

# FY19 CROSSCUTTING MODELING, SIMULATION, AND ANALYSIS PEER REVIEW OVERVIEW REPORT



October 10, 2019



U.S. DEPARTMENT OF  
**ENERGY**

NATIONAL ENERGY  
TECHNOLOGY LABORATORY

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# INTRODUCTION AND BACKGROUND

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The Crosscutting Modeling, Simulation, and Analysis Program focuses on developing and applying advanced computational tools at multiple scales (i.e., atomistic, device, process, grid, and market) to accelerate development and deployment of 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 fuel power generating systems. Computational design methods and concepts are required to significantly improve performance; reduce the costs of existing fossil energy power systems; and enable the development of new systems and capabilities, such as chemical looping combustion and fossil systems with integrated energy storage.

This effort combines theory, computational modeling, advanced optimization, experiments, and industrial input to simulate complex advanced energy processes, resulting in virtual prototyping. The research conducted in the Crosscutting Modeling, Simulation, and Analysis Program develops accurate and timely computational models of complex reacting flows and components relevant to advanced power systems. Model development and refinement is achieved through in-house research and partnerships to utilize expertise throughout the country.

## Office of Management and Budget Requirements and DOE 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 the National Energy Technology Laboratory (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 2019 (FY19) Crosscutting Modeling, Simulation, and Analysis Peer Review Meeting with independent technical experts to offer recommendations to strengthen projects during the period of performance. KeyLogic (NETL site-support contractor) convened a panel of academic and industry experts\* on September 10-11, 2019, to conduct a peer review of two Crosscutting Modeling, Simulation, and Analysis Program research projects.

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\* Please see “Appendix D: Peer Review Panel Members” for detailed panel member biographies. Please note that project-specific review panels comprised of four members were utilized for each day of the peer review; a total of six panel members supported the review, with two panel members participating both days.

TABLE 1. CROSSCUTTING MODELING, SIMULATION, AND ANALYSIS PEER REVIEW – PROJECTS REVIEWED

Project Number	Title	Lead Organization	Total Funding		Project Duration	
			DOE	Cost Share	From	To
FWP-1022423	The Institute for the Design of Advanced Energy Systems (IDAES)	NETL	\$29,272,000	\$0	01/01/2016	03/31/2021
FWP-1022405 Task 9	MFiX Suite Multiphase Code Development, Validation, Application	NETL	\$1,230,000 <sup>†</sup>	\$0	04/01/2019	03/31/2020
The projects were subject to recommendations-based evaluations. During recommendations-based evaluations, the independent panel provides recommendations to strengthen the performance of projects during the period of performance.			\$30,502,000	\$0		
			<b>\$30,502,000</b>			

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<sup>†</sup> Execution Year (EY) 2019

# OVERVIEW OF THE PEER REVIEW PROCESS

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Peer reviews are conducted to help ensure that the Office of Fossil Energy's (FE) 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 academic and industry experts to conduct a peer review of two research projects supported by the Crosscutting Modeling, Simulation, and Analysis Program. Throughout the peer review meeting, these recognized technical experts offered recommendations to strengthen the projects during the remaining period of performance. In consultation with NETL representatives, who chose the projects for review, KeyLogic selected an independent Peer Review Panel, facilitated the peer review meeting, and prepared this report to summarize the results.

## Pre-Meeting Preparation

Before the peer review, each project team submitted a Project Technical Summary (PTS) and project presentation. The Federal Project Manager (FPM) provided the Field Work Proposal (FWP), the latest quarterly report, and additional technical papers or publications as resources for the panel. The panel received these materials prior to the peer review meeting, which enabled the panel members to fully prepare for the meeting with the necessary background information to thoroughly evaluate the projects.

To increase the efficiency of the peer review meeting, multiple pre-meeting orientation teleconference calls were held with NETL, the Peer Review Panel, and KeyLogic staff to review the peer review process and procedures, evaluation criteria, and project documentation, as well as to allow for the Technology Manager to provide an overview of the program goals and objectives.

## Peer Review Meeting Proceedings

At the meeting, each project performer gave a presentation describing the project. The presentation was followed by a question-and-answer session with the panel and a closed panel discussion and evaluation. The time allotted for the presentation, the question-and-answer session, and the closed panel discussion was dependent on the project's complexity, duration, and breadth of scope.

During the closed sessions of the peer review meeting, the panel discussed each project to identify strengths, weaknesses, and recommendations in accordance with the Peer Review Evaluation Criteria. The panel offered a series of prioritized recommendations to strengthen the projects during the remaining period of performance based on the NETL Peer Review Evaluation Criteria<sup>‡</sup>.

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<sup>‡</sup> Please see "Appendix A: Peer Review Evaluation Criteria Form" for more information.

## SUMMARY OF KEY FINDINGS

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This section summarizes the overall key findings of the projects evaluated at the FY19 Crosscutting Modeling, Simulation, and Analysis Peer Review Meeting. The 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 an insight into the range of technology development and the relative progress that has been made by the project teams. The technical discussion enabled the panel to contribute to each project's development by identifying core issues and by making constructive recommendations to improve project outcomes. The panel generated several recommendations for NETL management to review and consider.

The panel offered several common strengths among the projects reviewed. Both projects are well aligned with the DOE goal of improving the performance/efficiency of coal-fired power generation by supporting existing coal-fired power plants and enabling the development of the next generation of advanced coal-based energy systems. The teams have highly qualified, experienced personnel to drive project development and established valuable collaborations with stakeholders to advance software capability and efficiently leverage available expertise. The panel indicated that there is significant potential for commercialization of the software, and the projects are using a state-of-the-art, open-source software foundation with high-performance computing architectures, which will facilitate effective and efficient development of the tools. In addition, integrating NETL's Institute for the Design of Advanced Energy Systems (IDAES) with the Multiphase Flow with Interphase eXchanges (MFiX) has the potential for a highly capable computational framework, targeting comprehensive simulation and optimization of advanced, coal-fired power plants.

The panel also noted several areas for improvement among the projects reviewed, such as defining a clear value proposition that will enable broader adoption and deployment of the tools. The panel suggested that the project teams should solicit additional user and stakeholder feedback and then formulate a value proposition based on the feedback that highlights the customer pain points addressed by the software. The value proposition should then be used to reemphasize key project focus areas that would provide the largest return on investment. Lastly, the panel noted that a skilled workforce is needed to develop and apply the software modeling tools, which is not scalable and could limit opportunities for expansion.

# PROJECT SYNOPSES

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For more information on the Crosscutting Modeling, Simulation, and Analysis Program and project portfolio, please visit the NETL website: <https://netl.doe.gov/coal/modeling-simulation-analysis>.

## **FWP-1022423**

### **THE INSTITUTE FOR THE DESIGN OF ADVANCED ENERGY SYSTEMS (IDAES)**

**Project Description:** The National Energy Technology Laboratory's (NETL) Institute for the Design of Advanced Energy Systems (IDAES) seeks to be the premier resource for the identification, synthesis, optimization, and analysis of innovative advanced energy systems at scales ranging from process to system to market to support the transformation of the national energy landscape to meet the U.S. Department of Energy's (DOE) three enduring strategic objectives: energy security, economic competitiveness, and environmental responsibility. IDAES will support technology innovation and maturation; enable identification, evaluation, and prioritization of research and development (R&D) concepts at earlier stages; enable the identification of cost and performance targets to enable new technologies to be successfully deployed in the market; enable the integrated and systematic consideration technology concepts in the context of broader energy systems and market needs and impacts; and support the more rapid maturation of cost-effective, low-carbon energy conversion systems.

## **FWP-1022405**

### **MULTIPHASE FLOW WITH INTERPHASE EXCHANGES (MFiX)**

**Project Description:** The project scope is to develop, validate, apply, publicly distribute, and support the Multiphase Flow with Interphase eXchanges (MFiX) suite of multiphase flow modeling software capable of modeling large-scale reactor systems that include complex chemical reactions and realistic geometry. These modeling tools will support the design and optimization of novel reactor systems that will meet the Advanced Reaction Systems (ARS) Field Work Proposal and Office of Fossil Energy (FE) goals. The project is developing and applying the Software Quality Assurance Program for the MFiX suite of software products to ensure that the software provides physically accurate predictions with known uncertainty. The Quality Assurance Program includes verification, validation, and uncertainty quantification processes and uses the capabilities of the Multiphase Flow Analysis Laboratory (MFAL) facilities for generation of high-quality validation data. In collaboration with industry and other partners, MFiX is applying computational tools and FE/National Energy Technology Laboratory (NETL) supercomputing resources to aid in understanding and optimizing circulating fluidized bed boiler performance under challenging operating conditions of interest to operators.



# APPENDIX A: PEER REVIEW EVALUATION CRITERIA

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## **PEER REVIEW EVALUATION CRITERIA AND GUIDELINES**

Peer reviews are conducted to ensure that the Office of Fossil Energy's (FE) research program, implemented by the National Energy Technology Laboratory (NETL), is compliant with the U.S. Department of Energy (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.

In the upcoming NETL peer review, a significant amount of information about the projects within its portfolio will be covered in a short period. For that reason, NETL has established a set of rules for governing the meeting so that everyone has an equal chance to accurately present their project accomplishments, issues, recent progress, and expected results for the remainder of the performance period (if applicable).

The following pages contain the criteria used to evaluate each project. Each criterion is accompanied by multiple characteristics to further define the topic. Each reviewer is expected to independently assess all the provided material for each project prior to the meeting and engage in discussion to generate feedback for each project during the meeting.

### **Recommendations-Based Evaluation**

At the meeting, the Facilitator and/or Panel Chairperson will lead the Peer Review Panel in identifying strengths, weaknesses, overall score, and prioritized recommendations for each project. The strengths and weaknesses shall serve as a basis for the determination of the overall project score in accordance with the Rating Definitions and Scoring Plan (see below). Under a recommendation-based evaluation, strengths and weaknesses shall be characterized as either "major" or "minor" during the Review Panel's discussion at the meeting. For example, a weakness that presents a significant threat to the likelihood of achieving the project's stated technical goal(s) and supporting objectives should be considered "major," whereas relatively less significant opportunities for improvement are considered "minor."

A recommendation shall emphasize an action that will be 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 (TRL-Based Evaluation). A recommendation should have as its basis one or more strengths or weaknesses. Recommendations shall be ranked from most important to least, based on the major/minor strengths/weaknesses.

<b>NETL Peer Review Evaluation Criteria</b>	
<b>1. Degree to which the project, if successful, supports the U.S. Department of Energy (DOE) Program's near- and/or long-term goals.</b>	<ul style="list-style-type: none"> <li>• Program goals are clearly and accurately stated.</li> <li>• Performance requirements<sup>1</sup> support the program goals.</li> </ul>
<b>2. Degree to which the project demonstrates alignment with a commercially relevant challenge or opportunity.</b>	<ul style="list-style-type: none"> <li>• The intended commercial application is clearly defined.</li> <li>• The technology value proposition has been validated by potential end-users.</li> <li>• The technology development plan and associated metrics and milestones meaningfully reduce the risk of market adoption.</li> <li>• The technology is ultimately technically and economically viable for the intended commercial application.</li> </ul>
<b>3. Degree to which there are sufficient resources to successfully complete the project.</b>	<ul style="list-style-type: none"> <li>• There is adequate funding, facilities, and equipment.</li> <li>• Project team includes personnel with the needed technical and project management expertise.</li> <li>• The project team is engaged in effective teaming and collaborative efforts, as appropriate.</li> </ul>
<b>4. Degree of project plan technical feasibility.</b>	<ul style="list-style-type: none"> <li>• Technical gaps, barriers, and risks to achieving the performance requirements are clearly identified.</li> <li>• Scientific/engineering approaches have been designed to overcome the identified technical gaps, barriers, and risks to achieve the performance requirements.</li> <li>• Remaining technical work planned is appropriate considering progress to date and remaining schedule and budget.</li> <li>• Appropriate risk mitigation plans exist, including Decision Points when applicable.</li> </ul>
<b>5. Degree to which progress has been made towards achieving the stated performance requirements.</b>	<ul style="list-style-type: none"> <li>• 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.</li> <li>• 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).</li> <li>• Milestones and reports effectively enable progress to be tracked.</li> <li>• Reasonable progress has been made relative to the established project schedule and budget.</li> </ul>
<b>6. Degree to which an appropriate basis exists for the technology's performance attributes and requirements.</b>	<ul style="list-style-type: none"> <li>• The TRL to be achieved by the end of the project is clearly stated<sup>2</sup>.</li> <li>• Performance attributes for the technology are defined<sup>2</sup>.</li> <li>• 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.</li> </ul>
<b>7. 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) and includes a plan for the commercialization of the technology.</b>	<i>(This criterion is not applicable to a Recommendations-Based Evaluation)</i>
<sup>1</sup> If it is appropriate for a project to not have cost/economic-related performance requirements, then the project will be evaluated on technical performance requirements only.	
<sup>2</sup> Supported by systems analyses appropriate to the targeted TRL.	

**Rating Definitions and Scoring Plan** (not applicable to TRL-based evaluation)

The Review Panel will be required to assign a score to the project, after strengths and weaknesses have been agreed upon. Intermediate whole number scores are acceptable if the Review Panel feels it is appropriate. The overall project score must be justified by, and consistent with, the identified strengths and weaknesses.

<b>NETL Peer Review Rating Definitions and Scoring Plan</b>	
<b>10</b>	<b>Excellent</b> - Several major strengths; no major weaknesses; few, if any, minor weaknesses. Strengths are apparent and documented.
<b>8</b>	<b>Highly Successful</b> - Some major strengths; few (if any) major weaknesses; few minor weaknesses. Strengths are apparent and documented, and outweigh identified weaknesses.
<b>5</b>	<b>Adequate</b> - Strengths and weaknesses are about equal in significance.
<b>2</b>	<b>Weak</b> - Some major weaknesses; many minor weaknesses; few (if any) major strengths; few minor strengths. Weaknesses are apparent and documented, and outweigh strengths identified.
<b>0</b>	<b>Unacceptable</b> - No major strengths; many major weaknesses. Significant weaknesses/deficiencies exist that are largely insurmountable.

# APPENDIX B: DOE TECHNOLOGY READINESS LEVELS

The following is a description of U.S. Department of Energy (DOE) Technology Readiness Levels (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.

<p><b>Technology Development</b></p>	<p><b>TRL 5</b></p>	<p>Laboratory-scale, similar system validation in relevant environment</p>	<p>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.</p>
<p><b>Technology Development</b></p>	<p><b>TRL 4</b></p>	<p>Component and/or system validation in laboratory environment</p>	<p>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.</p>
<p><b>Research to Prove Feasibility</b></p>	<p><b>TRL 3</b></p>	<p>Analytical and experimental critical function and/or characteristic proof of concept</p>	<p>Active research and development (R&amp;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.</p>
<p><b>Basic Technology Research</b></p>	<p><b>TRL 2</b></p>	<p>Technology concept and/or application formulated</p>	<p>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.</p>

	<b>TRL 1</b>	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.
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<sup>1</sup> Simulants should match relevant chemical and physical properties.

<sup>2</sup> Testing with as wide a range of actual waste as practicable and consistent with waste availability, safety, 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

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## Crosscutting Modeling, Simulation, and Analysis Peer Review September 10-11, 2019 NETL-Pittsburgh Building 922 Room 106A

### Tuesday, September 10, 2019

8:00 a.m. (no earlier)	<i>Panel Members Arrive at NETL-Pittsburgh for Security Check</i>
8:45 a.m.	<i>Morning Presenters Arrive, Visitors Escorted to NETL-Pittsburgh Building 922 Room 106A</i>
8:30 – 9:00 a.m.	Peer Review Panel Kickoff Session <i>DOE HQ/NETL, KeyLogic Peer Review Support Staff, and Panel Members Attend</i> <ul style="list-style-type: none"><li>- Facilitator Opening, Review Panel Introductions, Technology Manager Welcome, Peer Review Process and Meeting Logistics Presentation</li></ul>
9:00 – 9:40 a.m.	Project FWP-1022423 – IDAES Session 1 – Overview and Core Framework <i>David Miller, Andrew Lee – NETL, Carl Laird – Sandia National Laboratories</i>
9:40 – 10:15 a.m.	Project FWP-1022423 – IDAES Session 2 – Existing Fleet & Partnership Plant <i>Anthony Burgard – NETL, Debansu Bhattacharyya – West Virginia University</i>
10:15 – 10:30 a.m.	BREAK
10:30 – 11:45 a.m.	Question and Answer Session 1
11:45 – 12:30 p.m.	Working Lunch (Closed Discussion – Review Panel; Morning Session Recap) <i>DOE HQ/NETL and KeyLogic Peer Review Support Staff Attend as Observers</i>
12:30 – 1:00 p.m.	Project FWP-1022423 – IDAES Session 3 – Coal Plant of the Future <i>Carl Laird – Sandia National Laboratories, Jaffer Ghouse – NETL</i>
1:00 – 1:30 p.m.	Project FWP-1022423 – IDAES Session 4 – Grid & Infrastructure <i>John Sirola – Sandia National Laboratories, Alexander Dowling – University of Notre Dame</i>
1:30 – 1:45 p.m.	Project FWP-1022423 – IDAES Session 5 – Stakeholder Engagement & Outreach <i>John Shinn – Lawrence Berkeley National Laboratory</i>
1:45 – 2:00 p.m.	BREAK
2:00 – 3:15 p.m.	Question and Answer Session 2
3:15 – 4:45 p.m.	Closed Discussion (Recommendations-Based Evaluation; Review Panel) <i>DOE HQ/NETL and KeyLogic Peer Review Support Staff Attend as Observers</i>
4:45 p.m.	Adjourn

## Wednesday, September 11, 2019

- 8:00 a.m. (no earlier) *Panel Members Arrive at NETL-Pittsburgh for Security Check*
- 8:45 a.m. *Morning Presenters Arrive, Visitors Escorted to NETL-Pittsburgh Building 922 Room 106A*
- 8:30 – 9:00 a.m. Peer Review Panel Kickoff Session  
*DOE HQ/NETL, KeyLogic Peer Review Support Staff, and Panel Members Attend Facilitator Opening, Review Panel Introductions, Technology Manager Welcome, Peer Review Process and Meeting Logistics Presentation*
- 9:00 – 10:00 a.m. MFIX Session 1 – Program and Development Plan  
*Jordan Musser – NETL*
- 10:00 – 10:45 a.m. MFIX Session 2 – Verification and Validation; Nodeworks Toolsets  
*Avinash Vaidheeswaran – WVURC, William Fullmer – Leidos*
- 10:45 – 11:00 a.m. BREAK
- 11:00 – 11:45 a.m. Question and Answer Session 1
- 11:45 – 12:30 p.m. Working Lunch (Closed Discussion – Review Panel; Morning Session Recap)  
*DOE HQ/NETL and KeyLogic Peer Review Support Staff Attend as Observers*
- 12:30 – 1:00 p.m. MFIX Session 3 – Preprocessor Development, Outreach, and Stakeholder Support  
*Jeff Dietiker – Battelle*
- 1:00 – 1:45 p.m. MFIX Session 4 – Applications to Support the DOE Mission  
*Mehrdad Shabnam – NETL, William Rogers – NETL*
- 1:45 – 2:00 p.m. BREAK
- 2:00 – 2:45 p.m. Question and Answer Session 2
- 2:45 – 4:15 p.m. Closed Discussion (Recommendations-Based Evaluation; Review Panel)  
*DOE HQ/NETL and KeyLogic Peer Review Support Staff Attend as Observers*
- 4:15 – 4:45 p.m. Peer Review Panel Wrap-Up Session  
*DOE HQ/NETL, KeyLogic Peer Review Support Staff, and Panel Members Attend*
- 4:45 p.m. Adjourn



# APPENDIX D: PEER REVIEW PANEL MEMBERS

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## Crosscutting Modeling, Simulation, and Analysis Peer Review September 10-11, 2019 NETL-Pittsburgh Building 922 Room 106A

### September 10, 2019

#### **Michael Baldea, Ph.D.**

Dr. Michael Baldea is an Associate Professor and Fellow in Chemical Engineering at the University of Texas at Austin. His research focuses on modeling, simulation, optimization, and control of process and energy systems. Research in Dr. Baldea's group addresses theoretical challenges and problems of practical importance in process and energy systems engineering. Concepts from multiple fields – nonlinear systems, control, optimization, and numerical methods – are analyzed to develop new theory, algorithms, and software tools. The work follows three major thrusts: integrated decision-making in the chemical and energy supply chains, monitoring and optimizing process performance, and process integration and intensification.

Dr. Baldea formerly led research as a development specialist at Praxair Technology Center in Tonawanda, New York. While there, he initiated and led a research program focused on the dynamic modeling, optimization, and control of large-scale air separation plants. Among his achievements, he co-developed a novel optimization algorithm that is now commercially distributed as part of gPROMS, a platform for high-fidelity predictive modeling for process industries. Dr. Baldea received a diploma in Chemical Engineering and an M.S. in Interface Process Engineering from “Babes-Bolyai” University in Cluj-Napoca, Romania, and a Ph.D. in chemical engineering from the University of Minnesota – Twin Cities.

#### **Robert Button**

Robert Button is the principal of the consulting company RTO Tech, LLC, which specializes in process modeling and optimization software. He has more than 20 years of experience in process modeling and optimization, ranging from design and troubleshooting, offline optimization, scheduling, and operations management. Prior to his consulting business, Mr. Button was a Distinguished Engineering Associate at ExxonMobil. Mr. Button's responsibilities included the implementation of online optimization applications and he held the position of Global Lead for Refining Process Control and Optimization Practices. In total, he worked for ExxonMobil for 41 years (other positions included Senior Engineering Associate and Regional Process Control Specialist). Mr. Button received his B.Sc. in Chemical and Biomolecular Engineering at the Royal Melbourne Institute of Technology (RMIT) University in Australia.

#### **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. During his career at Aspen Technology, Dr. Lakshmanan was instrumental in the research and development 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 American Institute of Chemical Engineers (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 the Indian Institute of Technology, Madras.

### **Jerzy Sawicki, Ph.D., P.E.**

Dr. Jerzy Sawicki is the Vice President for Research at Cleveland State University (CSU), as well as the Donald E. Bently and Agnes Muszynska Endowed Chair and Professor of Mechanical Engineering. He is the Director of the Center for Rotating Machinery Dynamics and Control and his research interests are in structural dynamics, automatic control, rotor dynamics, turbomachinery, structural health monitoring, and engineering system modeling and simulation. He has published more than 200 peer-reviewed publications and 1 research monograph, has co-edited 3 major conference proceedings, and is the holder of 1 patent. Dr. Sawicki was the main advisor to 32 Ph.D. and M.S. students, and has supervised more than 10 post-doctoral researchers and visiting scholars.

In addition to serving on the board of several archival journals, Dr. Sawicki currently serves as the Editor-in-Chief for the American Society of Mechanical Engineers (ASME) Journal of Engineering for Gas Turbines and Power and as Chair of the ASME International Gas Turbine Institute (IGTI) Structure and Dynamics Committee. He is a Fellow of ASME and a U.S. representative to the ISO/TC 108/SC 2/WG 7 international committee, as well as a recipient of several Best Paper awards, the Siemens-Westinghouse Distinguished Speaker honor, and the University Distinguished Faculty Award for Research.

Dr. Sawicki holds a Ph.D. in Mechanical Engineering from Case Western Reserve University; an M.S. in Mechanical Engineering from Gdańsk University of Technology, Poland; and an M.S. in Applied Mathematics from the University of Gdańsk, Poland. He received the Ohio Outstanding Engineering Educator Award from the Ohio Society of Professional Engineers and is a registered professional engineer, licensed in Ohio.

**September 11, 2019****Robert Button**

Robert Button is the principal of the consulting company RTO Tech, LLC, which specializes in process modeling and optimization software. He has more than 20 years of experience in process modeling and optimization, ranging from design and troubleshooting, offline optimization, scheduling, and operations management. Prior to his consulting business, Mr. Button was a Distinguished Engineering Associate at ExxonMobil. Mr. Button's responsibilities included the implementation of online optimization applications and he held the position of Global Lead for Refining Process Control and Optimization Practices. In total, he worked for ExxonMobil for 41 years (other positions included Senior Engineering Associate and Regional Process Control Specialist). Mr. Button received his B.Sc. in Chemical and Biomolecular Engineering at the Royal Melbourne Institute of Technology (RMIT) University in Australia.

**Michael E. Mueller, Ph.D.**

Dr. Michael E. Mueller is an Assistant Professor in the Department of Mechanical and Aerospace Engineering at Princeton University. Dr. Mueller's research focuses on high-fidelity computational modeling of turbulent reacting flows, in which he utilizes a multi-fidelity approach leveraging full-fidelity direct numerical simulation (DNS) for the development of physics-based models for high-fidelity large eddy simulation (LES) applicable to practical engineering systems such as gas turbine combustors and reciprocating engines. Current areas of interest within his research group include multi-modal turbulent combustion, pollutant emissions, and combustion-affected turbulence. In addition, Dr. Mueller is active in areas of applied computational science, including the development of new approaches to uncertainty quantification and the development of new numerical algorithms and their implementation on emerging parallel computing architectures. Dr. Mueller received his Ph.D. from Stanford University in Mechanical Engineering, his M.S. from Stanford University in Mechanical Engineering, and his B.S. in Mechanical Engineering (Highest Honors) from the University of Texas at Austin.

**Muhammad Sami, Ph.D.**

Dr. Muhammad Sami joined ANSYS in 2000 and has expertise in computational fluid dynamics (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 has been assisting 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 (NO<sub>x</sub>, SO<sub>x</sub>, 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); involved with delivering advanced training courses in

multiphase, chemical reactions and user-defined code development in ANSYS FLUENT; and part of the ANSYS team that is testing the Reaction Design codes, Energico and Chemkin, for emission 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.

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