DOE-ID NEPA CX DETERMINATION
Idaho National Laboratory

CX Posting No.: DOE-ID-INL-20-035

SECTION A. Project Title: Develop High Fidelity Computation Models to Calculate the Effective Material Properties of Porous Cells

SECTION B. Project Description and Purpose:

Computational evaluation of effective material properties in heterogeneous materials (e.g., composites, multicomponent structures or functional graded additively manufactured components) has direct relevance in a vast number of applications, especially in the fields of thermal hydraulics, nuclear fuels, and materials. Metamodeling is a potential statistical technique to speed reactor design development and operational improvements by allowing understanding of the physical parameters that affect performance. The metamodel will be based on a full physics-based model for steady state and transient reactor conditions resulting in a model that reveal the physical parameters with greatest effect on performance. Meta modeling can further guide experimentation, data analysis and qualification processes. This project will specifically focus on 2-D and 3-D modeling of the thermal behavior of porous composite materials using a finite element method (FEM) as the computational modeling basis with at least two experimental datasets for validation. Furthermore, employing statistical experimental design approaches will further demonstrate accelerated development practices. Developed code verification packages, e.g., method of manufactured solutions (MMS), will be used as exact solutions to quantify discretization error, and grid convergence index (GCI) to estimate discretization uncertainty (i.e., solution verification). A code-to-code verification of meta model data outputs compared against BISON-generated data will provide additional comparative and validation information. The meta model will expand BISON material properties library detailing a range of porosity. The validated meta model for porous composite materials allows, through reduced complexities, a simplified but highly accurate solution for quicker response to operational events, especially unplanned and safety events.

The proposed project is aligned well with strategic interests of Idaho National Laboratory (INL) and the Department of Energy (DOE) by helping develop an understanding of the behaviors at microscale of new fuels and materials as well as microstructural integrity. Findings and their computational applications could decrease development time through data mining, high fidelity prediction of system behavior, and optimum experimentation techniques. The output of our developing meta model will also be used in supporting BISON as a material properties library detailing range of porosity. Also, in this collaborative research, code-to-code verification with BISON (which is a fuel performance code designed to have broad applicability). Several models for passive properties prediction of porous composite materials exists, however none of them address the properties of composite materials with heterogeneous heat generation. This research project will be a novel application.

Multiple programs/initiatives at the core of INL's business can benefit from novel rapid, validated, accurate, and reliable meta-computational models. Examples include: (1) To facilitate the design parameters and qualification of new fuel types/designs, thermal conductivity over a range of thermal loads needs to be evaluated over the length of a composite fuel compact. Applications include new- generation reactors using TRi-structural ISOtropic (TRISO) compacted fuel (e.g., advanced gas reactor (AGR), microreactors, light water reactor accident-tolerant designs) and Transient. Reactor Test Facility (TREAT) fuel particles distributed within a graphitic matrixed compact. Actual in-situ measurements are not yet feasible and achievable. High-fidelity, highly accurate, carefully FEM-verified meta-computational models will be validated per American Society of Mechanical Engineers (ASME), American Institute of Aeronautics and Astronautics (AIAA), and American Nuclear Society (ANS) codes. Once developed, these models are expected to decrease the thermal conductivity prediction uncertainty from 20% to approximately 5% for typical advanced gas reactor (AGR) conditions; (2) Thermoplastic material properties of porous media/composite functional coatings, e.g., thermal barrier coatings (TBC) or corrosion prohibitor coatings, are applicable to accident-tolerant fuel designs, small modular reactors (SMR), and microreactor designs. In an SMR, gas turbine efficiency increases by increasing the turbine inlet temperature. However, this would also increase the turbine component temperature, which can be critical. Porous media coatings such as TBC can protect the surface of the turbine blade. Running a numerous meta-model cases allows understanding the thermophysical properties of TBC materials to support critical to the design and advancement of gas turbines for the new generation of power plants; (3) Predicting thermal-mechanical properties under cyclic pressure and temperature gradients of functional graded additively manufactured components for fuel systems or heat exchanger (HX) components can lead to earlier design and materials down selection, especially compact HX (C-HX) in the secondary loop of SMRs. Availability of a specific meta-model allows for greater evaluations of the various design options quickly and accurately with more informed down selection tool. Furthermore, C-HX can be used as secondary heat exchanger in coupling Sodium Fast Reactors (SFRs) with supercritical CO2 (sCO2) Brayton cycles.

To reach the objectives of this project, our approach is divided into six tasks, detailing the interactive development and verification and validation processes will occur based on the physics-based scientific approach initially. All models and data generated will be peer reviewable. The main objective is to develop a validated metamodel demonstrated by thermomechanical properties of variable porous media with various application domains addressing INL's and DOE's mandate. Secondary objectives will be achieved by (1) providing a new thermal conductivity dataset on natural uranium-contained microencapsulated fuel particles within a graphitic matrix consisting of a packing factor range which will be of interest to new-generation reactor programs, like microreactors and accident-tolerant concepts; (2) inputting to BISON a composite database of thermal conductivity measurements of variable porous materials unique to the nuclear industry; and (3) improving current BISON models by adding predictive mechanical data on the effect of additive manufactured interlayers and these interlayers' measured effect on thermal conductivity.

Task 1: Development and Project Plan: The collaborative team will start by confirmation of the development objectives, specific project activities, responsibilities, technical, and operational management during a kick-off meeting. Also, during this process, detailed experimental test samples will be designed and/or collected, and scheduling will occur.

Task 2: Multi-dimensional composite models development and verification: The metamodel will be based on a full physics-based model for steady state and transient reactor conditions resulting in a model that reveal the physical parameters with greatest effect on performance. To analyze the thermal transport phenomena within the thermal boundary conditions, a 2-D system will be constructed. For this study, a unit half-cell is given with height, L, and width, W, and is oriented in the Cartesian $\boldsymbol{x}$-$\boldsymbol{y}$ plane with unit thickness out-of-plane. The bulk matrix material is defined as the first material phase with thermal conductivity k_1, where the pore phase is defined to have thermal conductivity $k2$. The pore pattern is circular, centered in the unit cell, with radius, R. Both the x=0 and x=W boundaries are given periodic boundary conditions for system symmetry, and the y=0 and y=L boundaries have enforced hot and cold boundary temperatures, T_H and T_C, respectively. By enforcing Dirichlet boundary conditions at the hot and cold boundaries, heat flow—per unit length—is used to define the relative pore size, where

$$\alpha = (\pi R^2)/(2WL) \quad (1)$$

The k_{eff} value is defined by overall heat flow through the system and the enforced boundary temperatures such that

$$k_{eff} = [(Q_H + Q_C)]/[2W(T_H - T_C)] \quad (2)$$

where the domain is assumed to have unit thickness out-of-plane.

In theory, Q_H=Q_C, but because this study is numerical in nature, the average of the two heat flow values is used in Eq. (2) to define the overall induced heat flow through the domain. To account for variable material properties of the matrix and porous phases in different TBCs, the ultimate system response quantity (SRQ) of interest in this analysis is the dimensionless effective thermal conductivity, k^*, which is merely the ratio of the effective thermal conductivity with the matrix material thermal conductivity, simply evaluated as

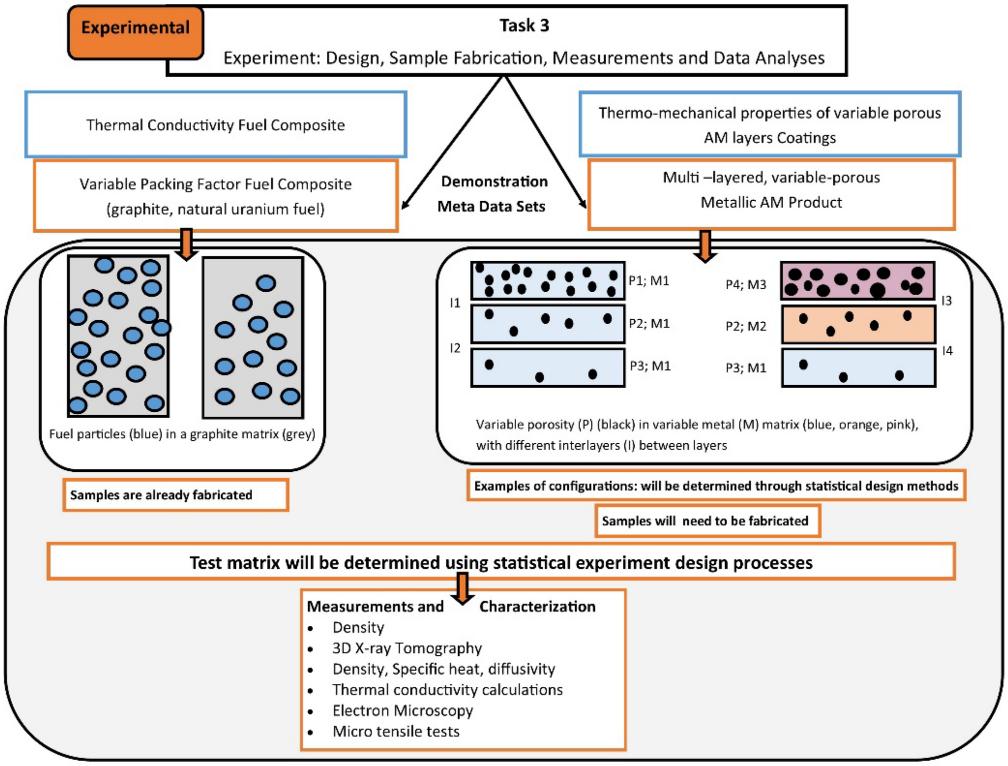
$$k^* = k_{eff}/k_1. \quad (3)$$

In order to verify the formally second order accurate solution, the MMS is employed for code verification.

Task 3: Experiment design, sample fabrication, measurements and data analyses: Two experimental systems were chosen for demonstration and validation purposes as it provides a demonstration of the wide application domain of the developed metamodel. The first experimental system will be applicable to a typical fuel composite consisting of microencapsulated uranium-containing fuel particles within a graphitic matrix with variable particle packing factor. These samples are already fabricated and available for this project. The second experimental system (samples need to be fabricated) will demonstrate the thermomechanical properties of multilayered, variable porosity, additive manufactured metallic products.

Statistical Analysis and Design: Possible experimental designs among many include: (1) Full factorial design, and (2) randomized complete block design (RCBD). Full factorial designs allow each possible design parameter combination to be assigned to at least one sample. But RCBDs work similarly except a higher-level parameter groups samples into blocks. Design parameters are randomly assigned to samples within each block to ensure complete representation. The inability to test statistically for interactions between design parameters is a limitation when only one sample (compact) is assigned to each design parameter combination. Main effects of design parameters also require multiple samples to be estimated. In the case where sample size is limited, fractional factorial and balanced incomplete block designs (BIBDs) may be considered. Fractional factorial designs work similarly to factorial designs, but systematically assign samples to design parameter combinations of most interest, or BIBDs might be used if there are not enough samples to observe all parameter combinations of interest within each blocking variable. Specific experimental designs will be identified for each experiment during a detailed design planning meeting at project kick-off.

General statistical analysis framework: Grouping variables often leads to systematically correlated samples. Multilevel mixed linear regression models account for these correlations and separate sources of measurement variation. These models also allow statistical inference about parameter effects, interactions, and parameter contributions to total measurement variation. Generic multilevel mixed linear regression models assume grouping variables are randomly selected from the entire population of grouping variables. It is also assumed that the measured response is continuous and has a linear relationship with all predictor variables. Other methods such as generalized linear models allow for non-continuous responses. Further, grouping variables must be independent, and correlation within the grouping variable must be preserved; however, models' correlation structures are flexible. We assume constant variation within each group, as well as normally distributed residuals at all levels, and independent predictor variables. In all cases, precision increases with the number of samples. Power calculations to detect effects can be used to optimally allocate samples relative to specific research questions.



Task 3.1. Transportation of Compacts from ISU (Pocatello) to Center for Advanced Energy Studies (CAES) (Idaho Falls): Task will be coordinated with ISU Radiation Safety Office and CAES Safety Officer. Rad safe already exists at CAES, with space for the compacts.
Task 3.2. Establish TC measurement technique: guidance from previous experiments performed by Utah State University. Consultation with researcher from that project (Dr. Colby Jensen) and staff from Irradiated Materials Characterization Laboratory (IMCL) (thermal properties group).
Task 3.3. Non-Destructive Examination: Two techniques are identified: X-ray tomography (CT), and electron microscopy/spectroscopy. Will be arranged at the Electron Microscopy Laboratory (EML) and CAES facilities, respectively. Specifications for X-ray CT will be determined with assistance from Dr. Josh Kane (EEST).
Task 3.4. Performing initial TC measurements: Stepwise procedure to be determined based on results from Task 1. Will be ASTM standard (or approved variation thereof) experimental technique. End task is to provide values for radial and axial thermal conductivity. Confirmatory tasks will also be performed by INL staff lead at IMCL, through the use of a newly developed thermal conductivity probe.
Task 3.5. Summary of results: Report with summary of data, including graphs, imaging, spectral analysis, tomography. Provide information for all relevant bulk property information, including (but not exclusive to): thermal conductivity, density, porosity.

Task 4: Statistical validation analysis against experimental data: Model validation will be performed to quantify the reliability of our model during the project by using experimental data. Quantitative comparison of computational responses and experimentally measured responses is the key aspect of our model validation. The validation metric operator (mathematical operator used to make the comparison) will be the temperature domain and the effective thermal conductivity. This is formulated as a difference operator, so the result is a statistical measure of the disagreement between computational and experimental responses. As shown in Figure 6, this assessment will be the first step of our model validation. The second step will utilize the model to perform predictions for the conditions of the intended use of the model. The third step is the evaluation of the model's accuracy based on the validation observation. The uncertainty involved in the available experimental data have already been evaluated and quantified. However, the replication uncertainties will be revisited to make sure the quantification accuracy is properly addressed. The computational results and experimental data will be compared statistically in different methods. The Area Metric Validation will be one of the methods to represent the mismatch between the experimental and computational results.

Task 5: Demonstration of novel integrated AM fuel system design down-selection using the validated meta model: This activity will use a concept design idea to test through application of the metamodel various options to down-select based on the enhanced thermodynamic properties. Currently it is an INL invention disclosure [6], and this modeling exercise will provide more data for validity of the proposed design options. This activity will, therefore, be a demonstration of how the newly developed model can be used in the design domain to decrease the need for experimentation, as well as to provide valuable data for strengthening patent applications, if selected.

Task 6: Final report and project close: The final report will summarize all tasks with final recommendations. The value proposition will be based on a measurement of the main objective, as well as the three secondary objectives identified as the objectives of this project.

Computational tasks will be completed at in-town office buildings or at the University of New Mexico. The experimental work described in Task 3 will be performed at the Center for Advanced Energy Studies, and Electron Microscopy Laboratory and Irradiated Materials Characterization Laboratory both at the

Materials and Fuels Complex using TRISO fuel compacts which were previously fabricated for the AGR project. Work at the Energy Innovation Laboratory will fabricate new additive manufacturing samples (metallic and ceramic) which contain no fuel.

SECTION C. Environmental Aspects or Potential Sources of Impact:

Air Emissions

N/A

Discharging to Surface-, Storm-, or Ground Water

N/A

Disturbing Cultural or Biological Resources

Section 106 of the National Historic Preservation Act (NHPA) requires the review of any proposed activity or project to determine if historic properties may be affected by the undertaking. The CRMO will conduct a Cultural Resource Review (CRR) for the proposed research activities.

Generating and Managing Waste

Some industrial waste is expected to be generated. No hazardous waste generation is anticipated. Waste generated at CAES will be managed by ISU personnel.

Releasing Contaminants

N/A

Using, Reusing, and Conserving Natural Resources

All applicable waste will be diverted from disposal in the landfill when possible. Project personnel will use every opportunity to recycle, reuse, and recover materials and divert waste from the landfill when possible. The project will practice sustainable acquisition, as appropriate and practicable, by procuring construction materials that are energy efficient, water efficient, are bio-based in content, environmentally preferable, non-ozone depleting, have recycled content and are non-toxic or less-toxic alternatives. New equipment will meet either the Energy Star or Significant New Alternatives Policy (SNAP) requirements as appropriate (see http://www.sftool.gov/GreenProcurement/ProductCategory/14).

SECTION D. Determine Recommended Level of Environmental Review, Identify Reference(s), and State Justification:
Identify the applicable categorical exclusion from 10 Code of Federal Regulation (CFR) 1021, Appendix B, give the appropriate justification, and the approval date.

For Categorical Exclusions (CXs), the proposed action must not: (1) threaten a violation of applicable statutory, regulatory, or permit requirements for environmental, safety, and health, or similar requirements of Department of Energy (DOE) or Executive Orders; (2) require siting and construction or major expansion of waste storage, disposal, recovery, or treatment or facilities; (3) disturb hazardous substances, pollutants, contaminants, or Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA)-excluded petroleum and natural gas products that pre-exist in the environment such that there would be uncontrolled or unpermitted releases; (4) have the potential to cause significant impacts on environmentally sensitive resources (see 10 CFR 1021). In addition, no extraordinary circumstances related to the proposal exist that would affect the significance of the action. In addition, the action is not “connected” to other action actions (40 CFR 1508.25(a)(1) and is not related to other actions with individually insignificant but cumulatively significant impacts (40 CFR 1608.27(b)(7)).

References: : National Environmental Policy Act (NEPA) Implementing Procedures, Final Rule, 10 CFR 1021 Appendix B to Subpart D, Categorical Exclusion B3.6,"Small-scale research and development, laboratory operations, and pilot projects."

Justification: Project activities are consistent with 10 CFR 1021 Appendix B to Subpart D, Categorical Exclusion B3.6, "Siting, construction, modification, operation, and decommissioning of facilities for small-scale research and development projects; conventional laboratory operations (such as preparation of chemical standards and sample analysis); and small-scale pilot projects (generally less than 2 years) frequently conducted to verify a concept before demonstration actions, provided that construction or modification would be within or contiguous to a previously disturbed or developed area (where active utilities and currently used roads are readily accessible). Not included in this category are demonstration actions, meaning actions that are undertaken at a scale to show whether a technology would be viable on a larger scale and suitable for commercial deployment."

Is the project funded by the American Recovery and Reinvestment Act of 2009 (Recovery Act) ☐ Yes ☒ No

Approved by Jason Sturm, DOE-ID NEPA Compliance Officer on: 5/14/2020