goals of the Current Study

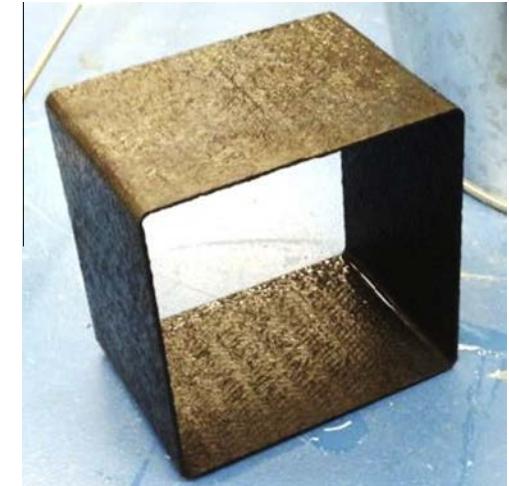
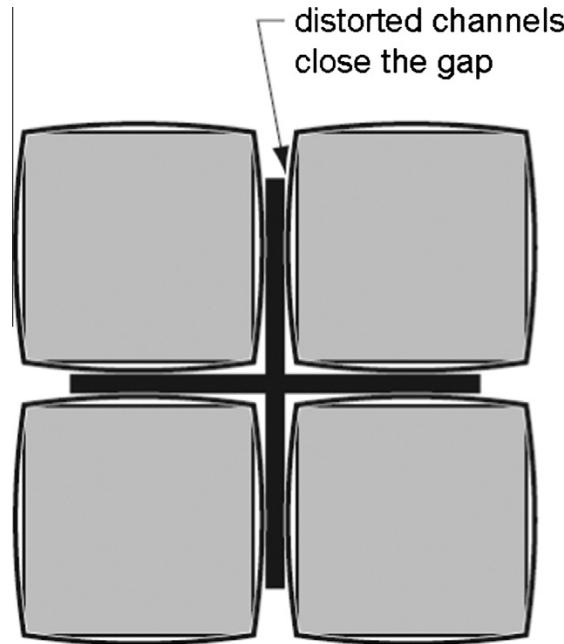
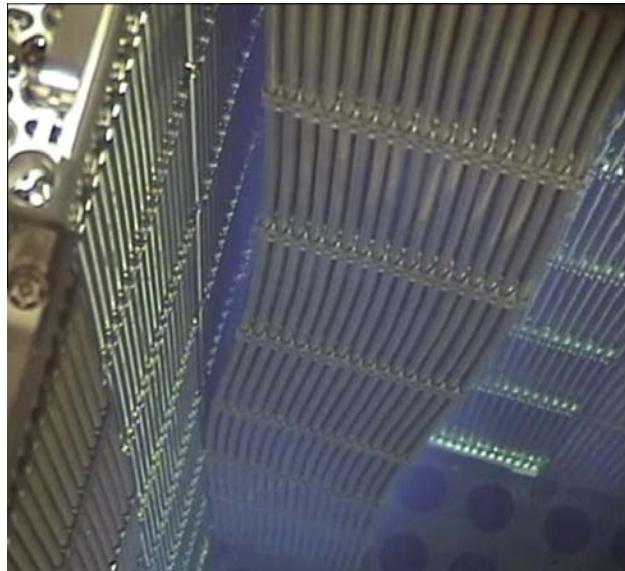
Main Objective: Provide thermal and neutronic boundary conditions for a study being to determine if the induced stress and deflection of a SiC/SiC channel box is acceptable

- Thermal boundary conditions needed because temperature gradient will cause thermal stress and bowing
- Neutron fast flux boundary conditions needed because of swelling of SiC-f/SiC-m when irradiated



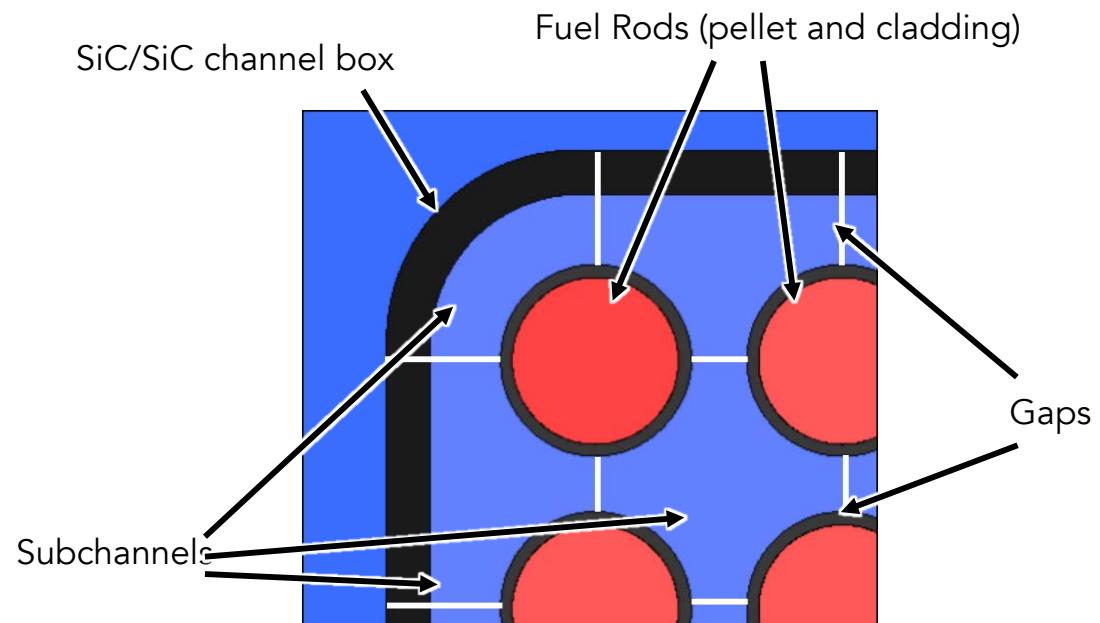
# Fuel Assembly and Channel Distortion

- Examples from Yueh and Terrani (2014)



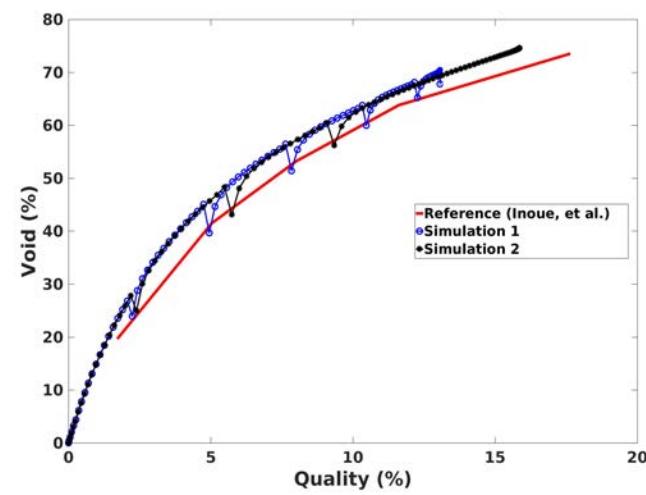
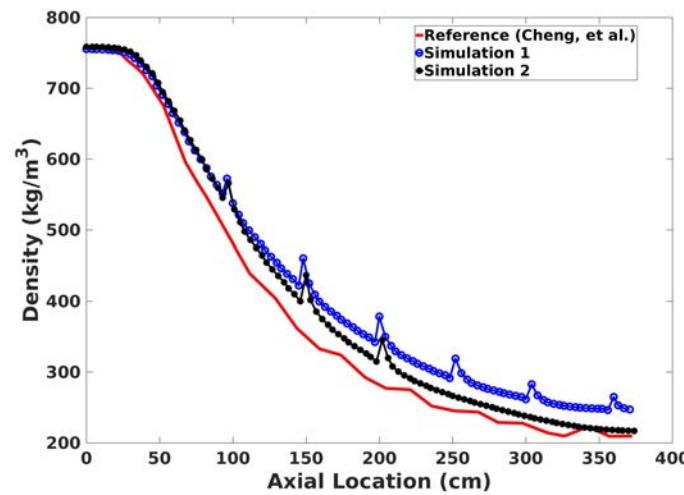
# Methodology

- Thermal hydraulic analysis performed using the Consortium for Advanced Simulation of Light Water Reactors (CASL) subchannel code CTF
  - Fuel assembly model created using a variety of publicly accessible open sources due to the fact that GE designs are proprietary
- Neutronic analysis performed using Serpent



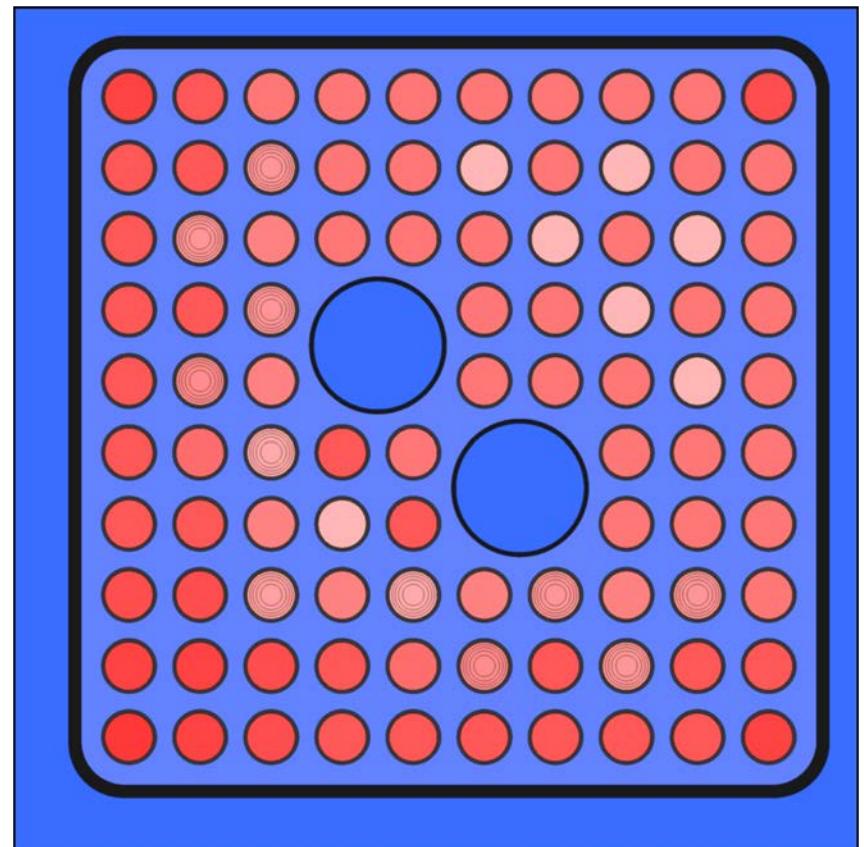
# CTF Models and Validation

- Two models developed for the study referred to as Simulation 1 and Simulation 2
- Both models have the same geometric inputs, except for assembly length
- Sources are P. Ferroni (MIT) and M. Fensin (Florida) theses



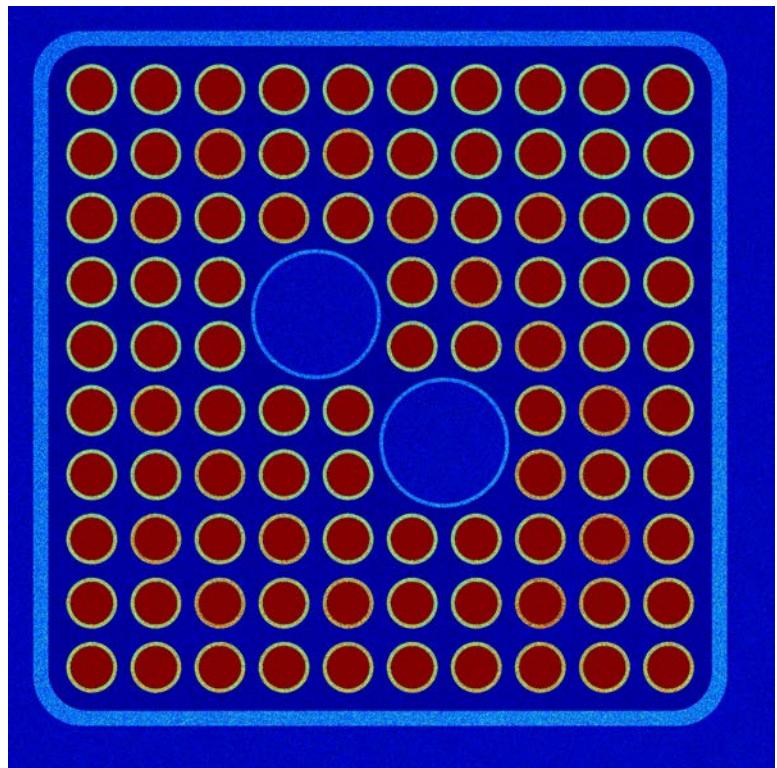
# Neutron Flux Analysis

- Goal of the neutronics analysis: determine spatial distribution of neutron flux in the SiC/SiC channel box for neutron energies greater than 0.1 MeV
- Models developed by defining fuel rod lattice geometry and material properties
- A layout of the lattice geometry is shown here, with different colors corresponding to different materials (including fuels with different enrichments and gadolinium contents)



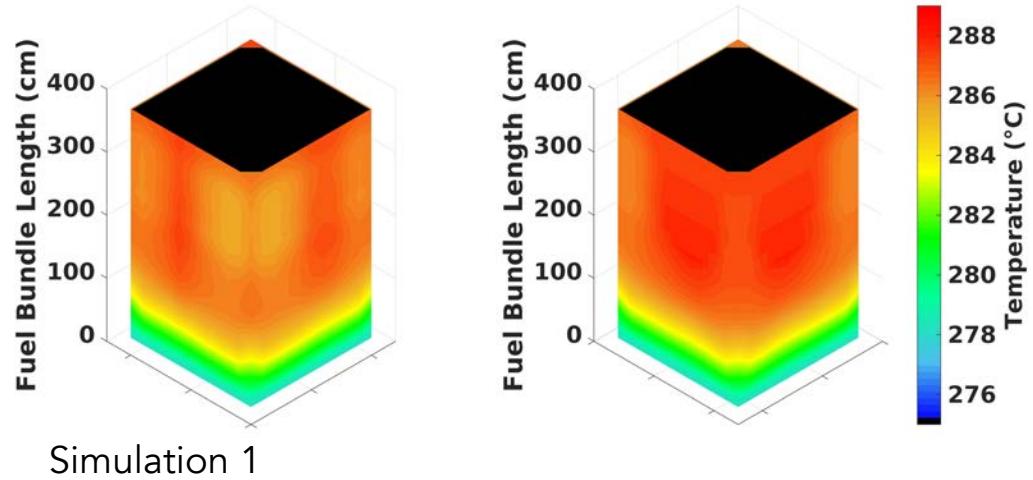
# Direct Energy Deposition in SiC/SiC Channel Box

- Used new photon transport features to enable estimate of direct energy deposition due to neutrons/photons in channel box
- Both total deposition and radial variation is important
- Channel box walls account for a very small fraction of direct deposition, and it is fairly uniform

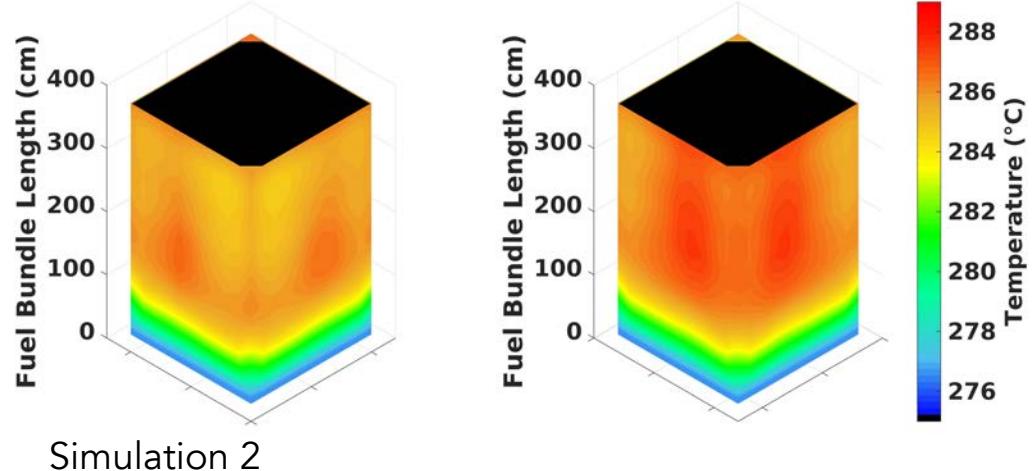


# CTF Results

- The temperature distributions in the channel box are shown for both simulations
  - The box is rotated so that all four sides can be seen
- The maximum temperature in each channel box is approximately equal to the coolant saturation temperature at the system pressure



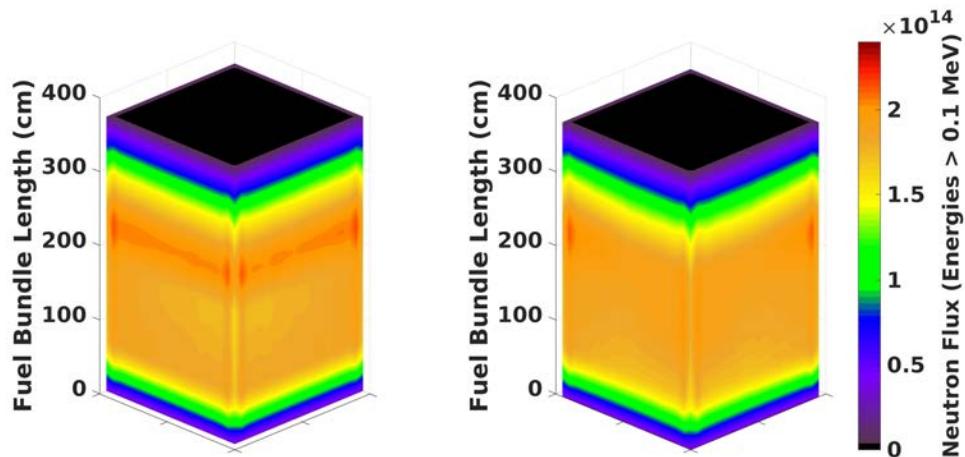
Simulation 1



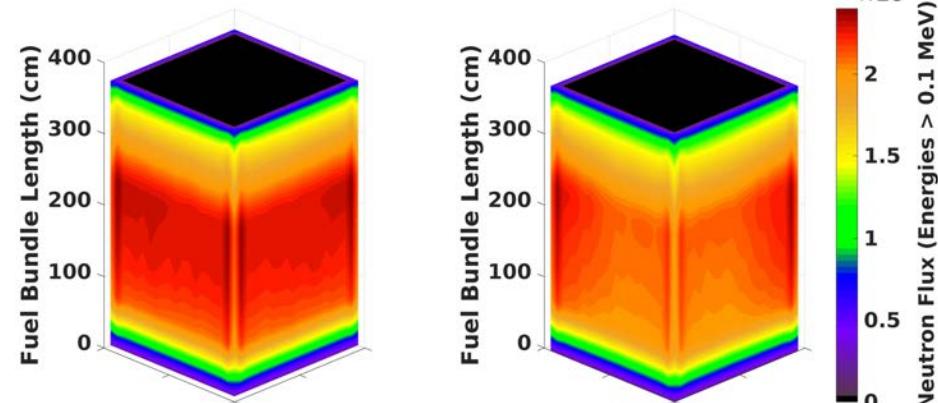
Simulation 2

# Neutron Flux

- Neutron flux only tallied for neutron energies greater than 0.1 MeV
- Significant axial variation of neutron flux due to different fuel enrichments and power in each axial zone
- Comparatively small radial neutron flux variation



Simulation 1



Simulation 2

# Summary of Channel Box Study

- Thermal and neutronic boundary conditions were generated for a SiC/SiC channel box in a BWR using CTF and Serpent
- Thermal hydraulic results showed that the temperature of the channel box varies significantly both axially and radially
- Neutronic results show that fast neutron flux also varies significantly radially and between each axial zone
- The conditions will induce swelling, stress and deflection in the channel box

**Preliminary Analysis of SiC  
BWR Channel Box  
Performance under Normal  
Operation**

Nuclear Technology  
Research and Development

Prepared for  
U.S. Department of Energy  
Nuclear Technology Research and  
Development Advanced Fuels Campaign  
G. Singh<sup>1,2</sup>, J. Gorton<sup>3</sup>, D. Schappel<sup>2</sup>, N.  
R. Brown<sup>3</sup>, Y. Kato<sup>1</sup>, K. Terrani<sup>1</sup>, and B.  
D. Wirth<sup>1,2</sup>

<sup>1</sup>Oak Ridge National Laboratory

<sup>2</sup>University of Tennessee Knoxville

<sup>3</sup>Pennsylvania State University

May 17, 2018

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