FISCAL YEAR 2023 SIMULATION-BASED ENGINEERING PEER REVIEW

OVERVIEW REPORT

October 24, 2022

Disclaimer

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1 INTRODUCTION AND BACKGROUND

The National Energy Technology Laboratory's (NETL) Simulation-Based Engineering (SBE) Program supports the development and application of new, innovative, physics- and chemistry-based models and computational tools at multiple scales (i.e., atomistic, device, process, grid, and market) to accelerate development and deployment of clean, advanced fossil fuel technologies. Research in this area provides the basis for the simulation of engineered devices and systems to better predict and optimize the performance of fossil energy electricity generation units. Computational design methods and concepts are vital to significantly improve performance; reduce the costs and emissions of fossil energy power systems; and enable the development, analysis, and optimization of new systems and capabilities. Current technologies of focus include integrated energy systems; advanced ultra-supercritical operation; biomass gasification; hydrogen storage and combustion; and carbon capture, utilization, and storage (CCUS).

NETL's SBE Program combines technical knowledge, software development, computational power, data repositories, experimental facilities, and unique partnerships to support research into timely and accurate solutions for complex fossil energy systems. Analysis and visualization tools are manipulated to gain scientific insights into complex, uncertain, high-dimensional, and high-volume datasets. The information generated is then collected, processed, and used to inform research that combines theory, computational modeling, advanced optimization, experiments, and industrial input with a focus on the following three research areas:

- **Multiphase Flow Science**—NETL has developed the Multiphase Flow with Interphase eXchanges (MFiX) software suite, which is the world's leading open-source design software for comparing, implementing, and evaluating multiphase flow constitutive models. These tools provide an accurate, validated, and cost-effective capability to design, optimize, scale up, and troubleshoot an extremely diverse range of multiphase flow applications. MFiX has been utilized for complex fossil energy applications, including gasification with biomass for hydrogen production (negative carbon emission), carbon capture using solid sorbents or liquid solvents, and chemical-looping combustion of gaseous and solid fuels. The MFiX software suite has more than 6,700 registered users and is the national leading platform for computational fluid dynamics (CFD) code.
- **Advanced Process Modeling and Optimization**—NETL's Institute for the Design of Advanced Energy Systems (IDAES) optimizes the design and operation of complex, interacting technologies and systems by providing rigorous modeling capabilities to increase efficiency, lower costs, increase revenue, and improve sustainability of power generation and electricity distribution. IDAES represents a paradigm shift as the only fully equation-oriented platform with integrated support for steady-state design, optimization, dynamic operations, data reconciliation, parameter estimation, and uncertainty quantification of complex energy and chemical processes. IDAES uniquely supports the process modeling life cycle, from conceptual design to dynamic optimization and control. IDAES enables users to efficiently search vast, complex design spaces that cannot be adequately explored with existing tools to discover the lowest

cost, most environmentally sustainable solutions. The extensible, open platform empowers users to create models of novel processes and rapidly develop custom analyses, workflows, and end-user applications.

- **Computational Design of Materials and Components**—Computational materials design utilizes modeling tools to enable rapid design and simulation of new and novel alloys suitable for high-temperature, high-pressure, corrosive environments of an advanced energy system. Computational methods are also used to provide validated models capable of simulating and predicting long-term performance and failure mechanisms of the newly developed materials, with specific emphasis on durability, availability, and cost. Similarly, component-scale modeling develops insight into fossil plant challenges and mitigation solutions using novel modeling tools. The program utilizes physically informed models of industrial components under cyclic loading, long-duration stress, and high-temperature exposure to generate practical and cost-effective solutions to reduce plant failures and extend plant life.

1.1 OFFICE OF MANAGEMENT AND BUDGET AND U.S. DEPARTMENT OF ENERGY REQUIREMENTS

In compliance with requirements from the Office of Management and Budget and in accordance with the U.S. Department of Energy (DOE) Strategic Plan, DOE and NETL are fully committed to improving the quality of research projects in their programs by conducting rigorous peer reviews. DOE and NETL conducted a Fiscal Year 2023 (FY 2023) Simulation-Based Engineering Peer Review Meeting with independent technical experts to offer recommendations to strengthen projects during the period of performance. KeyLogic, an NETL site-support contractor, convened a panel of six[a] academic and industry experts[b] on October 5–6, 2022, to conduct a peer review of two SBE Program research projects (reference Exhibit 1-1).

[a] Unique panels of three reviewers were utilized for each project during this peer review.

[b] Please see "Appendix D: Peer Review Panel Members" for panel member biographies.

Exhibit 1-1. FY 2023 Simulation-Based Engineering Peer Review—projects reviewed

Project Number	Title	Lead Organization	Total Funding		Project Duration	
			DOE	Cost Share	From	To
FWP-1022463	Computational Fluid Dynamics for Advanced Reactor Design (CARD)	National Energy Technology Laboratory	$1,895,000*	$0	04/01/2022	03/31/2023
FWP-1022423	The Institute for the Design of Advanced Energy Systems (IDAES)	National Energy Technology Laboratory	$1,535,000*	$0	04/01/2021	03/31/2026
Recommendations-Based Evaluation: During recommendations-based evaluations, the independent Review Panel provides recommendations to strengthen the performance of projects during the period of performance. * Execution Year 2022 (04/01/2022 to 03/31/2023); via NETL VUE.			**$3,430,000**	**$0**		
			$3,430,000			

2 OVERVIEW OF THE PEER REVIEW PROCESS

Peer reviews are conducted to help ensure that the Office of Fossil Energy and Carbon Management's (FECM) research program, implemented by NETL, is in compliance with requirements from the Office of Management and Budget and in accordance with the DOE Strategic Plan and DOE guidance. Peer reviews improve the overall quality of the technical aspects of research and development (R&D) activities, as well as overall project-related activities, such as utilization of resources, project and financial management, and commercialization.

KeyLogic convened a panel of six[c] academic and industry experts[d] to conduct a peer review of two research projects supported by the SBE Program. Throughout the peer review meeting, these recognized technical experts offered recommendations to strengthen the projects during the remaining period of performance. KeyLogic selected an independent Review Panel, facilitated the peer review meeting, and prepared this report to summarize the results.

2.1 PRE-MEETING PREPARATION

Before the peer review meeting, each project team submitted a Project Technical Summary (PTS) and project presentation(s). The Federal Project Manager (FPM)/Federal Point of Contact (FPOC) provided the Field Work Proposal (FWP), the latest quarterly report, and supplemental technical papers as additional resources for the Review Panel. The Review Panel received these materials prior to the peer review meeting, which enabled the Review Panel to fully prepare for the meeting with the necessary background information.

To increase the efficiency of the peer review meeting, multiple pre-meeting orientation sessions were held with NETL, the project teams, the Review Panel, and KeyLogic to review the peer review process and procedures, roles and responsibilities, peer review evaluation criteria, and project documentation. The Technology Manager also offered an overview presentation of the program goals and objectives and rationale behind selecting the projects for peer review.

2.2 PEER REVIEW MEETING PROCEEDINGS

At the meeting, each project team offered a series of presentations describing the project. The presentations were followed by multiple question-and-answer sessions with the Review Panel and a closed discussion and evaluation session for the Review Panel. The time allotted for the presentations, the question-and-answer sessions, and the closed discussion session was dependent on the project's complexity, duration, and breadth of scope.

During the closed discussion session of the meeting, the Review Panel discussed each project (identified in Exhibit 1-1) to identify strengths, weaknesses, and recommendations in accordance with the NETL Peer Review Evaluation Criteria.[e] The Review Panel offered

[c] Unique panels of three reviewers were utilized for each project during this peer review.

[d] Please see "Appendix D: Peer Review Panel Members" for panel member biographies.

[e] Please see "Appendix A: Peer Review Evaluation Criteria" for more information.

prioritized, actionable recommendations to strengthen the project during the remaining period of performance.

3 SUMMARY OF KEY FINDINGS

This section summarizes the overall key findings of the projects evaluated at the FY23 Simulation-Based Engineering Peer Review Meeting. The Review Panel concluded that the peer review provided an excellent opportunity to comment on the relative strengths and weaknesses of each project. The presentations and question-and-answer sessions provided additional clarity to complement the pre-meeting documentation. The peer review also provided insight into the range of technology development and the relative progress that has been made by the project teams. The technical discussion enabled the Review Panel to contribute to each project's development by identifying core issues and making constructive, actionable recommendations to improve project outcomes. The Review Panel generated 14 recommendations for NETL management to review and consider.

The Review Panel stated that the project teams are comprised of a strong team of engineers and other team members working to make improvements. The teams applied a strong strategy for execution over their respective period of performance, and they demonstrated a significant commitment, effort, and flexibility when listening to the stakeholder and user community. They used this feedback to learn and draw on needs from the community for continuing the development effort. Both projects have a strong publication and presentation record, making their tools and resources visible to the immediate user community (and in the general community). Finally, the Review Panel confirmed that the projects are aligned with DOE's near- and/or long-term goals and demonstrated noteworthy progress and accomplishments.

Regarding the Computational Fluid Dynamics for Advanced Reactor Design (CARD) research efforts, the Review Panel indicated the team has made significant improvements to the software and its applicability to real system issues/problems, noting that the improved computational time makes it more practical for real systems. In addition, the new graphics processing unit (GPU)-enabled computing with MFiX-Exa brings the software to the forefront of scientific computing.

Regarding the IDAES Integrated Platform, the Review Panel shared that, from a technology perspective, the platform exceeds commercially available process simulation and optimization environments widely used in the energy industry. Equation-oriented modeling and solution strategies enable fast process optimization by (1) using state-of-the-art optimization solvers that can tackle challenging models and (2) incorporating best-in-class modeling practices to mitigate numerical challenges. The ability to combine equation-oriented models and process/pilot/plant data-based models using machine learning-based approaches and surrogate models enables users to address a wide range of problems and provides the flexibility needed to create multi-scale models of complex systems at the appropriate level of model fidelity.

4 Project Synopses

For more information on the SBE Program and project portfolio, please visit the NETL website: https://netl.doe.gov/carbon-management/simulation-based-engineering.

Project Number FWP-1022463

Project Title	**Computational Fluid Dynamics for Advanced Reactor Design (CARD)**
Lead Organization	**National Energy Technology Laboratory**
Project Description	The National Energy Technology Laboratory's (NETL) Computational Fluid Dynamics for Advanced Reactor Design (CARD) research efforts focus on the development, enhancement, and application of NETL's suite of multiphase computational fluid dynamics (CFD) software tools. These next-generation fossil energy conversion technologies target process intensification, modularity, low emissions, feedstock flexibility, and increased efficiency—all supported by advanced manufacturing techniques. Science-based models are critical tools for reducing the risk, cost, and time tied to the development of novel fossil energy reactors. These tools, based on the NETL Multiphase Flow with Interphase eXchanges (MFiX) software suite, are used for design and analysis of novel reactors and devices for fossil energy application, and provide detailed predictions of reactor performance, including temperature, velocities, chemical composition, reaction rates, and heat transfer for both fluid and solid phases in the reactors. Understanding the performance of energy, environmental, and chemical process devices based on multiphase flow physics is challenging, and impacting their design early in the developmental process is critically important to control costs and reduce the risk of not meeting performance standards. Approximately 75% of the manufacturing cost of any product is committed at the conceptual design stage, even when the incurred cost may be small. Computational models can be used to simulate a multiphase device to help understand its performance before the design is finalized, thereby reducing cost. Use of computational models is valuable when empirical scale-up information is not available when reactors at the appropriate scale have not been built. Furthermore, it is well known that traditional scale-up methods do not work well for multiphase flow reactors. These factors point toward the critical need for science-based models with quantified uncertainty for reducing the cost and time required for development of multiphase flow devices.

PROJECT NUMBER FWP-1022423

Project Title	Institute for Design of Advanced Energy Systems (IDAES)
Lead Organization	National Energy Technology Laboratory
Project Description	The Institute for Design of Advanced Energy Systems (IDAES) Integrated Platform helps companies, technology developers, and researchers to model, design, and optimize complex systems. As an optimization-based integrated process modeling platform, IDAES enables rigorous analysis of multi-scale, dynamic processes and operating scenarios to improve efficiency of existing systems and develop next-generation energy systems. The IDAES Integrated Platform addresses the capability gap between state-of-the-art simulation packages and general algebraic modeling languages (AMLs) by integrating an extensible, equation-oriented process model library within the open-source, U.S. Department of Energy (DOE)-funded Pyomo AML, which addresses challenges in formulating, manipulating, and solving large and structured optimization problems. IDAES includes tools for (1) process synthesis and conceptual design, including process intensification; (2) process design, optimization, and integration; (3) process control and dynamic optimization; (4) use of advanced solvers and computer architectures; (5) automated development of thermodynamic, physical property, and kinetic submodels from experimental data; (6) integration of multi-scale models; (7) comprehensive, end-to-end uncertainty quantification, including stochastic optimization; (8) maintenance of complete provenance information; and (9) the ability to support multiple scales, from materials to process to market.

APPENDIX A: PEER REVIEW EVALUATION CRITERIA

Peer reviews consist of a formal evaluation of selected National Energy Technology Laboratory (NETL) projects by an independent panel of subject matter experts (SMEs) and are conducted to ensure that the Office of Fossil Energy and Carbon Management's (FECM) research program, implemented by NETL, is compliant with Office of Management and Budget (OMB) guidance, the U.S. Department of Energy (DOE) Strategic Plan, and DOE guidance. Peer reviews reduce project risk (e.g., cost, schedule, technology development) and improve the overall quality of the technical aspects of research and development (R&D) activities, as well as overall project-related activities, such as utilization of resources, project and financial management, and commercialization. NETL uses the peer review findings to guide and redirect projects, as appropriate, underscoring NETL's commitment to funding and managing a portfolio of high-quality research.

NETL PEER REVIEW—RECOMMENDATIONS-BASED EVALUATION

At the meeting, the peer review facilitator leads the Review Panel in identifying strengths[f], weaknesses[g], and prioritized recommendations. A recommendation emphasizes an action that is considered by the project team and/or DOE to correct or mitigate the impact of weaknesses, expand upon a project’s strengths, or progress along the technology maturation path. A recommendation has as its basis one or more strengths or weaknesses. Recommendations are ranked from most important to least.

[f] A strength is an aspect of the project that, when compared to the evaluation criterion, reflects positively on the probability of successful accomplishment of the project’s goal(s) and objectives.

[g] A weakness is an aspect of the project that, when compared to the evaluation criterion, reflects negatively on the probability of successful accomplishment of the project’s goal(s) and objectives.

Exhibit A-1. NETL Peer Review evaluation criteria

Evaluation Criteria
1. Degree to which the project, if successful, supports the U.S. Department of Energy (DOE) Program's near- and/or long-term goals.
• Program goals are clearly and accurately stated. • Performance requirements[1] support the program goals. • The intended commercial application is clearly defined. • The technology is ultimately technically and economically viable for the intended commercial application.
2. Degree to which there are sufficient resources to successfully complete the project.
• There is adequate funding, facilities, and equipment. • Project team includes personnel with the needed technical and project management expertise. • The project team is engaged in effective teaming and collaborative efforts, as appropriate.
3. Degree of project plan technical feasibility.
• Technical gaps, barriers, and risks to achieving the performance requirements are clearly identified. • Scientific/engineering approaches have been designed to overcome the identified technical gaps, barriers, and risks to achieve the performance requirements. • Remaining technical work planned is appropriate considering progress to date and remaining schedule and budget. • Appropriate risk mitigation plans exist, including Decision Points when applicable.
4. Degree to which progress has been made towards achieving the stated performance requirements.
• The project has tested (or is testing) those attributes appropriate for the next Technology Readiness Level (TRL). The level of technology integration and nature of the test environment are consistent with the aforementioned TRL definition. • Project progress, with emphasis on experimental results, shows that the technology has, or is likely to, achieve the stated performance requirements for the next TRL (including those pertaining to capital cost, if applicable). • Milestones and reports effectively enable progress to be tracked. • Reasonable progress has been made relative to the established project schedule and budget.
5. Degree to which an appropriate basis exists for the technology's performance attributes and requirements.
• The TRL to be achieved by the end of the project is clearly stated.[2] • Performance attributes for the technology are defined.[2] • Performance requirements for each performance attribute are, to the maximum extent practical, quantitative, clearly defined, and appropriate for and consistent with the DOE goals as well as technical and economic viability in the intended commercial application.
6. The project Technology Maturation Plan (TMP) represents a viable path for technology development beyond the end of the current project, with respect to scope, timeline, and cost. *(This criterion is not applicable to a recommendations-based evaluation)*

[1] If it is appropriate for a project to not have cost/economic-related performance requirements, then the project is evaluated on technical performance requirements only.

[2] Supported by systems analyses appropriate to the targeted TRL.

APPENDIX B: DOE TECHNOLOGY READINESS LEVELS

Exhibit B-1. Description of DOE TRLs

Relative Level of Technology Development	Technology Readiness Level	TRL Definition	Description
System Operations	TRL 9	Actual system operated over the full range of expected mission conditions	The technology is in its final form and operated under the full range of operating mission conditions. Examples include using the actual system with the full range of wastes in hot operations.
System Commissioning	TRL 8	Actual system completed and qualified through test and demonstration	The technology has been proven to work in its final form and under expected conditions. In almost all cases, this Technology Readiness Level (TRL) represents the end of true system development. Examples include developmental testing and evaluation of the system with actual waste in hot commissioning. Supporting information includes operational procedures that are virtually complete. An Operational Readiness Review (ORR) has been successfully completed prior to the start of hot testing.
	TRL 7	Full-scale, similar (prototypical) system demonstrated in relevant environment	This represents a major step up from TRL 6, requiring demonstration of an actual system prototype in a relevant environment. Examples include testing full-scale prototype in the field with a range of simulants in cold commissioning (1). Supporting information includes results from the full-scale testing and analysis of the differences between the test environment, and analysis of what the experimental results mean for the eventual operating system/environment. Final design is virtually complete.
Technology Demonstration	TRL 6	Engineering/pilot-scale, similar (prototypical) system validation in relevant environment	Engineering-scale models or prototypes are tested in a relevant environment. This represents a major step up in a technology's demonstrated readiness. Examples include testing an engineering-scale prototypical system with a range of simulants (1). Supporting information includes results from the engineering-scale testing and analysis of the differences between the engineering-scale, prototypical system/environment, and analysis of what the experimental results mean for the eventual operating system/environment. TRL 6 begins true engineering development of the technology as an operational system. The major difference between TRL 5 and 6 is the step-up from laboratory scale to engineering scale and the determination of scaling factors that will enable design of the operating system. The prototype should be capable of performing all the functions that will be required of the operational system. The operating environment for the testing should closely represent the actual operating environment.

Relative Level of Technology Development	Technology Readiness Level	TRL Definition	Description
Technology Development	TRL 5	Laboratory-scale, similar system validation in relevant environment	The basic technological components are integrated so that the system configuration is similar to (matches) the final application in almost all respects. Examples include testing a high-fidelity, laboratory scale system in a simulated environment with a range of simulants (1) and actual waste (2). Supporting information includes results from the laboratory scale testing, analysis of the differences between the laboratory and eventual operating system/environment, and analysis of what the experimental results mean for the eventual operating system/environment. The major difference between TRL 4 and 5 is the increase in the fidelity of the system and environment to the actual application. The system tested is almost prototypical.
Technology Development	TRL 4	Component and/or system validation in laboratory environment	The basic technological components are integrated to establish that the pieces will work together. This is relatively "low fidelity" compared with the eventual system. Examples include integration of ad hoc hardware in a laboratory and testing with a range of simulants and small-scale tests on actual waste (2). Supporting information includes the results of the integrated experiments and estimates of how the experimental components and experimental test results differ from the expected system performance goals. TRL 4–6 represent the bridge from scientific research to engineering. TRL 4 is the first step in determining whether the individual components will work together as a system. The laboratory system will probably be a mix of on hand equipment and a few special purpose components that may require special handling, calibration, or alignment to get them to function.
Research to Prove Feasibility	TRL 3	Analytical and experimental critical function and/or characteristic proof of concept	Active research and development (R&D) is initiated. This includes analytical studies and laboratory-scale studies to physically validate the analytical predictions of separate elements of the technology. Examples include components that are not yet integrated or representative tested with simulants (1). Supporting information includes results of laboratory tests performed to measure parameters of interest and comparison to analytical predictions for critical subsystems. At TRL 3 the work has moved beyond the paper phase to experimental work that verifies that the concept works as expected on simulants. Components of the technology are validated, but there is no attempt to integrate the components into a complete system. Modeling and simulation may be used to complement physical experiments.

Relative Level of Technology Development	Technology Readiness Level	TRL Definition	Description
	TRL 2	Technology concept and/or application formulated	Once basic principles are observed, practical applications can be invented. Applications are speculative, and there may be no proof or detailed analysis to support the assumptions. Examples are still limited to analytic studies. Supporting information includes publications or other references that outline the application being considered and that provide analysis to support the concept. The step up from TRL 1 to TRL 2 moves the ideas from pure to applied research. Most of the work is analytical or paper studies with the emphasis on understanding the science better. Experimental work is designed to corroborate the basic scientific observations made during TRL 1 work.
Basic Technology Research	TRL 1	Basic principles observed and reported	This is the lowest level of technology readiness. Scientific research begins to be translated into applied R&D. Examples might include paper studies of a technology's basic properties or experimental work that consists mainly of observations of the physical world. Supporting Information includes published research or other references that identify the principles that underlie the technology.

[1] Simulants should match relevant chemical and physical properties.

[2] Testing with as wide a range of actual waste as practicable and consistent with waste availability, safety, as low as reasonably achievable (ALARA), cost, and project risk is highly desirable.

Source: U.S. Department of Energy, "Technology Readiness Assessment Guide." Office of Management. 2011.

APPENDIX C: MEETING AGENDA

FY 2023 Simulation-Based Engineering Peer Review
October 5–6, 2022
Virtual Meeting

WEDNESDAY, OCTOBER 5, 2022

COMPUTATIONAL FLUID DYNAMICS FOR ADVANCED REACTOR DESIGN (CARD)

**** All times Eastern ****

11:00–11:15 a.m.	**Peer Review Panel Kickoff Session** *DOE HQ/NETL, KeyLogic Peer Review Support, and Review Panel Attend* Facilitator Opening, Review Panel Introductions, NETL Welcome, Peer Review Process and Meeting Logistics
11:15 a.m.–12:00 p.m.	**Computational Fluid Dynamics for Advanced Reactor Design (CARD)** **Session 1 – Overview, Program and Development Plan, Outreach, and Stakeholder Support** Presenter: Jeff Dietiker
12:00–12:45 p.m.	**Question and Answer Session 1**
12:45–1:00 p.m.	**BREAK**
1:00–2:00 p.m.	**Computational Fluid Dynamics for Advanced Reactor Design (CARD)** **Session 2 – Quality Assurance (MFAL Connection), Applications Supporting the DOE Mission, Exa-Scale Computing** Presenters: Avinash Vaidheeswaran, William Rogers, Mary Ann Clarke, Jordan Musser
2:00–2:45 p.m.	**Question and Answer Session 2**
2:45–3:00 p.m.	**BREAK**
3:00–4:30 p.m.	**Closed Discussion (Recommendations-Based Evaluation; Review Panel)** *DOE HQ/NETL and KeyLogic Peer Review Support Attend as Observers*
4:30–4:45 p.m.	**Peer Review Panel Wrap-Up Session (Logistics/Process Feedback)** *DOE HQ/NETL, KeyLogic Peer Review Support, and Review Panel Attend*
4:45 p.m.	**Adjourn**

THURSDAY, OCTOBER 6, 2022

INSTITUTE FOR DESIGN OF ADVANCED ENERGY SYSTEMS INTEGRATED PLATFORM (IDAES)

**** All times Eastern ****

11:00–11:15 a.m.	**Peer Review Panel Kickoff Session** *DOE HQ/NETL, KeyLogic Peer Review Support, and Review Panel Attend* Facilitator Opening, Review Panel Introductions, NETL Welcome, Peer Review Process and Meeting Logistics
11:15 a.m.–12:00 p.m.	**Institute for Design of Advanced Energy Systems Integrated Platform (IDAES)** **Session 1 – Overview and Scope** Presenters: David Miller, John Shinn
12:00–12:45 p.m.	**Question and Answer Session 1**
12:45–1:00 p.m.	**BREAK**
1:00–2:00 p.m.	**Institute for Design of Advanced Energy Systems Integrated Platform (IDAES)** **Session 2 – Key Capabilities and Applications** Presenters: Alex Dowling, John Siirola, Tony Burgard, Larry Biegler, Debangsu Bhattacharyya, Chrysanthos Gounaris
2:00–2:45 p.m.	**Question and Answer Session 2**
2:45–3:00 p.m.	**BREAK**
3:00–4:30 p.m.	**Closed Discussion (Recommendations-Based Evaluation; Review Panel)** *DOE HQ/NETL and KeyLogic Peer Review Support Attend as Observers*
4:30–4:45 p.m.	**Peer Review Panel Wrap-Up Session (Logistics/Process Feedback)** *DOE HQ/NETL, KeyLogic Peer Review Support, and Review Panel Attend*
4:45 p.m.	**Adjourn**

APPENDIX D: PEER REVIEW PANEL MEMBERS

FY 2023 Simulation-Based Engineering Computational Fluid Dynamics for Advanced Reactor Design (CARD) Peer Review
October 5, 2022
Virtual Meeting

HAMID ARASTOOPOUR, PH.D.

Dr. Hamid Arastoopour is the Henry R. Linden Professor of Engineering and Director of Wanger Institute for Sustainable Energy Research (WISER) at Illinois Institute of Technology (IIT) in Chicago, Illinois. Since 1985, he has been a member of the chemical engineering faculty at IIT, where he served as chairman of the department from 1989 to 2003, and Dean of the Armour College of Engineering from 2003 to 2008.

Dr. Arastoopour began his research activities at the Institute of Gas Technology (IGT) in the experimental measurement, mathematical modeling, and simulation of pneumatic conveying and fluidized bed systems associated with coal conversion and gasification processes. His main research expertise is in the area of computational fluid dynamics (CFD) of multiphase flow and particle technology—an area motivated by energy and environmentally related applications and documented in more than 100 publications and 13 U.S. patents.

He currently serves on the editorial board of Powder Technology Journal and is a fellow of the American Institute of Chemical Engineers (AIChE). He has received several national awards, including the Donald Q. Kern Award in Heat Transfer and Energy Conversion, the Fluor Daniel Lectureship in Fluidization and Fluid/Particle Systems, the Fluidization Processes Recognition Award, and the Ernest W. Thiele Award. He also received IIT's Excellence in Teaching Award in 1992.

CHRIS BOYCE, PH.D.

Dr. Chris Boyce, an Assistant Professor of Chemical Engineering at Columbia University in the City of New York, teaches undergraduate and graduate courses in fluid mechanics. His research involves examining the fundamentals of multiphase flows to spark advances in energy, health, and the environment, and using magnetic resonance imaging (MRI) and computational modeling to gain insights into complex systems.

Dr. Boyce discovers and characterizes instabilities and other flow anomalies existing in multiphase granular flows and analyzes how they couple with chemical reactions. He develops and utilizes MRI and computational techniques to study these flows and seeks to be a leader in the exploitation of MRI capabilities to provide insight into engineering systems by truly seeing inside of them. The fundamental physics insight from Dr. Boyce's research is relevant to understanding geologic flows surrounding volcanos and earthquakes, as well as to developing new technologies in the energy, pharmaceuticals, mining, and filtration industries. Because of the many length scales, applications, techniques, and areas of science involved in his work, he collaborates with a variety of engineers, physicists, chemists, and geologists. In the long term, Dr. Boyce aims to transfer insights and techniques from his work into areas more directly relevant to physiology and human health.

Dr. Boyce received a B.S. in chemical engineering and physics from Massachusetts Institute of Technology (MIT) in 2011. He studied as a Gates Cambridge Scholar at the University of Cambridge, where he earned his Ph.D. in 2015 and won the Danckwerts-Pergamon Prize for the best Ph.D. thesis in chemical engineering. He held post-doctoral positions at Princeton University and ETH Zurich before joining the faculty of Columbia Engineering in 2018.

MUHAMMAD SAMI, PH.D.

Dr. Muhammad Sami joined Ansys in 2000 and has expertise in CFD multiphase reacting flows, particulate flows, dense flows, combustion, and emissions. Before Ansys, he received his Ph.D. in mechanical engineering from Texas A&M University. As an Ansys Customer Excellence (ACE) team member, he assists clients in the power, water, and energy sector in their usage of Ansys CFD products. This interaction includes technical support, consulting, software application field testing, and technical paper presentations at conferences.

For almost 20 years, Dr. Sami has been using CFD tools to model engineering problems dealing with turbulence, heat transfer, combustion, and multiphase and particulate flows. A mechanical engineer by profession, he has been working with Ansys (formerly Fluent Inc.) since 2000 on a variety of engineering projects in the power generation and environmental industry, and since 2010 he has been working mostly with clients from the oil and gas industry. Dr. Sami's main area of interest is multi-pollutant (nitrogen oxides [NO_X], sulfur oxides [SO_X], and mercury) reduction from fossil fuel and biomass combustion in industrial and utility boilers. He is currently working on in-cylinder engine modeling (reactive flows with moving mesh); is actively involved with delivering advanced training courses in multiphase, chemical reactions, and user-defined code development in Ansys Fluent; and is part of the Ansys team that is testing the Reaction Design codes (Energico and Chemkin) for emissions predictions from gas turbine engines and utility boilers. In addition, Dr. Sami has also worked with water industry clients on modeling the ultraviolet (UV) reactors used in the water treatment of industrial and residential water supply.

FY 2023 Simulation-Based Engineering Institute for the Design of Advanced Energy Systems (IDAES) Peer Review
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AJAY LAKSHMANAN, PH.D.

Dr. Ajay Lakshmanan has more than 25 years of experience in the development of algorithms and software for process modeling, simulation, and optimization. Dr. Lakshmanan is currently the Senior Director of Product Management at Aspen Technology Inc., and is responsible for the Aspen HYSYS product line—the leading process simulator used in the oil and gas and refining industry. During his career at Aspen Technology, Dr. Lakshmanan was instrumental in the research and development (R&D) of refinery reactor models and modeling frameworks that enable process synthesis, design, analysis, optimization, and planning. Dr. Lakshmanan has authored several peer-reviewed publications and conference presentations on conceptual design, process modeling, and optimization, and has delivered invited talks at Foundations of Computer Aided Process Design (FOCAPD) conferences and served as a panel member in discussions on the Validation of Computer Codes at the AIChE annual conference. Dr. Lakshmanan has also served as the process design area Chair for the Computing and Systems Technology section of the AIChE annual meeting and as a member of the International Programming Committee at the FOCAPD and Process Systems Engineering (PSE) conferences. Dr. Lakshmanan received his Ph.D. in chemical engineering from Carnegie Mellon University and a Bachelor of Technology in chemical engineering from Indian Institute of Technology, Madras.

IGNASI PALOU-RIVERA, PH.D.

Dr. Ignasi Palou-Rivera is the Technology Platform Director of the Rapid Advancement in Process Intensification Deployment (RAPID) Manufacturing Institute—a part of AIChE in partnership with the U.S. Department of Energy (DOE). The RAPID Institute focuses on the promotion of modular chemical process intensification (MCPI), with the goal of reducing the capital and energy intensity of the U.S. process industries.

Dr. Palou-Rivera holds a Ph.D. in chemical engineering from the University of Wisconsin-Madison, and an Engineer Degree from the Universitat Politècnica de Catalunya in Barcelona. His technical background spans the areas of process modeling and optimization; techno-economic, life cycle, and sustainability analysis of fuels and chemicals; and R&D management. Before joining RAPID, he was part of several industrial and academic organizations, such as LanzaTech, Argonne National Laboratory, BP Refining Technology, and AspenTech. Dr. Palou-Rivera is a Senior Member of AIChE and has been heavily involved in volunteer positions with the Computing and Systems Technology (CAST) Division. He also is the current Chair of the Sustainable Engineering Forum (SEF).

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