

Final Report Strategic Center for Coal Fuel Cells FY 2011 Peer Review Meeting



Meeting Summary and Recommendations Report

Morgantown, West Virginia
February 14–18, 2011

**FINAL REPORT
STRATEGIC CENTER FOR COAL
FUEL CELLS
FY2011 PEER REVIEW MEETING**

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MEETING SUMMARY AND RECOMMENDATIONS REPORT

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EXECUTIVE SUMMARY

The mission of the U.S. Department of Energy's (DOE) Office of Clean Coal (OCC) is to ensure the availability of ultraclean, near-zero emission, abundant, and low-cost domestic energy from coal in order to fuel economic prosperity, strengthen energy security, and enhance environmental quality.¹ The OCC research and development effort is administered by the Office of Fossil Energy's National Energy Technology Laboratory (NETL) through eight technology areas; one of these areas—the Fuel Cells Program—is the subject of this report.

The NETL Fuel Cells Program manages a research, development, and demonstration (RD&D) portfolio designed to remove environmental concerns over the future use of coal by developing highly efficient, economical, and robust fuel cell technologies. The Fuel Cells Program goals include the following:

- By 2010, reduce the cost of the fuel cell power block to \$400/kW (2000 dollars, assuming 250 MW per year production).
- By FY2015, test module proof-of-concept stacks (>250kW) that are building blocks for multi-megawatt-class, coal based fuel cell systems with a minimum 50% higher heating value (HHV) efficiency, nitrogen oxide emissions of less than 0.5 ppm, that are suitable for integration with high-efficiency gasification and carbon capture.
- This work will enable Multi-Megawatt scale coal-based (IGFC) Integrated Gasification Fuel Cell systems capable of 50%–60% HHV efficiency with carbon capture for commercial scale demonstration in the 2020 time frame.

In compliance with requirements from the Office of Management and Budget, DOE and NETL are fully committed to improving the quality of research projects in their programs. To aid this effort, DOE and NETL conducted a FY2011 Fuel Cells Peer Review Meeting with independent technical experts to assess ongoing research projects and, where applicable, to make recommendations for individual project improvement.

In cooperation with Leonardo Technologies, Inc., the American Society of Mechanical Engineers (ASME) convened a panel of eight leading academic and industry experts on February 14–18, 2011, to conduct a five-day Peer Review of selected Fuel Cells Program research projects supported by NETL.

Overview of Office of Fossil Energy Fuel Cells Program Research Funding

The total funding of the 17 projects reviewed, over the duration of the projects, is \$166,066,211. Of this amount, \$124,137,312 (75%) is funded by DOE, while the remaining \$41,928,899 (25%) is funded by project partner cost sharing.

The 17 projects that were the subject of this Peer Review are summarized in Table ES-1 and in Section II of this report.

¹ U.S. Department of Energy, Office of Fossil Energy, Office of Clean Coal, Office of Clean Coal Strategic Plan (Washington D.C.: U.S. Department of Energy, September 2006), http://fossil.energy.gov/programs/powersystems/publications/OCC_Strategic_Plan_external_Sept06.pdf.

TABLE ES-I FUEL CELLS PROJECTS REVIEWED

Reference Number	Project No.	Title	Lead Organization	Principal Investigator	Total Funding		Project Duration	
					DOE	Cost Share	From	To
1	FC26-08NT0003894	SECA Coal-Based Systems – UTC Power	UTC Power Corporation	Tom Skiba	\$29,992,500	\$9,261,931	10/1/2008	6/30/2011
2	DE-FE0000528	Techno-Economic Analysis of Scalable Coal-Based Fuel Cells	University of Akron	Steven Chuang	\$1,370,977	\$342,984	9/1/2009	8/31/2013
3	DE-FE0004001.410.01.13and29	Analysis of Integrated Gasification Fuel Cell (IGFC) Plant Configurations	National Energy Technology Laboratory - Office of Program Planning and Analysis (OPPA)	W. Morgan Summers	\$290,000	\$0	11/15/2009	2/18/2011
4	FC26-04NT41837	SECA Coal-Based Systems - FuelCell Energy	FuelCell Energy, Inc.	Hossein Ghezeli-Ayagh	\$56,999,889	\$28,378,916	2/27/2004	2/28/2011
5	FC26-08NT0004113	Validation of Novel Planar Cell Design for Megawatt-Scale SOFC Power Systems	NexTech Materials, Ltd.	Michael J. Day	\$450,000	\$112,500	10/1/2008	9/30/2011
6	FC26-08NT0005177	Viscous Glass/Composite SOFC Sealants	Alfred University	Scott Misture	\$250,000	\$88,310	10/1/2008	9/30/2011
7	DE-FE0000982	Improved Flow Field Structures for Direct Methanol Fuel Cells	NuVant Systems Inc.	Bogdan Gurau	\$913,985	\$228,496	9/17/2009	9/29/2011
8	DE-FE0000303	SECA Coal-Based Systems - Rolls-Royce	Rolls-Royce Fuel Cell Systems (US) Inc.	Richard Goettler	\$9,504,885	\$2,499,971	9/1/2009	6/30/2011
9	DE-FE0000773	Rolls-Royce Solid Oxide Fuel Cell (SOFC) Model Development	Rolls-Royce Fuel Cell Systems (US) Inc.	Greg Rush	\$1,233,680	\$308,420	10/1/2009	9/30/2011
10	FC26-08NT0004104	Solid Oxide Fuel Cell Cathodes: Unraveling the Relationship Between Structure, Surface Chemistry & Oxygen Reduction	Trustees of Boston University	Srikanth Gopalan	\$450,001	\$114,926	10/1/2008	9/30/2011
11	FC26-08NT0004105	Investigation of Cathode Electrocatalytic Activity using Surfaced Engineered Thin Film Samples and High Temperature Property Measurements	Carnegie Mellon University	Paul Salvador	\$688,588	\$172,195	9/30/2008	9/29/2011
12	FWP-40552 (Task 1)	SECA Core Technology Program: Task 1 - SOFC Component Development	Pacific Northwest National Laboratory (PNNL)	Jeffrey Stevenson	\$14,450,000	\$0	10/1/2007	9/30/2011
13	FY10.MSE.1610248.621	Solid Oxide Fuel Cell Research and Development: Impact of Minor Species from Coal Syngas on SOFC Performance	National Energy Technology Laboratory-Office of Research and Development (ORD)	Kirk Gerdes	\$461,807	\$0	10/1/2009	9/30/2010
14	FC26-08NT0006557	Theory, Investigation and Stability of Cathode Electrocatalytic Activity	Georgia Tech Research Corporation	Meilin Liu	\$600,000	\$150,000	9/3/2008	8/31/2011

Executive Summary

Reference Number	Project No.	Title	Lead Organization	Principal Investigator	Total Funding		Project Duration	
					DOE	Cost Share	From	To
15	FEAA066	Reliability of Materials and Components for Solid Oxide Fuel Cells	Oak Ridge National Laboratory (ORNL)	Edgar Lara-Curzio	\$5,400,000	\$0	10/1/2000	9/30/2011
16	FC26-08NT0004117	Chemistry of SOFC Cathode Surfaces: Fundamental Investigation and Tailoring of Electronic Behavior	Massachusetts Institute of Technology	Bilge Yildiz	\$600,000	\$150,000	9/30/2008	9/29/2011
17	DE-FE0005132	Small Scale SOFC Demonstration using Bio-based and Fossil Fuels	Technology Management, Inc.	Robert Ruhl	\$481,000	\$120,250	10/1/2010	9/30/2011
TOTALS					\$124,137,312	\$41,928,899		

Note: Funding amounts and project durations have been obtained from project summaries submitted by the principal investigator.

NETL FUEL CELLS PROGRAM OVERVIEW

The NETL Fuel Cells Program aims to operate coal-based IGFC power systems at efficiencies of 50%–60% HHV while achieving nearly 100% carbon capture. Efforts are focused on the R&D required to provide fuel cells that will improve efficiency and the cost effectiveness of IGFC and other related processes by decreasing fuel cell cost, increasing fuel cell reliability, and improving fuel cell manufacturing processes. The program has advanced the solid oxide fuel cell (SOFC) technology, which has the potential to provide step-change improvements in coal-based power generation thermal efficiency, cost of electricity, environmental emissions, and water consumption, along with the ability to capture carbon. The program's mission is to have fuel cell systems ready for demonstration in a Clean Coal Power Initiative (CCPI) by 2020.

Research efforts will be focused in the following areas:

Cost Reduction – The Fuel Cells Program is sponsoring R&D that will lead to substantially improved power density and more reliable and robust systems using the state-of-the-art national laboratory facilities and the nation's university and small business infrastructure. The strategy is to have fuel cell technology demonstrated in small- to medium-scale applications before use in large-scale, coal-based central power generation to ensure sufficient operating experience is collected prior to substantial capital investment.

Coal-based Systems – This element focuses on the scale-up and integration of the fuel cell technology, resulting in the operation of module proof-of-concept stacks (>250 kW) that are building blocks for multi-megawatt-class coal based IGFC systems by 2015. IGFC systems using advanced gasification technology have the potential to achieve efficiencies approaching 60%, with carbon capture and near-zero emissions, including a near-zero water footprint.

Overview of the Peer Review Process

NETL requested that ASME assemble a Fuel Cells Peer Review Panel (hereinafter referred to as the Panel) of recognized technical experts to provide recommendations on how to improve the management, performance, and overall results of each individual research project. Each project team prepared a detailed project information form containing an overview of the project's purpose, objectives, and achievements, and a presentation to be given at the Peer Review Meeting. The Panel received the project information forms and presentations prior to the Peer Review Meeting.

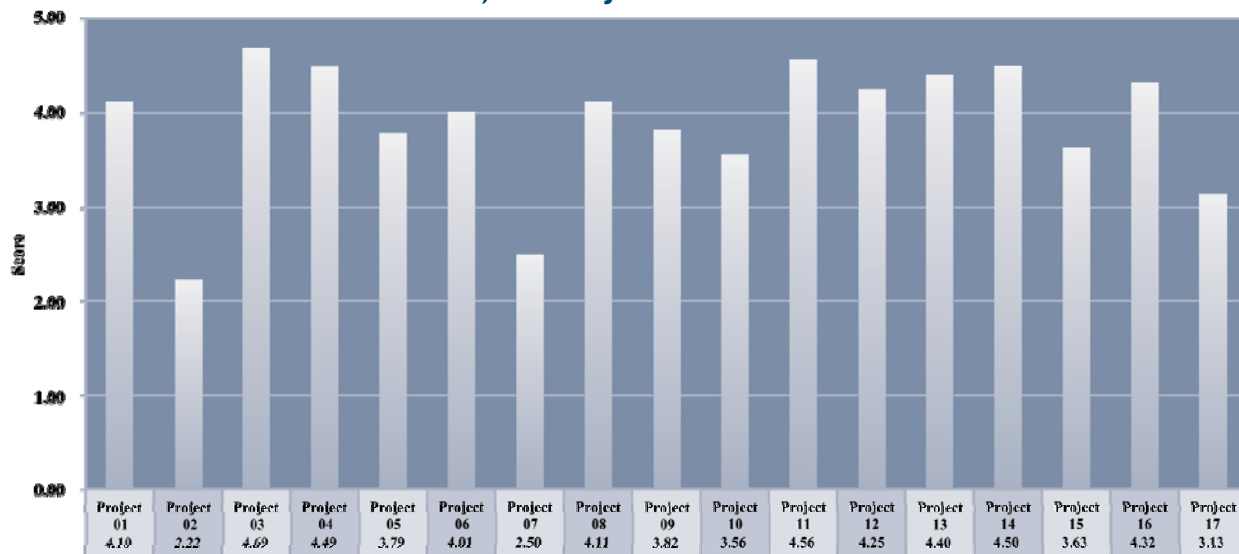
At the meeting, each research team made an uninterrupted 45- to 120-minute PowerPoint presentation that was followed by a 40- to 60-minute question-and-answer session with the Panel. After the principal investigator and project team left the room, the Panel had a 30- to 40-minute discussion about the strengths, weaknesses, recommendations, and action items for each project. To facilitate a full and open discourse of project-related material between the project team and the Panel, all sessions were limited to the Panel, ASME project team members, and DOE/NETL personnel and contractor support staff.

After the group discussions, each panel member individually evaluated the 17 projects, providing written comments based on a predetermined set of review criteria. For each of the nine review criteria, the individual reviewer was asked to score the project as one of the following:

- Effective (5)
- Moderately Effective (4)
- Adequate (3)
- Ineffective (2)
- Results Not Demonstrated (1)

The Panel occasionally had divergent views of a project. In the extreme case, this divergence is reflected in projects receiving ratings ranging from 1 to 4 or 2 to 5 in a particular criterion. This result should not be taken as an indication that the Panel was indecisive; rather, this reflects the varied backgrounds and differing perspectives of a diverse Panel. Such diversity is a strength allowing the Panel, as a whole, to review a wide range of projects on varied topics with a comparable overall level of expertise.

Figure ES-2 shows the overall average score, combining all nine review criteria, for each of the 17 projects.

FIGURE ES-2 AVERAGE SCORING, BY PROJECT

The “Project Average” in Table ES-3 shows the score for each criterion averaged across all 17 projects. The “Highest Project Rating” and “Lowest Project Rating” columns portray the highest and lowest scores, respectively, received by an individual project in a given criterion. The highest-ranking review criteria, Scientific and Technical Merit; Existence of Clear, Measurable Milestones; and Anticipated Benefits, if Successful, all earned average scores across all projects of 4.1. Two criteria, Utilization of Government Resources and Technical Approach, received average scores of 4.0. These scores indicate that NETL is continuously working to pursue strong, relevant research and development (R&D) and clearly demonstrate NETL’s efforts to ensure that ambitious R&D goals are achievable. The lowest-ranking review criterion was Potential Technology Risks Considered, indicating that several projects did not fully consider project risks and ways to mitigate them.

TABLE ES-3 AVERAGE SCORING, BY REVIEW CRITERION

Criterion	Project Average	Highest Project Rating	Lowest Project Rating
1. Scientific and Technical Merit	4.1	4.9	2.3
2. Existence of Clear, Measurable Milestones	4.1	5.0	2.5
3. Utilization of Government Resources	4.0	5.0	2.0
4. Technical Approach	4.0	4.9	2.1
5. Rate of Progress	3.9	4.8	2.4
6. Potential Technology Risks Considered	3.5	4.4	2.0
7. Performance and Economic Factors	3.6	4.6	1.9
8. Anticipated Benefits, if Successful	4.1	4.8	2.6
9. Technology Development Pathways	3.7	4.6	2.1

Note: The score for each project in a given criterion is, by definition, the average of *all reviewer ratings* for that criterion.

For more on the overall evaluation process and the nine review criteria, see Section III.

Each project was categorized based on its stage of development, which ranged from fundamental research to proof-of-concept, as described in Table ES-4. This categorization enabled the Panel to appropriately score the Performance and Economic Factors and Technology Development Pathway criteria by providing context for the anticipated level of economic and developmental data for each project.

TABLE ES-4 DESCRIPTION OF DEVELOPMENT STAGES

Stage of Research	Description
Fundamental Research	The project explores and defines technical concepts or fundamental scientific knowledge. Projects are laboratory-scale and, traditionally but not exclusively, are the province of academia.
Applied Research	The project presents a laboratory- or bench-scale proof of the feasibility of potential applications of a fundamental scientific discovery.
Prototype Testing	The project develops and tests a prototype technology or process in the laboratory or field, maintaining predictive modeling or simulation of performance and evaluating scalability.
Proof-of-Concept	The project develops and tests a pilot-scale technology or process for field testing and validation at full scale, but is not indicative of a long-term commercial installation.
Major Demonstration <i>*not applicable in this peer review</i>	The project develops a commercial-scale demonstration of energy and energy-related environmental technologies, generally with the intent of becoming the initial representation of a long-term commercial installation.

A summary of key project findings as they relate to individual projects can be found in Section IV of this report. Process considerations and recommendations for future project reviews are found in Section V.

For More Information

For more information concerning the contents of this report, contact the NETL Federal Project Manager and Peer Review Coordinator, José D. Figueroa, at (412) 386-4966 or Jose.Figueroa@netl.doe.gov.

MEETING SUMMARY AND RECOMMENDATIONS

I. INTRODUCTION

In fiscal year (FY) 2011, the American Society of Mechanical Engineers (ASME) was invited to provide an independent, unbiased, and timely peer review of selected projects within the U.S. Department of Energy (DOE) Office of Fossil Energy Fuel Cells Program (administered by the Office of Fossil Energy's National Energy Technology Laboratory [NETL]). On February 14–18, 2011, ASME convened a panel of eight leading academic and industry experts to conduct a five-day peer review of selected Fuel Cells research projects supported by NETL. This report contains a summary of the findings from that review.

Compliance with Office of Management and Budget Requirements

DOE, the Office of Fossil Energy, and NETL are fully committed to improving the quality and results of their projects. The peer review of selected projects within the Fuel Cells Program was designed to comply with requirements from the Office of Management and Budget.

ASME Center for Research and Technology Development

All requests for peer reviews are organized under ASME's Center for Research and Technology Development (CRTD). CRTD's Director of Research, Dr. Michael Tinkleman, with advice from the chair of the ASME Board on Research and Technology Development, selects an executive committee of senior ASME members that is responsible for reviewing and approving all panel members and ensuring that there are no conflicts of interest within the Panel or the review process. In consultation with NETL, ASME formulates the review meeting agenda, provides information advising the principal investigators (PIs) and their colleagues on how to prepare for the review, facilitates the review session, and prepares a summary of the results. A more extensive discussion of the ASME peer review methodology used for the Fuel Cells Peer Review Meeting is provided in Appendix A. A copy of the meeting agenda is provided in Appendix B, and profiles of the panel members are provided in Appendix C.

Overview of the Peer Review Process

ASME was selected as the independent organization to conduct a five-day peer review of 17 Fuel Cells Program projects. ASME performed this project review work as a subcontractor to prime NETL contractor Leonardo Technologies, Inc. NETL selected the 17 projects, while ASME organized an independent review panel of eight leading academic and industry experts. Prior to the meeting, project PIs submitted their PowerPoint presentations and an 11-page written summary (project information form) of their project's purpose, objectives, and progress. This project information is given to the Panel prior to the meeting, which allows the Panel to come to the meeting fully prepared with the necessary project background information.

At the meeting, each research team made a 45- to 120-minute oral presentation, followed by a 40- to 60-minute question-and-answer (Q&A) session with the Panel and a 30- to 40-minute Panel discussion of each project. The length of the presentation and Q&A session was primarily a function of the perceived time required for the PI to go through the presentation material, which depended on a number of factors, such as the project's complexity, duration, and breadth of scope. Based on lessons learned from prior peer reviews and the special circumstances associated with Fuel Cells Program research, both the PI presentations and Q&A sessions with the Panel for the Fuel Cells Peer Review were held as closed sessions, limited to the Panel, ASME project team members, and DOE/NETL personnel and contractor support staff. The closed sessions ensured open discussions between the PIs and the Panel. Panel members were also instructed to hold the discussions that took place during the Q&A session as confidential.

Each member of the Panel individually evaluated the project and provided written comments based on a predetermined set of review criteria. This publically available document, prepared by ASME, provides a general overview of the Fuel Cells Peer Review and the projects reviewed therein.

Peer Review Criteria and Peer Review Criteria Forms

ASME developed a set of agreed-upon review criteria to be applied to the projects reviewed at this meeting. ASME provided the Panel and PIs with these review criteria in advance of the Peer Review Meeting, and assessment sheets with the review criteria were pre-loaded (one for each project) onto laptop computers for each panel member. During the meeting, the panel members assessed the strengths and weaknesses of each project before providing both recommendations and action items. A more detailed explanation of this process and a sample peer review criteria form are provided in Appendix D.

The following sections of this report summarize findings from the Fuel Cells Peer Review Meeting, organized as follows:

- II. *Summary of Projects Reviewed in FY 2011 Fuel Cells Peer Review:*
A list of the 17 projects reviewed and the selection criteria
- III. *An Overview of the Evaluation Scores for the Fuel Cells Program:*
Average scores and a summary of evaluations, including analysis and recommendations
- IV. *Summary of Key Project Findings:*
An overview of key findings from project evaluations
- V. *Process Considerations for Future Peer Reviews*
Lessons learned in this review that may be applied to future reviews

II. SUMMARY OF PROJECTS REVIEWED IN FY2011 FUEL CELLS PEER REVIEW

NETL selected key projects within the Fuel Cells Program, including projects being conducted at NETL, to be reviewed by the independent Peer Review Panel. The selected projects are listed below along with the name of the organization leading the research. A short summary of each of the above projects is presented in Appendix E.

PROJECTS REVIEWED

01: FC26-08NT0003894

SECA Coal-Based Systems – UTC Power
UTC Power Corporation

02: DE-FE0000528

Techno-Economic Analysis of Scalable Coal-Based Fuel Cells
University of Akron

03: DE-FE0004001.410.01.13AND29

Analysis of Integrated Gasification Fuel Cell (IGFC) Plant Configurations
National Energy Technology Laboratory – Office of Program Planning and Analysis

04: FC26-04NT41837

SECA Coal-Based Systems - FuelCell Energy
FuelCell Energy, Inc. (FCE)

05: FC26-08NT0004113

Validation of Novel Planar Cell Design for Megawatt-Scale SOFC Power Systems
NexTech Materials, Ltd.

06: FC26-08NT0005177

Viscous Glass/Composite SOFC Sealants
Alfred University

07: DE-FE0000982

Improved Flow Field Structures for Direct Methanol Fuel Cells
NuVant Systems Inc.

08: DE-FE0000303

SECA Coal-Based Systems - Rolls-Royce
Rolls-Royce Fuel Cell Systems (US) Inc.

09: DE-FE0000773

Rolls-Royce Solid Oxide Fuel Cell (SOFC) Model Development
Rolls-Royce Fuel Cell Systems (US) Inc.

10: FC26-08NT0004104

Solid Oxide Fuel Cell Cathodes: Unraveling the Relationship Between Structure, Surface Chemistry & Oxygen Reduction
Trustees of Boston University

I1: FC26-08NT0004105

Investigation of Cathode Electrocatalytic Activity using Surfaced Engineered Thin Film Samples and High Temperature Property Measurements
Carnegie Mellon University

I2: FWP-40552 (TASK 1)

SECA Core Technology Program: Task 1 - SOFC Component Development
Pacific Northwest National Laboratory (PNNL)

I3: FY10.MSE.1610248.621

Solid Oxide Fuel Cell Research and Development: Impact of Minor Species from Coal Syngas on SOFC Performance
National Energy Technology Laboratory-Office of Research and Development (ORD)

I4: FC26-08NT0006557

Theory, Investigation and Stability of Cathode Electrocatalytic Activity
Georgia Tech Research Corporation

I5: FEAA066

Reliability of Materials and Components for Solid Oxide Fuel Cells
Oak Ridge National Laboratory (ORNL)

I6: FC26-08NT0004117

Chemistry of SOFC Cathode Surfaces: Fundamental Investigation and Tailoring of Electronic Behavior
Massachusetts Institute of Technology

I7: DE-FE0005132

Small Scale SOFC Demonstration using Bio-based and Fossil Fuels
Technology Management, Inc.

III. AN OVERVIEW OF THE EVALUATION SCORES FOR THE FUEL CELLS PROGRAM

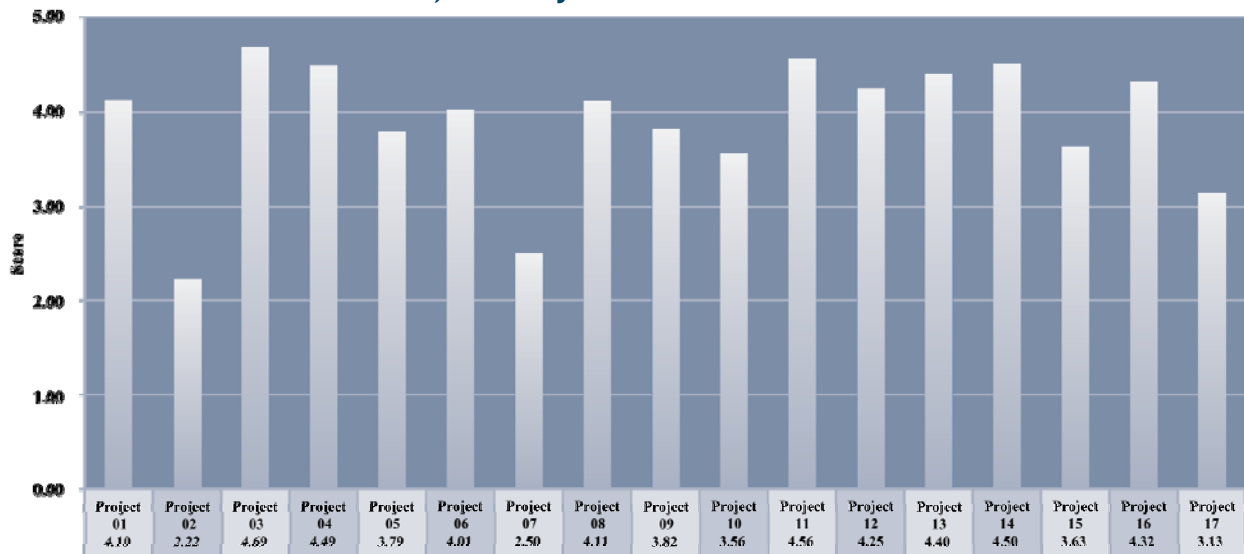
For each of the nine review criteria, individual reviewers were asked to score the project as one of the following:

- Effective (5)
- Moderately Effective (4)
- Adequate (3)
- Ineffective (2)
- Results Not Demonstrated (1)

The average scores for all the projects and across each rating criterion indicate that, overall, the Fuel Cells Program is adequate and has opportunities for improvement. The program consists primarily of well-managed and well-staffed projects aimed at developing innovative and marketable technologies that have considerable potential to provide valuable benefits to the fuel cells industry.

Figure 1 shows the average project scores, combining the average of the nine review criteria for each of the 17 projects reviewed. As Figure 1 illustrates, it is relatively easy to look at the scores for an individual project and gain an impression of how well the project performed. While it is not the intent of this review to directly compare one project with another, an average score exceeding 3.0 generally indicates that a specific project was viewed favorably by the Panel. Fifteen of the seventeen projects reviewed from the Fuel Cells Program met or exceeded this score. Conversely, a specific project was viewed less favorably by the Panel if the average score was below 3.0. Two of the seventeen projects fit within this category.

FIGURE I AVERAGE SCORING, BY PROJECT



General conclusions about the Fuel Cells Program can also be drawn by looking at the average scores for each of the nine review criteria, which are shown in Table 1. The “Project Average” in Table ES-3 shows the score for each criterion averaged across all 17 projects. The “Highest Project Rating” and “Lowest Project Rating” columns portray the highest and lowest scores, respectively, received by an individual project in a given criterion.

TABLE 1 AVERAGE SCORING, BY REVIEW CRITERION

Criterion	Project Average	Highest Project Rating	Lowest Project Rating
1. Scientific and Technical Merit	4.1	4.9	2.3
2. Existence of Clear, Measurable Milestones	4.1	5.0	2.5
3. Utilization of Government Resources	4.0	5.0	2.0
4. Technical Approach	4.0	4.9	2.1
5. Rate of Progress	3.9	4.8	2.4
6. Potential Technology Risks Considered	3.5	4.4	2.0
7. Performance and Economic Factors	3.6	4.6	1.9
8. Anticipated Benefits, if Successful	4.1	4.8	2.6
9. Technology Development Pathways	3.7	4.6	2.1

Note: The score for each project in a given criterion is, by definition, the average of *all reviewer ratings* for that criterion.

All of the criteria received average scores between 4.1 and 3.5, reflecting NETL’s efforts to fund and manage projects that are developing innovative and scientifically rigorous technologies. The lowest-ranking review criterion was Potential Technology Risks Considered, indicating that several projects did not fully consider project risks and ways to mitigate them. The highest-ranking review criterion, Existence of Clear, Measureable Milestones, earned average scores across all projects of 4.10, indicating that NETL is continuously working to pursue research and development (R&D) with measurable, quantitative milestones that clearly demonstrate NETL’s efforts to ensure that progress is made toward project goals.

A copy of the Peer Review Criteria Form and a detailed explanation of the review process are provided in Appendix D.

IV. SUMMARY OF KEY FINDINGS

This section summarizes key findings from across the 17 projects evaluated at the FY 2011 Fuel Cells Peer Review.

General Project Strengths

The Panel was very impressed by the high-quality projects they reviewed from DOE's Fuel Cells Program. These projects have ambitious goals and significant potential to advance fuel cell technology toward applications in coal-based power generation. The Panel found the Program to be essentially on track and to have a well balanced portfolio of fundamental science, national laboratory research, and large-scale industry demonstration projects. The Panel was particularly impressed with the top-notch science being performed and the use of modeling to support experimentation in many of the projects. Based on the progress made to date in the Program, the Panel was optimistic about the future of fuel cell development and the ultimate potential for gains in coal gasification based power plant efficiency resulting from the use of fuel cells for power plants both with and without carbon capture.

Table 1 displays the spread of average scores across all 17 projects among the nine individual criteria. All of the criteria received averages ranging from 3.5 to 4.1. This signifies that, overall, the Fuel Cells Program ranked well above "adequate" in all criterion areas, with five criteria receiving above "outstanding" (4.0) performance. As depicted in Figure 1, 10 of the 17 reviewed projects received average ratings of 4.0 or above, also indicative of an exemplary DOE Program.

The five criteria that earned average scores across all projects of 4.0 or higher include Scientific and Technical Merit; Existence of Clear, Measureable Milestones; Utilization of Government Resources; Technical Approach; and Anticipated Benefits, if Successful. These high scores reflect the Panel's view that, overall, the projects were based on innovative, high-quality science and technical approaches that measured success using meaningful performance targets aligned with Fuel Cells Program targets. The Panel found that the program has leveraged its resources toward relevant research and development initiatives that, if successful, could contribute significantly to achieving DOE goals. The remaining criteria received ratings of 3.5 or above—well above adequate—signifying that the program overall was strong in all areas and that, on average, projects more than adequately considered costs, economics, risk factors, and technology development pathways.

The highest-rated project was project 03, "Analysis of Integrated Gasification Fuel Cell (IGFC) Plant Configurations" conducted by the NETL Office of Program Planning and Analysis (OPPA). This project received an average rating across the nine criteria of 4.7 out of 5.0. Three other projects—project 11, "Investigation of Cathode Electrocatalytic Activity using Surface Engineered Thin Film Samples and High Temperature Property Measurements" conducted by Carnegie Mellon University; project 14, "Theory, Investigation and Stability of Cathode Electrocatalytic Activity" conducted by Georgia Tech Research Corporation; and project 4, "SECA Coal-Based Systems FuelCell Energy" conducted by FuelCell Energy—received average scores above 4.5. In addition to these top four projects, five additional projects received ratings of "outstanding" or above (4.0 or greater). In general, high-scoring projects were characterized by knowledgeable principal investigators, innovative technical approaches, strong collaborative efforts, and thorough consideration of commercialization pathways.

General Project Weaknesses

Although the projects evaluated in the Fuel Cells Program received above average ratings in all nine criteria, four areas fell short of an "outstanding" score: Rate of Progress (3.9), Potential

Technology Risks Considered (3.5), Performance and Economic Factors (3.6), and Technology Development Pathways (3.7). The scores in these four areas indicate that the Panel found that one or more projects were behind schedule and that some project teams did not sufficiently identify and consider the economics, risks, and commercial viability of their technologies.

The predominant recurring theme that arose during the Fuel Cells Peer Review was the lack of attention paid in many projects to coal-based fuel cells applications. While the Fuel Cells Program has clearly established natural-gas-fired applications as the nearer-term goal for the program, the Panel considered it a weakness if the team failed to consider the impact that coal-based contaminants can have on fuel cells, as this deficiency could lead to the development of technologies that may not have the flexibility or durability to be used in coal-based systems.

Another major theme identified by the Panel was the lack of risk and cost analyses associated with technology scale-up. The Panel found that some project teams were paying insufficient attention to the competing technologies present in the target market and the performance metrics and cost of electricity the technology under development needs to achieve in order to be competitive. Other recurring issues included insufficient testing periods and the listing of milestones as activities rather than performance-based targets, though this was sometimes related to the short duration or to the exploratory nature of projects. In a couple of instances, projects were deemed to have had too broad a scope and needed to be refocused in order to successfully help DOE to achieve its program goals.

The Panel noted that the issues related to the three lowest-ranking criteria above may be due to the inherent difficulty in thoroughly evaluating cost and economic factors for projects that are in the fundamental research stages of technology development. However, some of the basic science projects received some of the highest scores across the board due to the fact that the principal investigator and project team were acknowledging and considering the long-term goals and applications of their technology.

Issues for Future Consideration

While the majority of the recommendations provided by the Panel were technical in nature and specific to the particular project's technology or approach, several overarching themes emerged, addressing some of the general weaknesses discussed above.

The Panel recognized that coal-based fuel cells such as IGFCs are a much longer-term goal for the Fuel Cells Program; however, they felt that project teams could have increased their consideration of coal and the presence of trace contaminants in the syngas to be delivered to the fuel cell system. At the very least, project teams should develop a more thorough understanding of the types of contaminants and their impacts on the technology being studied. This would better enable the project team, and the Fuel Cells Program as a whole, to be better positioned to develop technology that is suitable for coal-based fuel cell systems. The Panel also acknowledged that while a technology may only work under natural gas conditions, if successfully commercialized, it would still be helping to pave the way for the longer-term deployment and widespread use of coal-based fuel cells.

The Panel also emphasized the importance of defining the cost and performance parameters necessary for successfully scaling up and commercializing the technologies as well as running longer-term tests under more realistic operating conditions. Additional recommendations included the need to restate milestones as measureable cost and performance targets.

V. PROCESS CONSIDERATIONS FOR FUTURE PEER REVIEWS

The Panel and DOE/NETL managers involved in the Fuel Cells Peer Review offered positive feedback on the review process and constructive comments for improving future peer reviews. These comments were provided at the conclusion of the Peer Review Meeting. The following is a brief summary of ideas recommended for consideration when planning future peer review sessions.

General Process Comments

All involved agreed that the current peer review process is effective, especially the meeting organization and facilitation. The panel members appreciated the early availability of the project information and background, as it gave them ample time prior to the Peer Review Meeting to read the project information documents. The Panel commented that they knew when to expect information, and what to expect as far as the meeting agenda and the length of the days. They suggested that these practices continue to enable the members to fit the integral step of project information review into their busy schedules prior to the Meeting.

Many panel members found the openness of the NETL Technology Manager when asked for clarifying input on a broader programmatic issue to be beneficial to the overall review process, as the context he provided enabled the Panel to provide more accurate feedback on the specific project being reviewed.

Meeting Agenda

The Panel appreciated the amount of flexibility afforded to the overall meeting agenda, as it enabled the presentations to remain on time without shortchanging presentations, question and answer sessions, and Panel discussions. While panel members found the two-hour presentations quite long, members agreed that such long presentations are necessary for some projects, and felt that short breaks between the presentation and Q&A would help panel members to retain their focus.

Presentations

The Panel recognized that the project presentations and the review process were enhanced by the DOE presentation template and DOE's efforts to familiarize the principal investigators (PIs) with the peer review process. The panel members had suggestions regarding the organization and structure of the presentations. Overall, the Panel recommended that DOE/NETL encourage the PIs to focus their presentations more on the assumptions that were made and the progress that has been achieved. The Panel also suggested that the PI be required to include a slide that details the project's contributions to the state of the art and DOE program goals.

Specifically, the Panel recommended that DOE/NETL inform the PIs that less important project management administrative items (e.g., budget/cost progress, Gantt charts, and earned value analysis) should be placed at the end of the presentations since this information can be understood from the project information forms. The Panel also recommended that complex slides of equations be eliminated if possible.

The Panel recommended limiting the number of slides used in each 45-minute presentation to between 25 and 35 slides. Each presenter should be advised to spend several minutes on each slide; it was difficult for reviewers to digest the information on each slide when presenters were quickly clicking through highly technical presentations.

Evaluation Process and Criteria

While the Panel noted that their introduction to the review process was quick and effective, some reviewers found the potential subjectivity of the numerical scores and resulting differences in ratings among panel members to be a challenge. The ability to view preliminary project ratings during the Panel discussion session was cited as helpful for identifying and mitigating these discrepancies in criteria interpretation among individual panel members.

The Panel expressed some difficulty scoring the projects objectively using the 5-point rating scale. Panel members recommended potentially redefining the rating system, or suggested that reviewers be given a broader range of scoring options, such as a 6- or 7-point scale with a stronger rating option than “Effective.” They also felt that the scoring process uses a “one size fits all” rating scale when in reality, the nature and expectations of projects from industry, national laboratories, and universities are very different. For example, the Panel felt that it is sometimes difficult for fundamental, university-based research projects to have clear, measurable milestones.

Review Panel

The Panel acknowledged that the diverse areas of the panel members’ expertise offered other members needed insight on various topics during discussion, allowing them to provide more accurate and comprehensive ratings and comments. The Panel enjoyed the learning experience and camaraderie of collaborating with their colleagues in the fuel cells field and thanked ASME and DOE for the opportunity to participate in this Peer Review. The Panel appreciated the professionalism of all parties involved with the Peer Review and valued panel members’ ability to cooperate and remain professional despite occasional differences of opinion. The Panel also suggested altering the seat assignments from day to day, in order to provide a fresh perspective for panel members throughout the week.

APPENDICES

APPENDIX A: ASME PEER REVIEW METHODOLOGY

The American Society of Mechanical Engineers (ASME) has been involved in conducting research since 1909, when it started work on steam boiler safety valves. Since then, the Society has expanded its research activities to a broad range of topics of interest to mechanical engineers. ASME draws on the impressive breadth and depth of technical knowledge among its members and, when necessary, experts from other disciplines for participation in ASME-related research programs. In 1985, ASME created the Center for Research and Technology Development (CRTD) to coordinate ASME's research programs.

As a result of the technical expertise of ASME's membership and its long commitment to supporting research programs, the Society has often been asked to provide independent, unbiased, and timely reviews of technical research by other organizations, including the federal government. After several years of experience in this area, the Society developed a standardized approach to reviewing research projects. This section provides a brief overview of the review procedure established for the DOE/ NETL fiscal year (FY) 2011 Fuel Cells Peer Review.

ASME Knowledge and Community Sector

One of the five sectors responsible for the activities of ASME's 127,000 members worldwide—the Knowledge and Community Sector—is charged with disseminating technical information, providing forums for discussions to advance the mechanical engineering profession, and managing the Society's research activities.

Board on Research and Technology Development

ASME members with suitable industrial, academic, or governmental experience in the assessment of priorities for research and development, as well as in the identification of new or unfulfilled needs, are invited to serve on the Board on Research and Technology Development (BRTD) and to function as liaisons between BRTD and the appropriate ASME sectors, boards, and divisions. The BRTD has organized more than a dozen research committees in specific technical areas.

Center for Research and Technology Development

CRTD has undertaken the mission to plan and manage ASME's collaborative research activities effectively to meet the needs of the mechanical engineering profession, as defined by the ASME members. The CRTD is governed by the BRTD, and day-to-day operations of the CRTD are handled by the director of research and his staff. The director of research serves as staff to the Peer Review Executive Committee, handles all logistical support for the Panel, provides facilitation of the actual review meeting, and prepares all summary documentation.

Fuel Cells Peer Review Executive Committee

For each set of projects reviewed, the BRTD convenes a Peer Review Executive Committee to oversee the review process. The Executive Committee is responsible for guaranteeing that all ASME rules and procedures are followed, reviewing and approving the qualifications of those asked to sit on the Panel, ensuring that there are no conflicts of interest in the review process, and reviewing all documentation coming out of the project review. There must be at least three members of the Peer Review Executive Committee, all of whom must have experience relevant to the program being reviewed. Members of the FY2011 Fuel Cells Peer Review Executive Committee were as follows:

- **Richard T. Laudenat, Chair.** Mr. Laudenat is the immediate past senior vice president of the ASME Knowledge and Communities Sector. He was previously a vice president of the ASME Energy Conversion Group and was a member of the ASME Energy Committee.
- **William Stenzel,** Sargent & Lundy. Mr. Stenzel is a former chair of the ASME Power Division and past member of the ASME Energy Committee.
- **William Worek,** University of Illinois. Dr. Worek is a past vice president of the ASME Energy Resources Group and former chair of the ASME Solar Energy Division. He currently serves on the ASME Mechanical Engineering Department Heads Committee and was recently elected to serve as a member of the ASME Board on Research and Technology Development.

Fuel Cells Peer Review Panel

The Fuel Cells Peer Review Executive Committee accepted résumés for proposed Fuel Cells Peer Review Panel members from CRTD, from a call to ASME members with relevant experience in this area, and from the DOE/NETL program staff. From these sources, the ASME Peer Review Executive Committee selected an eight-member review panel and agreed that they had the experience necessary to review the broad range of projects under this program and did not present any conflicts of interest. Panel members and qualifications are described in Appendix C.

Meeting Preparation and Logistics

Prior to the meeting, the project team for each project being reviewed was asked to submit an 11-page Project Information Form that detailed project goals, purpose, and accomplishments to date. A standard set of specifications for preparing this document was provided by CRTD. These Project Information Forms were collected and provided to the Panel prior to the meeting.

Also in advance of the review meeting, CRTD gave the project teams a standard PowerPoint presentation template and set of instructions for the oral presentations they were to prepare for the Panel. The Panel was also given hard-copy handouts of these PowerPoint slides.

The Project Information Forms and presentations for all projects were provided to the Panel well in advance of the meeting to help them to better prepare for their roles.

Project Presentations, Evaluations, and Discussion

At the Fuel Cells Peer Review Meeting, presenters were held to a specific time limit (ranging from 45 to 120 minutes) to allow sufficient time for all presentations within the five-day meeting period. After each presentation, the project team participated in a 40- to 60-minute question-and-answer session with the Panel.

The Panel then spent 30–40 minutes evaluating the projects based on the presentation material. To start, each reviewer scored the project against a set of predetermined peer review criteria. The following nine criteria were used:

- Scientific and Technical Merit
- Existence of Clear, Measurable Milestones
- Utilization of Government Resources
- Technical Approach
- Rate of Progress
- Potential Technology Risks Considered
- Performance and Economic Factors
- Anticipated Benefits if Successful
- Technology Development Pathways

For each of these review criteria, individual panel members scored each project as one of the following:

- Effective (5)
- Moderately Effective (4)
- Adequate (3)
- Ineffective (2)
- Results Not Demonstrated (1)

To facilitate the evaluation process, Leonardo Technologies, Inc. (LTI) provided the Panel with laptop computers that were preloaded with Peer Review Criteria Forms for each project. The Panel then discussed the project for the purpose of defining project strengths, project weaknesses, recommendations, and action items that the team must address to correct a project deficiency. After discussing and scoring the projects on these criteria, each panel member provided written comments reiterating and expanding on the discussions about each project.

APPENDIX B: MEETING AGENDA

FY11 Fuel Cells Peer Review



Waterfront Place Hotel
Morgantown, WV
February 14-18, 2011

AGENDA

Monday, February 14, 2011 –

- | | |
|--------------------|---|
| 7:00 – 7:30 a.m. | Registration – |
| 7:30 – 8:30 a.m. | Peer Review Panel Kick Off Meeting – Open to NETL and ASME staff only
- Review of ASME Process – Michael Tinkleman/Ross Brindle, ASME
- Role of Panel Chair – James Sorensen, ASME
- Role of NETL – José Figueroa, NETL
- Meeting logistics/completion of forms – Justin Strock/Nicole Ryan, IBM |
| 8:30 – 9:15 a.m. | Overview – Open to NETL and ASME staff only
- Fuel Cells Technology Manager – Shailesh Vora, National Energy Technology Laboratory (NETL) |
| 9:15 – 9:30 a.m. | BREAK – |
| 9:30 – 11:30 a.m. | 01 - Project # NT0003894 – SECA Coal-Based Systems - UTC Power –
<i>Thomas Skiba, UTC Power Corporation</i>
Q&A
Discussion, evaluation, and written comments |
| 11:30 – 12:30 p.m. | |
| 12:30 – 1:10 p.m. | |
| 1:10 – 2:10 p.m. | Lunch (on your own) |
| 2:10 – 2:55 p.m. | 02 - Project # FE0000528 – Techno-Economic Analysis of Scalable Coal-Based Fuel Cells –
<i>Steven S.C. Chuang and Felipe Guzman, University of Akron</i>
Q&A
Discussion, evaluation, and written comments |
| 2:55 – 3:35 p.m. | |
| 3:35 – 4:05 p.m. | |

Monday, February 14, 2011 –

- 4:05 – 4:20 p.m. **BREAK –**
- 4:20 – 5:05 p.m. **03 - Project # DE-FE0004001.410.01.13and29** – Analysis of Integrated Gasification Fuel Cell (IGFC) Plant Configurations –
Kristin Gerdes, National Energy Technology Laboratory (NETL)
Dale Keairns, Booz Allen Hamilton (BAH)
- 5:05 – 5:45 p.m. Q&A
- 5:45 – 6:15 p.m. Discussion, evaluation, and written comments

Tuesday, February 15, 2011 –

- 7:00 – 7:30 a.m. **Registration –**
- 7:30 – 9:30 a.m. **04 - Project # NT41837** – SECA Coal-Based Systems - FuelCell Energy –
Hossein Ghezal-Ayagh, FuelCell Energy, Inc. (FCE)
- 9:30 – 10:30 a.m. Q&A
- 10:30 – 11:10 a.m. Discussion, evaluation, and written comments
- 11:10 – 11:25 a.m. **BREAK –**
- 11:25 – 12:10 p.m. **05 - Project # NT0004113** – Validation of Novel Planar Cell Design for Megawatt-Scale SOFC Power Systems –
Michael J. Day and Scott Swartz, NexTech Materials, Ltd.
- 12:10 – 12:50 p.m. Q&A
- 12:50 – 1:20 p.m. Discussion, evaluation, and written comments
- 1:20 – 2:20 p.m. **Lunch (on your own)**
- 2:20 – 3:05 p.m. **06 - Project # NT0005177** – Viscous Glass/Composite SOFC Sealants –
Scott Mixture, Alfred University
- 3:05 – 3:45 p.m. Q&A
- 3:45 – 4:15 p.m. Discussion, evaluation, and written comments
- 4:15 – 4:30 p.m. **BREAK –**
- 4:30 – 5:15 p.m. **07 - Project # FE0000982** – Improved Flow Field Structures for Direct Methanol Fuel Cells –
Bogdan Gurau, NuVant Systems Inc.
- 5:15 – 5:55 p.m. Q&A
- 5:55 – 6:25 p.m. Discussion, evaluation, and written comments

Wednesday, February 16, 2011 –

- 7:00 – 7:30 a.m. **Registration –**
- 7:30 – 9:30 a.m. **08 - Project # FE0000303** – SECA Coal-Based Systems - Rolls-Royce –
Richard Goettler, Rolls-Royce Fuel Cells Systems Inc. (US)
- 9:30 – 10:30 a.m. Q&A
- 10:30 – 11:10 a.m. Discussion, evaluation, and written comments

Wednesday, February 16, 2011 –

- 11:10 – 11:25 a.m. **BREAK –**
- 11:25 – 12:10 p.m. **09 - Project # FE000773** – Rolls-Royce Solid Oxide Fuel Cell (SOFC) Model Development –
Ben Haberman and Carlos Martinez-Baca, Rolls-Royce Fuel Cells Systems Inc. (US)
- 12:10 – 12:50 p.m. Q&A
- 12:50 – 1:20 p.m. Discussion, evaluation, and written comments
- 1:20 – 2:20 p.m. **Lunch (on your own)**
- 2:20 – 3:05 p.m. **10 - Project # NT0004104** – Solid Oxide Fuel Cell Cathodes: Unraveling the Relationship
Between Structure, Surface Chemistry & Oxygen Reduction –
Srikanth Gopalan, Trustees of Boston University
- 3:05 – 3:45 p.m. Q&A
- 3:45 – 4:15 p.m. Discussion, evaluation, and written comments
- 4:15 – 4:30 p.m. **BREAK –**
- 4:30 – 5:15 p.m. **11 - Project # NT0004105** – Investigation of Cathode Electrocatalytic Activity using Surfaced
Engineered Thin Film Samples and High Temperature Property Measurements –
Paul Salvador, Carnegie Mellon University
- 5:15 – 5:55 p.m. Q&A
- 5:55 – 6:25 p.m. Discussion, evaluation, and written comments

Thursday, February 17, 2011 –

- 7:00 – 7:30 a.m. **Registration –**
- 7:30 – 8:15 a.m. **12 - Project # FWP-40552 (Task 1)** – SECA Core Technology Program: Task 1 - SOFC
Component Development –
Jeffry W. Stevenson, Pacific Northwest National Laboratory (PNNL)
- 8:15 – 8:55 a.m. Q&A
- 8:55 – 9:25 a.m. Discussion, evaluation, and written comments
- 9:25 – 9:40 a.m. **BREAK –**
- 9:40 – 10:25 a.m. **13 - Project # FY10.MSE.1610248.621** – Solid Oxide Fuel Cell Research and Development:
Impact of Minor Species from Coal Syngas on SOFC –
Kirk Gerdes, National Energy Technology Laboratory (NETL)
- 10:25 – 11:05 a.m. Q&A
- 11:05 – 11:35 a.m. Discussion, evaluation, and written comments
- 11:35 – 12:35 p.m. **Lunch (on your own)**
- 12:35 – 1:20 p.m. **14 - Project # NT0006557** – Theory, Investigation and Stability of Cathode Electrocatalytic
Activity –
Meilin Liu, Georgia Tech Research Corporation
- 1:20 – 2:00 p.m. Q&A
- 2:00 – 2:30 p.m. Discussion, evaluation, and written comments

Thursday, February 17, 2011 –

- 2:30 – 2:45 p.m. **BREAK –**
- 2:45 – 3:30 p.m. **15 - Project # FEAA066** – Reliability of Materials and Components for Solid Oxide Fuel Cells –
Edgar Lara-Curzio and Amit Shyam, Oak Ridge National Laboratory (ORNL)
- 3:30 – 4:10 p.m. **Q&A**
- 4:10 – 4:40 p.m. Discussion, evaluation, and written comments

Friday, February 18, 2011 –

- 7:00 – 7:30 a.m. **Registration –**
- 7:30 – 8:15 a.m. **16 - Project # NT0004117** – Chemistry of SOFC Cathode Surfaces: Fundamental Investigation
and Tailoring of Electronic Behavior –
Bilge Yildiz, Massachusetts Institute of Technology
Clemens Heske, University of Nevada, Las Vegas
- 8:15 – 8:55 a.m. **Q&A**
- 8:55 – 9:25 a.m. Discussion, evaluation, and written comments
- 9:25 – 9:40 a.m. **BREAK –**
- 9:40 – 10:25 a.m. **17 - Project # FE0005132** – Small Scale SOFC Demonstration using Bio-based and Fossil Fuels –
Michael Petrik, Technology Management, Inc.
- 10:25 – 11:05 a.m. **Q&A**
- 11:05 – 11:35 a.m. Discussion, evaluation, and written comments
- 11:35 – 11:50 a.m. **BREAK –**
- 11:50 – 1:15 p.m. **Meeting Wrap-up Session**



APPENDIX C: PEER REVIEW PANEL MEMBERS

After reviewing the scientific areas and issues addressed by the 17 projects to be reviewed, the Center for Research and Technology Development (CRTD) staff and the American Society of Mechanical Engineers (ASME) Peer Review Executive Committee identified the following areas of expertise as the required skill sets of the fiscal year (FY) 2011 Fuel Cells Peer Review Panel:

- General/Solid Oxide Fuel Cells (SOFC)
- Special Configurations (IGFC/DMFC/DCFC/RRFCs)
- Cost Analysis
- Integration with Central Power Plants
- Coal Gasification/Synthesis Gas (Syngas)
- Component/Prototype Design; Fabrication; Bench Test
- System Design, Analysis, Testing
- Scale-up; Manufacturing Process
- Anode or Cathode Design or Function
- Cell or Stack Design or Analysis
- Materials; Analysis; Disposition
- Emissions Testing; Carbon Dioxide (CO₂) Capture; Sequestration
- Surface Chemistry; Electrochemistry
- Membranes; Solid Membranes
- Catalysts; Electrocatalytics
- Thin Films; Structures
- High Temperature; High Pressure
- Modeling/Electrochemical
- Modeling/Fluid Flow
- Liquid Methanol; Biofuels
- Contaminants (from Coal)

These required reviewer skill sets were then put into a matrix format and potential panel members were evaluated on whether their expertise matched the required skills. This matrix also ensures that all the necessary skill sets are covered by the Panel. The Panel selection process also helps to guarantee that the Panel represents the distinct perspectives of both academia and industry.

Considering the areas of expertise listed above, the CRTD carefully reviewed the résumés of all those who had served on prior ASME Review Panels for DOE (acknowledging the benefit of their previous experience in this peer review process), a number of new submissions from DOE, and those resulting from a call to ASME members with relevant experience. It was determined that five individuals who had served on prior ASME Peer Review Panels were qualified to serve on the Fuel Cells Peer Review Panel.

Appropriate résumés were then submitted to the Fuel Cells Peer Review Executive Committee for review. The following eight members were selected for the FY2011 Fuel Cells Peer Review (* indicates a prior panel member):

- James C. Sorensen,* Sorensenergy, LLC – *Chair*
- Thomas L. Cable,* Ph.D., NASA Glenn Research Center
- Minking K. Chyu,* Ph.D., University of Pittsburgh
- Wayne Huebner, Ph.D., Missouri University of Science and Technology
- William R. Owens,* Ph.D., *formerly of* Princeton Energy Resources International
- John H. Pavlish, University of North Dakota
- Michael von Spakovsky,* Ph.D., Virginia Polytechnic Institute and State University
- Ronald W. Wolk, Wolk Integrated Technical Services

Panel members reviewed presentation materials prior to the meeting and spent five days at the meeting evaluating projects and providing comments. Panelists received an honorarium for their time as well as reimbursement of travel expenses. A brief summary of their qualifications follows.

FY2011 Fuel Cells Peer Review Panel Members**James C. Sorensen, Panel Chair**

Mr. Sorensen is a consultant with a primary focus on clean coal and supporting technologies, including integrated gasification combined cycle (IGCC), oxyfuel combustion, and coal-to-liquids. Prior to founding Sorensenergy, LLC, he worked for Air Products & Chemicals, including positions as director of New Markets with responsibility for Syngas Conversion Technology Development and Government Systems; and director of Gasification and Energy Conversion. In the latter position, he had commercial responsibility for numerous studies involving air separation unit (ASU)/gas turbine integration for IGCC. Mr. Sorensen was responsible for the sale of the ASU for the Tampa Electric Polk County IGCC facility, which included the first commercial application of the Air Products cycle for nitrogen integration of the ASU with the gas turbine. He was also involved with gas turbine integration associated with Air Products' ion transport membrane oxygen program. Prior responsibilities included project management of Air Products' baseload liquid natural gas projects, commercial management of synthetic natural gas production, and general management of the membrane systems department.

Mr. Sorensen's technical interests include IGCC, oxyfuel combustion, gas-to-liquids, and air separation and hydrogen/syngas technology. His programmatic interests include Electric Power Research Institute CoalFleet, Fossil Energy Research & Development, DOE's Clean Coal Power Initiative, DOE's FutureGen program, and commercial projects. His areas of expertise include project conception and development, consortium development and management, technology and government sales and contracting, research and development program management, technology consulting and training, proposal preparation and review, commercial contract development, and intellectual property.

Mr. Sorensen is the founding chairman of the Gasification Technologies Council and is vice chairman of both the Council on Alternate Fuels and Energy Futures International. Mr. Sorensen holds eight U.S. patents, one of which involves ASU/gas turbine integration for IGCC. He has international experience with customers and partners in Algeria, Chile, China, Germany, Great Britain, Indonesia, Japan, The Netherlands, and elsewhere; and is also well published in the area of clean coal. He received a B.S. in chemical engineering from the California Institute of Technology, an M.S. in chemical engineering from Washington State University, and an M.B.A. from the Harvard Business School.

Thomas L. Cable, Ph.D.

Dr. Cable is a specialist in solid oxide fuel cells (SOFCs) and regenerative fuel cells, with 22 years of laboratory and project management experience. His areas of expertise include anode and cathode compositions and microstructures, solid electrolytes, sulfur-tolerant anodes and sulfur-tolerant catalysts for steam reforming of natural gas and heavy hydrocarbons (JP8 and diesel), and mixed ionic/electronic conducting ceramic membranes for oxygen separation.

Dr. Cable has been employed as the chief scientist in the Solid Oxide Fuel Cells Ceramics Branch of the University of Toledo/NASA Glenn Research Center since 2003. In this position, he serves as the technical lead in the development of new, all-ceramic SOFC designs for aeronautic applications. Prior to this position, Dr. Cable was employed as chief scientist at McDermott Technology Inc. from 1999 to 2003, where he was principal investigator in cell development of the SOFC stack design; responsible for all intellectual property; and co-director of the DOE Solid State Energy Conversion Alliance, a 10-year, \$75 million contract for the development of a 10 kW auxiliary power unit. Dr. Cable was a research scientist at BP Chemicals from 1997 to 1999, a group leader in materials research at Technology Management, Inc. from 1993 to 1997, a project leader and senior project leader at BP America, Inc. from 1987 to 1992, and a senior project engineer at Standard Oil Co. of Ohio from 1984 to 1987.

Dr. Cable holds 28 U.S. patents, including four patents in SOFC designs, three in the direct conversion of hydrocarbon with SOFCs, two in sulfur-tolerant SOFC anodes and catalysts, eleven in single- and dual-phase membranes for conversion of hydrocarbons to synthesis gas, and eight in single- and dual-phase membranes for separation of oxygen. Dr. Cable has presented at approximately 10 conferences, has published eight reports and journal articles, and is a member of the American Ceramic Society (Electronics Division) and the Electrochemical Society.

Dr. Cable received a B.S. in chemistry and chemical engineering and a Ph.D. in chemical and fuels engineering from the University of Utah. His dissertation research investigated the deactivation of catalysts used for the hydrodesulfurization process during coal liquefaction. He also completed a post-doctoral fellowship at Brigham Young University, during which he supervised graduate students in Fischer-Tropsch catalysis for the conversion of carbon monoxide and hydrogen to gasoline under the direction of Professor Calvin Bartholomew.

Minking K. Chyu, Ph.D.

Dr. Chyu is chair of the Department of Mechanical Engineering and Materials Science and the Leighton Orr Endowed Professor of Engineering at the University of Pittsburgh. Dr. Chyu's primary research focus is thermo-fluid issues related to power and propulsion system, material processing, microsystem technology, transport phenomena, energy and power systems, gas turbines, and fuel cells. Major projects he has conducted include convective cooling of gas turbine airfoils, thermal control of rotating machinery, thermal measurement and imaging techniques, and transport phenomena in adaptive flow control and fabrication of microstructures.

Dr. Chyu has received numerous honors and awards, including DOE-NETL Faculty Fellow from 2007 to the present, associate fellow of the American Society of Aeronautics and Astronautics (2005), ASME Engineer of the Year Award (2002), and DOE Advanced-Turbine-System Faculty Fellow (1998–1999). Dr. Chyu is also a fellow of ASME, a member of the Heat Transfer Technical Committee in Gas Turbines (K-14), and an advisory board member of the Center for Advanced Energy and Environment, National Tsing Hua University in Taiwan. Dr. Chyu served as associate editor of the *ASME Journal on Heat Transfer*, served on National Science Foundation Propane Review Panels from 2003 to 2005, and is a member of the Scientific Council for the International Centre for Heat and Mass Transfer. Dr. Chyu has over 70 publications and over 100 symposium and conference papers, has been conference chair or organizer of nearly 30 conferences, served as an invited lecturer on more than 40 occasions, has won over 30 grants, and has graduated 12 Ph.D. and 20 M.S. students.

Dr. Chyu received a B.S. in nuclear engineering at the National Tsing Hua University in Taiwan, an M.S. in applied mechanics at the University of Cincinnati, and a Ph.D. in mechanical engineering from the University of Minnesota.

Wayne Huebner, Ph.D.

Dr. Huebner is a professor and the chair of the Ceramic Engineering Department, and a senior investigator of the Materials Research Center at the Missouri University of Science and Technology (Missouri S&T). Prior to teaching at Missouri S&T, Dr. Huebner was an assistant professor of Ceramic Science and Engineering at the Pennsylvania State University from 1985 to 1991.

Dr. Huebner's research interests include the preparation, characterization, and theoretical understanding of electronic ceramics, in particular ferroelectrics, piezoelectrics, varistors, thermistors, superionic conductors, and solid oxide electrolytes; fuel cells; and oxygen separation membranes.

Dr. Huebner received the American Ceramic Society's 1995 Karl Schwartzwalder Professional Achievement in Ceramic Engineering Award, the Missouri S&T Outstanding Teaching Award (1993–1994), the Dr. Edward F. Tuck Excellence Award (1994–1995), and the McDonnell Douglas Faculty Excellence Award (1993–1994). Dr. Huebner holds a patent for Method of Manufacture of Multiple-Element Piezoelectric Transducer and has published numerous articles in peer-reviewed academic journals.

Dr. Huebner received his B.S and Ph.D. in ceramic engineering from the University of Missouri-Rolla.

William R. Owens, Ph.D.

Dr. Owens is an energy consultant with emphasis on fossil and renewable energy systems. He was formerly vice president of fossil energy projects at Princeton Energy Resources International. He has over 48 years of engineering expertise in energy-related industries, with 27 years as a director, planner, and manager of 13 task order contracts for DOE. He has extensive experience in system engineering principles, cost estimation, project economics, environmental control technologies, project management, and project control of power generation systems, including conventional and emerging technologies. This experience includes fuel cells, turbines, gasifiers, and fluidized bed combustors. Dr. Owens' experience includes systems with bituminous coal, anthracite coal, and subbituminous western coals. He has worked with alternate fuel systems including natural gas, hydrogen, gasifier fuel-gas, oil, and oil-shale systems. Dr. Owens has provided DOE with detailed support in outreach programs, deregulation of the electric utility industry, and international programs.

Dr. Owens was a senior director in a Clean Coal Technology proposal, for which he was responsible for the project coordination, project economics, financial plan including the negotiations with venture capitalists, and commercialization plan. Dr. Owens has provided DOE with detailed support in outreach programs, deregulation of the electric utility industry, and international programs.

Dr. Owens is the author of more than 50 technical publications and reports on the research, engineering, and application of advanced fossil energy power generation systems. He has a B.S. from Pennsylvania State University, an M.S. from Drexel University, and a Ph.D. from the University of Maryland. All of his degrees are in mechanical engineering.

John H. Pavlish

Mr. Pavlish is a senior research advisor, the director of a multiyear, multimillion-dollar Center for Air Toxic Metals Program, and the Manager of the Energy Conversion Systems Group at the Energy and Environmental Research Center. Prior to his current position, he served as unit leader/systems engineer at Black & Veatch Engineers-Architects in Kansas City, Missouri.

Mr. Pavlish's principal areas of interest and expertise include research and consultation on air toxic issues; hazardous air pollutants, with emphasis on mercury; carbon dioxide capture and the coal combustion process; the effects of fuel quality and ash on combustion, gasification, and power plant system performance; generation recovery; steam generator performance and reliability; emission reduction control technologies and flue gas-processing equipment; and economic and feasibility analyses on control technologies and energy conversion systems.

Mr. Pavlish is a registered professional engineer in the state of Kansas, a member of ASME, and a member of the Air & Waste Management Association (AWMA). He serves on numerous professional and technical committees, including the BiNational Strategy Utility Mercury Reduction Committee, Minnesota Pollution Control Agency (MPCA) Research Advisory Committee, MPCA Utilities and Taconite Subcommittee, and B&W Advanced Emissions Control Development Air Toxics Program Advisory Committee.

Mr. Pavlish has authored and coauthored numerous publications including peer-reviewed journal articles. He was the program manager and technical coordinator for the conferences on Air Quality: Mercury, Trace Elements, and Particulate Matter, in 1998 and 2000. Mr. Pavlish has served as a session chair at various conferences, most recently at the AWMA International Specialty Conference on Mercury.

Mr. Pavlish received his B.S. in mechanical engineering from North Dakota State University and has completed over half of the M.S. requirements in mechanical engineering from the University of Kansas. He received an A.A.S. in power and machinery from the University of Minnesota - Crookston.

Michael von Spakovsky, Ph.D.

Dr. von Spakovsky has over 18 years of teaching and research experience in academia and over 17 years of industry experience in mechanical engineering, power utility systems, aerospace engineering, and software engineering. In January of 1997, Dr. von Spakovsky joined the mechanical engineering faculty at Virginia Polytechnic Institute and State University as professor and director of the Energy Management Institute (now the Center for Energy Systems Research). He teaches undergraduate- and graduate-level courses in thermodynamics, kinetic theory, fuel cell systems, and energy system design. Prior to teaching at Virginia Polytechnic Institute and State University, Dr. von Spakovsky worked at the National Aeronautics and Space Administration, and in the power utility industry, first as an engineer and then as a consultant. He was also both an educator and researcher at the Swiss Federal Institute of Technology in Lausanne, Switzerland where he led a research team in the modeling and systems integration of complex energy systems and taught classes in the thermodynamics of indirect and direct energy conversion systems.

Dr. von Spakovsky's research interests include computational methods for modeling and optimizing complex energy systems; methodological approaches for the integrated synthesis, design, operation, control, and diagnosis of such systems (stationary power as well as, for example, high-performance aircraft systems); theoretical and applied thermodynamics with a focus on the unified quantum theory of mechanics and thermodynamics; and fuel cell applications for both transportation and distributed power generation.

Dr. von Spakovsky has been a contributing author of more than 170 publications, including articles in scholarly journals and conference proceedings; and has given talks, seminars, and short courses (e.g., on fuel cells) worldwide. Included among his various professional activities and awards are member of the American Institute of Aeronautics and Astronautics, fellow of ASME, chair of ASME's Advanced Energy Systems Division, elected member of Sigma Xi and Tau Beta Pi, associate editor of the *International Journal of Fuel Cell Science and Technology*, editor-in-chief of the *International Journal of Thermodynamics*, and chairman of the executive committee for the International Center of Applied Thermodynamics. Dr. von Spakovsky holds a B.S. in aerospace engineering from Auburn University and an M.S. and Ph.D. in mechanical engineering from the Georgia Institute of Technology.

Ronald W. Wolk

Mr. Wolk is a principal at Wolk Integrated Technical Services. His previous positions include director of the Advanced Fossil Power Systems Department at the Electric Power Research Institute (EPRI), Program Manager of the Clean Liquid and Solid Fuels Program at EPRI, and Associate Laboratory Director at Hydrocarbon Research, Inc. He has extensive experience in assessing, developing, and commercializing advanced generation and fuel conversion technologies, including fuel cell, gas turbine, distributed power generation, and integrated gasification combined cycle technology systems. His current work includes the evaluation of advanced fuel cell technology and R&D program planning for hydrogen-fueled combustion turbines.

Mr. Wolk serves on the National Research Council (NRC) Committee on R&D Opportunities for Advanced Fossil-Fueled Energy Complexes and continues to work with NRC on issues relating to fuel cells and coal gasification. He has over 200 published articles, papers, patents, and technical presentations. Mr. Wolk holds B.S. and M.S. degrees in chemical engineering from the Polytechnic Institute of Brooklyn (now Polytechnic University).

APPENDIX D: PEER REVIEW CRITERIA FORM

PEER REVIEW CRITERIA FORM

U. S. DEPARTMENT OF ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY
FY11 FUEL CELLS PEER REVIEW

February 14 – 18, 2011

Project Title:	
Performer:	
Presenter:	
Name of Peer Reviewer:	
Date of Review:	

The following pages contain the criteria used to evaluate each project. The criteria have been grouped into three (3) major categories: (1) **Project Overview**; (2) **Technical Discussion**; and (3) **Technology Benefits**. Additionally, each criterion is accompanied by multiple characteristics to further define the topic.

The Reviewer is expected to provide a **rating** and **substantive comments** which support that rating for each criterion. Please note that if a rating of "*Results Not Demonstrated*" is selected, **justifying comments must be included**. To assist with determining the criterion adjectival rating, descriptions of those ratings are provided below.

RATING DEFINITIONS	
Effective	Effective projects set ambitious goals, achieve results, are well-managed and enhance the likelihood of meeting program goals and objectives.
Moderately Effective	In general, a project rated Moderately Effective has set ambitious goals and is well-managed, and is achieving results. Better results could be realized by focusing on key technical issues, more efficient use of resources, and improvements in overall management.
Adequate	Adequate describes a project that needs to set more ambitious goals, achieve better results, improve accountability or strengthen its management practices.
Ineffective	Ineffective projects are unable to achieve results due to a lack of clarity regarding the project's purpose or goals, poor management, or some other significant weakness (e.g., technical problem).
Results Not Demonstrated	Results Not Demonstrated indicates that a project has not been able to develop acceptable performance goals or collect data to determine whether it is performing.

PEER REVIEW RATING CRITERIA

Please evaluate the project against each of the nine (9) criteria listed below. Definitions for these nine (9) criteria are provided on page 4. For each criterion, select the appropriate rating by typing an "X" in the applicable cell. Definitions for the five ratings are provided on page 1.

NOTE: If you rate any criterion as "Results Not Demonstrated," a justification for this rating is required. Please include your justification in the box at the end of this table.

CRITERIA		RATINGS				
(Criteria Definitions, refer to Page 4)		(Rating Definitions, refer to Page 1)				
		Effective	Moderately Effective	Adequate	Ineffective	Results Not Demonstrated*
PROJECT OVERVIEW						
1	Scientific and Technical Merit					
2	Existence of Clear, Measurable Milestones					
3	Utilization of Government Resources					
TECHNICAL DISCUSSION						
4	Technical Approach					
5	Rate of Progress					
6	Potential Technology Risks Considered					
7	Performance and Economic Factors					
TECHNOLOGY BENEFITS						
8	Anticipated Benefits, if Successful					
9	Technology Development Pathways					
*Please explain why the project was rated "Results Not Demonstrated" for a particular criterion.						

COMMENTS

Please provide your comments for each of the areas in the blocks below. Please substantiate your comments (i.e., facts on why you are making the statement). General statements without explanation (e.g., great project) are not sufficient. Please avoid any use of clichés, colloquialisms or slang.

Strengths:
Weaknesses:
Recommendations:
Action Items:
General Comments:

CRITERIA DEFINITIONS**PROJECT OVERVIEW****1: Scientific and Technical Merit**

- The underlying project concept is scientifically sound.
- Substantial progress or even a breakthrough is possible.
- A high degree of innovation is evident.

2: Existence of Clear, Measurable Milestones

- At least two measurable milestones per budget period exist.
- Milestones are quantitative and clearly show progression towards project goals.
- Each milestone has a title, planned completion date and a description of the method/process/measure used to verify completion.

3: Utilization of Government Resources

- Research team is adequate to address project goal and objectives.
- Sound rationale presented for teaming or collaborative efforts.
- Equipment, materials, and facilities are adequate to meet goals.

TECHNICAL DISCUSSION**4: Technical Approach**

- Technical approach is sound and supports stated project goal and objectives.
- A thorough understanding of potential technical challenges and technical barriers is evident.

5: Rate of Progress

- Progress to date against stated project goal, objectives, milestones, and schedule is reasonable.
- Continued progress against possible technical barriers is likely.
- There is a high likelihood project goal, objectives, and expected outcomes and benefits will be achieved.
- The budget is on track to achieve project goal and objectives.

6: Potential Technology Risks Considered

- Potential risks to the environment or public associated with widespread technology deployment have been considered.
- Project risks are identified and effective measures to address and mitigate these risks, including potential technical uncertainties and barriers, are presented.
- Scientific risks are within reasonable limits.

7: Performance and Economic Factors *

- Appropriate technology cost and performance assessments are conducted consistent with the level of technology development.
- Implementation cost estimates, if warranted, are sensible given uncertainties.
- There is a high likelihood of meeting ultimate DOE cost and performance goals.

TECHNOLOGY BENEFITS**8: Anticipated Benefits, if Successful**

- There exist clear statements of potential benefits if research is successful.
- Technologies being developed can benefit other programs.
- Project will make a significant contribution towards meeting near- and long-term program cost and performance goals.

9: Technology Development Pathways *

- Researchers know and can describe a “real world” application and adequately discuss requirements (additional research, potential partners, and resources) for the next level of technology development.
- Market analyses, if appropriate, indicate the technology being developed is likely to be implemented if research is successful.
- Potential barriers to commercialization have been identified and addressed, if appropriate.

* Additional details to be considered for Criterion 7 (Performance and Economic Factors) and 9 (Technology Development Pathways) for specific Technology Development Stages are described on the next page.

**TECHNOLOGY DEVELOPMENT STAGES FOR
ECONOMIC ANALYSIS & TECHNOLOGY DEVELOPMENT PATH**

Research, Development, and Demonstration (RD&D) projects can be categorized based on the level of technology maturity. Listed below are five (5) technology development categories of RD&D projects managed by the National Energy Technology Laboratory. These technology maturation categories are often termed "stages," which provide a basis for establishing a rational and structured approach to decision-making and identifying performance criteria that must be met before proceeding to a subsequent stage of development.

Fundamental Research—Explores and defines technical concepts or fundamental scientific knowledge; laboratory-scale; traditionally but not exclusively the province of academia.

Applied Research—Laboratory- or bench-scale proof of the feasibility of multiple potential applications of a given fundamental scientific discovery.

Prototype Testing—Prototype technology development and testing, either in the laboratory or field; predictive modeling or simulation of performance; evaluation of scalability.

Proof-of-Concept—Pilot-scale development and testing of technology or process; field testing and validation of technology at full-scale, but in a manner that is not designed or intended to represent a long-term commercial installation.

Major Demonstration *—Commercial-scale demonstration of energy and energy-related environmental technologies; generally a first-of-a-kind representation of a long-term commercial installation.

Table 1 describes economic analysis and technology development sub-criteria for each of the five technology development stages. These sub-criteria are examples of the types of information that is typically determined in technology research and development projects.

Please note that the Economic Analysis and Technology Development Path are examples of the types of information that should be provided for the projects being reviewed. Projects are not expected to address all sub-criteria for a given Technology Development Stage, but should address at least one of them.

Table 1. Economic Analysis and Technology Development Sub-Criteria

Technology Development Stage	Economics Analysis Sub-Criteria	Technology Development Path Sub-Criteria
Fundamental Research	<ul style="list-style-type: none"> • Material costs available • Potential cost benefits over conventional systems identified 	<ul style="list-style-type: none"> • Scientific feasibility proven • Application(s) considered • Potential technology developers identified
Applied Research	<ul style="list-style-type: none"> • Component or sub-system costs estimated • First-order cost-benefit analysis available • Material and energy balances calculated 	<ul style="list-style-type: none"> • Conceptual process proposed • Potential applications well defined • Process feasibility established
Prototype Testing	<ul style="list-style-type: none"> • Conceptual process costs developed • Market analysis completed • Risk assessment completed 	<ul style="list-style-type: none"> • Process test data available • Engineering scale-up data developed • Optimum operating conditions identified
Proof-of-Concept	<ul style="list-style-type: none"> • Process contingency costs identified • Full-scale process costs, including O&M calculated • Full-scale installation costs developed 	<ul style="list-style-type: none"> • Major technology components thoroughly tested and evaluated • Technology demonstration plans firmly established • Major component optimization studies performed
Major Demonstration*	<ul style="list-style-type: none"> • Installation costs determined 	<ul style="list-style-type: none"> • Business and commercialization plans developed

* Not relevant to this Peer Review.

APPENDIX E: FUEL CELLS PROJECT SUMMARIES

Presentation ID Number	Project Number	Title
01	FC26-08NT0003894	SECA Coal-Based Systems - UTC Power
02	DE-FE0000528	Techno-Economic Analysis of Scalable Coal-Based Fuel Cells
03	DE-FE0004001.410.01.13and29	Analysis of Integrated Gasification Fuel Cell (IGFC) Plant Configurations
04	FC26-04NT41837	SECA Coal-Based Systems - FuelCell Energy
05	FC26-08NT0004113	Validation of Novel Planar Cell Design for Megawatt-Scale SOFC Power Systems
06	FC26-08NT0005177	Viscous Glass/Composite SOFC Sealants
07	DE-FE0000982	Improved Flow Field Structures for Direct Methanol Fuel Cells
08	DE-FE0000303	SECA Coal-Based Systems - Rolls-Royce
09	DE-FE0000773	Rolls-Royce Solid Oxide Fuel Cell (SOFC) Model Development
10	FC26-08NT0004104	Solid Oxide Fuel Cell Cathodes: Unraveling the Relationship Between Structure, Surface Chemistry & Oxygen Reduction
11	FC26-08NT0004105	Investigation of Cathode Electrocatalytic Activity using Surfaced Engineered Thin Film Samples and High Temperature Property Measurements
12	FWP-40552 (Task 1)	SECA Core Technology Program: Task 1 - SOFC Component Development
13	FY10.MSE.1610248.621	Solid Oxide Fuel Cell Research and Development: Impact of Minor Species from Coal Syngas on SOFC Performance
14	FC26-08NT0006557	Theory, Investigation and Stability of Cathode Electrocatalytic Activity
15	FEAA066	Reliability of Materials and Components for Solid Oxide Fuel Cells
16	FC26-08NT0004117	Chemistry of SOFC Cathode Surfaces: Fundamental Investigation and Tailoring of Electronic Behavior
17	DE-FE0005132	Small Scale SOFC Demonstration using Bio-based and Fossil Fuels

01: FC26-08NT0003894

Project Number	Project Title		
FC26-08NT0003894	SECA Coal-Based Systems - UTC Power		
Contacts	Name	Organization	Email
<i>DOE/NETL Project Mgr.</i>	Briggs White	NETL – Power Systems Division	Briggs.White@netl.doe.gov
<i>Principal Investigator</i>	Tom Skiba	UTC Power Corporation	Tom.Skiba@UTCPower.com
<i>Partners</i>	Delphi Automotive Systems, LLC United Technologies Research Center		
Stage of Development			
<input type="checkbox"/> Fundamental R&D	<input type="checkbox"/> Applied R&D	<input checked="" type="checkbox"/> Prototype Testing	<input type="checkbox"/> Proof of Concept
			<input type="checkbox"/> Demonstration

Technical Background

Solid oxide fuel cell (SOFC) and stack technology has been identified as a candidate for use in highly efficient, economically competitive central generation power plant facilities fueled by coal synthesis gas (syngas). However, existing SOFC stack and system designs are not easily scalable to multi-megawatt levels.

In order to meet the performance, durability, and cost requirements of an integrated gasification fuel cell (IGFC) power plant, the SOFC cell and stack design must be improved. The baseline stack design is the Generation 3 (Gen 3) stack from Delphi, which involves stacks of 30 cells, each cell with an active area of 105 cm². To meet the power generation needs of an IGFC power plant, the active area of each cell must be increased, the number of cells per stack increased, and stack design needs to be made amenable for integration into stack modules. In parallel, material improvements to stack components will help to increase the performance of each cell, resulting in improved power density, and thus, reduced cost per kW.

The Gen 3 stack has demonstrated durability of several thousand hours with low degradation rates, but improvements are needed to meet IGFC lifetime requirements of >40,000 hours. To meet cost requirements, high-volume manufacturing processes and avoidance of exotic materials must be considered in the stack design.

Progress has been made to advance SOFC cell and stack technology to meet the Solid State Energy Conversion Alliance's (SECA) goals for large stationary units. Key achievements in this budget period include the following:

- Scaled up cells from 105 cm² (active area) to 403 cm² without increasing cell thickness for Generation 4 (Gen 4) stacks
- Expanded cell and stack fabrication and testing capability for large footprint Gen 4 stacks
- Fabricated and tested Gen 4 stacks
- Completed design for 25 kW SECA Phase 1 test article
- Demonstrated 5 kW Gen 4 stack module
 - Produced 5,064 W (506 MW per cm²) at 0.81 V per cell
 - Fuel = 48.5% hydrogen (H₂), 3% water (H₂O), rest nitrogen (N₂)

- Developed low-cost, high-volume manufacturing processes (e.g., stamping and laser welding) for Gen 4 stack components
- Fabricated stack modules for end-of-phase testing (25 kW)
- Demonstrated 10,000 hours continuous durability in Generation 3.2 (Gen 3.2) stack
- Demonstrated 200 thermal cycles in Gen 3.2 stack
- Completed an initial downselect of the 250–1,000 kW SOFC power module operating on pre-reformed natural gas based on performance, durability, operability, and cost
- Developed the conceptual design of an atmospheric IGFC system with a solid oxide fuel cell / gas turbine / steam turbine (SOFC/GT/ST) cycle achieving an efficiency of 57% higher heating value (HHV)

CELL DEVELOPMENT

All standard cell production has moved to the larger 403 cm² footprint, while the former smaller cells (105 cm²) are still being fabricated for product and process development purposes. Delphi continues to work closely with commercial suppliers of raw materials, unfired (green) tape, and thick film pastes to ensure a consistent flow of incoming raw material components.

Delphi also continues to research and develop lanthanum strontium cobalt ferrite (LSCF) cathode-based, anode-supported cells to further improve performance. The current focus of high-performance cathode (HPC) development has been to reduce the non-charge transfer part of the cell impedance by developing ways to enhance the ionic conductivity of cathode layers, refine the grain structure, and reduce the cathode tortuosity to achieve an optimized microstructure. Cathode development efforts have also focused on the evaluation of low-cost cathode powders, verification and optimization of new cathode powders with improved performance, and improvement in electrochemical performance with a modified barrier layer. Anode development has focused on modifications for increasing robustness to contaminants, such as sulfur, as well as improving the mechanical strength of the cell.

STACK DEVELOPMENT

Design of a next-generation stack has been completed. This design incorporates larger active area cells to increase power density and reduce stack cost. Key stack features include the following:

- 4x active area increase
- Very low pressure drop (anode and cathode)
- Stamped metallic cassette components including interconnects
- Laser-welded cassette repeating unit configuration
- Low-cost, conventionally processed balance of stack components

Testing continues on Gen 3 and Gen 4 stacks for performance and durability evaluation; multiple Gen 4 stacks have been fabricated and tested. A 25-cell Gen 4 stack produced 5 kW of power at a power density of 506 MW per cm² at 0.81 V per cell with 48.5% H₂, 3% H₂O, and the rest N₂, which is consistent with the performance of a Gen 3.2 stack.

Forty-cell Gen 4 stacks are also being fabricated and tested. A 40-cell Gen 4 stack produced 7,452 W at 0.81 V per cell with 48.5% H₂, 3% H₂O, and the rest N₂. Fuel utilization tests showed a minimal drop in power in going from a low fuel utilization to 80% fuel utilization.

Multiple stacks have been evaluated for durability. A 30-cell Gen 3.2 stack has been tested for steady-state durability for 9,700 hours on 48.5% H₂, 3% H₂O, rest N₂ reformat and a current of 333 mA per cm². The total degradation was found to be 1.12% per 500 hours with most of the degradation in the initial 800 hours. To mitigate this degradation, development is ongoing and a solution is being implemented. While the stack test was terminated due to a facilities shutdown, the overall result is encouraging.

Thirty-cell Gen 3.2 stacks have also been evaluated for thermal cycling with improved seals. The stacks underwent a two-hour heat-up with a performance evaluation conducted after each thermal cycle; minimal degradation was observed after 200 thermal cycles. Development has also focused on improvements in glass/ceramic seals and substrate coatings, which have demonstrated good results for repeating unit to repeating unit sealing in a stack. Coupon-level testing has demonstrated higher shear strength and thermal cycling stability, and multiple stacks tested with the improved repeating unit to repeating unit seals confirmed improved thermal cycling capability with no measurable leakage in the seals. In addition, low-cost coatings and interconnects have been developed and implemented, and coupon-level tests have demonstrated stable and acceptable area specific resistance (ASR), which has been tested for >9,700 hours in Gen 3.2 stack durability tests.

SYSTEM CONCEPTS

A power module consisting of multiple integrated SOFC stacks is the building block for larger power plants. Studies on the power module focused on analyzing the influence of operating parameters and fuel methane content. Turn-down strategies were also developed and process designs were revised with additional actuators as needed to operate at all power levels—from rated to net zero output—while satisfying all operating constraints. After investigating several different design system variants, a design was chosen that offers the best combination of recycle blower inlet temperature, desulfurization performance, and heat exchanger area.

The chosen power module design should be suitable for integration into an IGFC power plant, but as an interim step, a proof of concept (POC) 5 MW system must be developed. Notional studies of several 5 MW, ambient pressure POC systems were completed. A total of four systems were designed, each achieving an efficiency of greater than 58% based on the HHV of coal gas and net alternating current (AC) power greater than 5 MW. All of the systems have a bottoming cycle, but two systems use a conventional steam cycle while two use an Organic Rankine Cycle. The systems are designed to use either an oxy-burner for carbon separation or a conventional exhaust gas burner combining anode and cathode exhaust.

IGFC design activities focused on integrating the developed subsystem models into an integrated simulation model. Three such models were developed for the two atmospheric and the pressurized power block designs. The integrated models were validated against the original component models and yielded the same results. IGFC system design activities also focused on heat integration for the three power systems, which included integrating the syngas expander and optimizing heat integration. The final design achieves an approximately five percentage point gain over the non-heat integrated models. All three systems produce greater than 120 MW net AC power at an efficiency greater than 50% HHV: the IGFC system with steam turbine and air blower achieves approximately 51% HHV efficiency and the gas turbine systems achieve greater than 57% HHV efficiency. A sensitivity analysis was also carried out to demonstrate that all three IGFC designs maintain their key performance requirements over a comfortably wide range of key operating parameters.

SUMMARY

Development continues on cell and stack technology for meeting SECA requirements for coal-gas-based power plants. Gen 4 stacks are being fabricated using high-volume manufacturing processes and tested with encouraging results; durability stacks with improved cell and stack material sets have demonstrated 9,700 hours of steady-state durability; progress is being made in interconnect and seal development; and processes for high-volume manufacturing are being used to fabricate 40-cell Gen 4 stacks. Progress is being made in technology development, design, and manufacturing processes to get these stacks closer to meeting production requirements.

To address the system integration issues of an IGFC power plant, a system study was performed to develop a power module and POC system. This work was used to define and describe the 100+ MW baseline and 5 MW POC system fuel cell power block, the fuel cell module sizing, and the design of the fuel cell stack integration into the fuel cell module. Additional work continues on the selection of non-fuel cell components and subsystems.

Relationship to Program

This project will support important advances within the SOFC systems development and analysis focus of the NETL Fuel Cells Program. Fuel cells are able to produce electricity at high efficiencies and with little to no environmental impact—historically, fuel cells have obtained AC power efficiencies greater than 40%. SOFC fuel cell technology operates at high temperatures, increasing electrical efficiency to greater than 50% and enabling system simplification and fuel flexibility, which makes SOFCs very attractive for operation on coal gas. Heat recovery subsystems can further increase the overall efficiency of the system. Furthermore, compared with a traditional integrated gasification combined cycle (IGCC) power plant, the IGFC uses less water in the balance of plant, and because the fuel and oxidant effluent streams are maintained separately, carbon sequestration technologies may be utilized to minimize the impact of power generation on the environment.

Phase I of this project will support the SECA goals of developing large-scale power plants utilizing SOFC technology by increasing the size of SOFC cells and stacks combined with using material improvements to increase performance to drive down costs; improving stack module design to allow for integration into large stationary power plants; conducting system studies and modeling to provide for a power plant design that meets DOE requirements for cost and efficiency; and testing scaled stacks and stack arrays to provide an understanding of performance and durability expected in IGFC systems. These investigations will provide the basis for work in subsequent phases where the concepts will be built and demonstrated at a larger scale.

Primary Project Goal

The primary project goal is to deliver and test a ≥ 25 kW SOFC stack array incorporating scaled cells and to propose a stack module concept that is amenable to integration in large stationary power plants. The stack array should be tested in accordance with the guidance provided in the DOE-approved test plan and the SECA minimum requirements, and the performance and cost evaluated with respect to the metrics specified therein. The stack module should also be suitable for integration into a 250–1,000 kW fuel cell power module and a 5 MW POC system.

The effort associated with scale-up to larger, multi-megawatt coal-based systems is significant. The Phase I project will have a positive impact toward the program goals by investigating and demonstrating the viability of the technology at a larger scale.

Objectives

The objectives of this Phase I effort include the following:

- Perform cell and stack scale-up, performance enhancement, and cost reduction culminating in the fabrication, delivery, and verification testing of scaled-up SOFC stacks to meet the performance and cost requirements of multi-megawatt fuel cell modules.
- Design an advanced IGFC power plant that will generate electric power from coal while meeting electrical efficiency and cost goals, and utilize the baseline system to complete a system cost analysis.
- Develop a stack module concept for an SOFC stationary system that integrates a large-cell stack design that considers packaging and serviceability to provide a design configuration that is scalable for large SOFC power plants.

02: DE-FE0000528

Project Number	Project Title			
DE-FE0000528	Techno-Economic Analysis of Scalable Coal-Based Fuel Cells			
Contacts	Name	Organization	Email	
<i>DOE/NETL Project Mgr.</i>	Maria Reidpath	NETL – Power Systems Division	Maria.Reidpath@netl.doe.gov	
<i>Principal Investigator</i>	Steven Chuang	The University of Akron	chuang@uakron.edu	
<i>Partners</i>	FirstEnergy Corp.			
Stage of Development				
<input type="checkbox"/> Fundamental R&D	<input checked="" type="checkbox"/> Applied R&D	<input type="checkbox"/> Prototype Testing	<input type="checkbox"/> Proof of Concept	<input type="checkbox"/> Demonstration

Technical Background

The University of Akron Fuel Cell Laboratory pioneered the development of a laboratory-scale coal-based fuel cell, which allows the direct use of high-sulfur-content coal as fuel. The initial research and coal fuel cell technology development, *Coal-based Fuel Cell* by S. S. C. Chuang, demonstrated that it is feasible to electrochemically oxidize carbon to carbon dioxide (CO₂) producing electricity.

Electrochemical oxidation of carbon from coal in a fuel cell (i.e., carbon-based fuel cell) is an attractive one-step concept for electric power generation that could offer high overall energy efficiency; minimization of nitrogen oxide (NO_x) emissions, due to its operating temperature range (700°C–1,000°C); and production of high-purity CO₂ streams for direct CO₂ sequestration. The high energy efficiency (η) of the carbon-based fuel cell can be attributed to the favorable thermodynamics of the reaction of carbon (C) and oxygen (O₂), $C + O_2 \rightarrow CO_2$, which exhibits a positive entropy change ($\Delta S^\circ = 1.6 \text{ J/mol K}$ at 600°C) and allows for efficiencies ($\eta = \Delta GT / \Delta H_{298}$) slightly exceeding 100%. Since the carbon fuel and CO₂ product exist in different phases, the carbon chemical potential (activity) remains constant, which, at least in principle, facilitates achieving complete fuel conversion in a single pass with theoretical voltages remaining constant (i.e., minimal Nernst loss).

The key innovative concept of this coal-based fuel cell technology is that carbon in coal can be converted through an electrochemical oxidation reaction into manageable CO₂, efficiently generating electricity without involving coal gasification, reforming, and water-gas shift reaction. This novel coal-based fuel cell technology is a highly efficient, super clean, multi-use electric generation technology, which promises to provide low-cost electricity by expanding the utilization of U.S. coal supplies and relieving dependence on foreign oil. Scaling up this coal-based fuel cell technology to the MW scale for the nation's electric power supply requires two key elements: (1) developing the manufacturing technology for the components of the coal-based fuel cell, and (2) long-term testing of a kilowatt-scale fuel cell pilot plant. This project is expected to develop a scalable coal-based fuel cell manufacturing process through testing and simulation that will demonstrate the feasibility of building a large-scale coal-based fuel cell power plant. The success of this project will attract industrial investment for the commercialization of this technology for diverse applications, ranging from small-scale batteries to mW-scale power generation units.

Relationship to Program

This project will support important advances within the solid oxide fuel cell (SOFC) systems development and analysis focus of the NETL Fuel Cells Program. Successful development of a coal-based fuel cell stack could offer the following benefits:

- Demonstrate the technical feasibility of converting high-sulfur coal into electricity with high overall energy efficiency, minimization of NO_x emissions due to its operating temperature range (700°C–1,000°C), and production of high-purity CO₂ streams for sequestration.
- Attract industrial investment for the commercialization of this technology for applications ranging from small-scale battery replacement to the mW-scale power generation.
- Decrease the nation's dependence on foreign oil, reduce pollution and CO₂ emissions, and increase power generation efficiency above 50%.

Primary Project Goal

The primary goal of this project is to demonstrate the technical feasibility of building a 250 kW pilot-plant coal-based fuel cell with industry participation. This project will address initial development, scaling, and manufacturing of the core technology.

Objectives

The project has the following objectives:

- *Develop low-cost interconnect and cathode current collector materials* – Interconnect and cathode current collector materials for the coal-based fuel cell must possess high electrical conductivity and long-term durability. Initial tests have shown that ferrite steel coated with a thin silver (Ag) layer could serve as both interconnect and cathode current collectors. These materials are very promising because of the low cost of ferrite. Research efforts will focus on optimizing the amount of Ag to be coated and determining the degradation characteristics of interconnect and cathode current collectors. The performance of interconnect and cathode current collector materials will be characterized by electrochemical impedance spectroscopy (EIS), measuring the voltage-current characteristics of the fuel cells under practical conditions in hydrogen (H₂) and coke. The structure and chemical composition of the interconnect and cathode current collector materials will be characterized by X-ray diffraction (XRD) and X-ray fluorescence (XRF) spectroscopy.
- *Develop a kilowatt-scale fuel cell manufacturing technology* – The project's current fuel cell is manufactured by tape casting and laminated techniques. A co-casting technique will be developed to eliminate the lamination step that involves casting the multilayers: anode layer, interlayer, and electrolyte layer. The manufacturing processes will be scaled up from laboratory scale of 4 in x 4 in to the pilot scale of 3 ft x 10 in. The composition of each layer will be optimized to avoid racking and de-lamination. The process will be streamlined and a computer-controller algorithm and device will be incorporated.
- *Design a coal injection and fly ash withdraw system* – The injection of coal and removal of fly ash from the anode chamber of the fuel cell constitute one of the most challenging tasks in developing the coal-based fuel cell stack. This system will enable the continuous operation of the coal-based fuel cell. Two different prototypes will be built and tested for further modification. The most efficient prototype will be incorporated with a computer-controlled system.
- *Design a kilowatt-scale fuel cell system and simulate its performance* – A kilowatt-scale fuel cell system will be designed and its performance will be simulated. The fuel cells fabricated according to the co-casting technique will be attached to either a zirconia or steel frame for measuring fuel cell performance. The anodes of the fuel cell can attach to the metal frame

with a ceramic seal, a seal with a comparable coefficient of thermal expansion (CTE) as the metal used. Another approach is securing the anode, cathode, and electrolyte with a metal tube, a metal framework, a metal structure, or a metal plate. By varying the makeup of the steel, stable conductivity for continuous operation is possible. The cathode is exposed to the static air and the fuel cell remains constant at 750°C for all testing. The composition of the fuel cell exhaust is analyzed by a mass spectrometer (MS [Pfeiffer Vacuum Omnistar, GSD 301]) and gas chromatograph (GC [SRI 8610C]) equipped with helium ionization (HID). The fuel cell current and voltage are measured simultaneously by a Labview system every 0.25 seconds. The mass/electron (m/e) ratios monitored by MS were 2 (H₂), 15 (methane [CH₄]), 28 (carbon monoxide [CO]), 32 (O₂), 40 (argon [Ar]) and 44 (CO₂). The composition of gases at the exhaust of the fuel cell is characterized by GC and MS during steady-state operation of the fuel cell.

- *Evaluate the durability of the kW fuel cell components* – The long-term durability of the kW fuel cell components for the system will be tested and evaluated by simulating the performance of individual components—fuel cell, interconnects, and seals—for more than 300 hours.
- *Design a 250 kW fuel cell pilot plant* – A 250 kW fuel cell pilot plant will be designed and its performance will be simulated. The design and simulated data will be used for the cost analysis.

03: DE-FE0004001.410.01.13and29

Project Number	Project Title			
DE-FE0004001.410.01.13and29	Analysis of Integrated Gasification Fuel Cell (IGFC) Plant Configurations			
Contacts	Name	Organization	Email	
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<i>Partners</i>	Kristin Gerdes, NETL Office of Program Planning and Analysis (OPPA) Dale Keairns, Booz Allen Hamilton Richard Newby, Booz Allen Hamilton			
Stage of Development				
<input type="checkbox"/> Fundamental R&D	<input checked="" type="checkbox"/> Applied R&D	<input type="checkbox"/> Prototype Testing	<input type="checkbox"/> Proof of Concept	<input type="checkbox"/> Demonstration

Technical Background

A series of system studies that include performance estimates and economic assessments were formulated into a pathway study for coal-based, integrated gasification fuel cell (IGFC) power systems with carbon capture and sequestration (CCS). The results quantify the performance and cost benefits for a series of projected gains made through the development of advanced technologies or improvements in plant operation and maintenance, representing the potential future benefits of IGFC technology development. As such, the results provide DOE with a basis to select the most appropriate development path for IGFC, and to measure and prioritize the contribution of its research and development (R&D) program to future power systems technology.

The IGFC plants in this study apply advanced, planar, solid oxide fuel cell (SOFC) technology and incorporate anode off-gas oxycombustion for nearly complete carbon capture. The SOFC simulations utilize the expected operating conditions and performance capabilities of planar SOFC technology, having split cathode and anode off-gas steams and operating initially at atmospheric pressure. The power plant cost and performance estimates reflect performance projections based on the current state of SOFC development, and project a pathway of SOFC technology development advances. The following fuel cell system advances are incorporated in a cumulative manner:

- Reduced SOFC stack performance degradation
- Reduced stack overpotential
- SOFC cost reduction
- Improved inverter efficiency
- Pressurized SOFC

Advances in IGFC plant operation are also included in the pathway as improved plant availability and capacity factor achieved through advanced component monitoring, improved maintenance practices, and plant operation experience.

Two parallel pathways of IGFC development are characterized, both incorporating CCS, and overall plant performance and cost is estimated along these pathways in a consistent technical and economic manner. The first pathway applies conventional coal gasification technology (ConocoPhillips E-Gas™). This gasification technology produces syngas having limited methane (CH₄) content, roughly 6 mol%. Increased synthesis gas (syngas) CH₄ content is projected to benefit the performance of the IGFC plant. The pathway for the conventional gasifier IGFC follows both SOFC technology advances and an enhancement in the gasifier technology to generate syngas having higher CH₄ content (10% CH₄). The second pathway applies an advanced, catalytic coal gasification technology projected to produce syngas having high CH₄ content of roughly 30 mol%, greatly improving the IGFC performance. This pathway follows similar advances in SOFC technology development as used for the pathway with a conventional gasifier.

The potential benefit of an alternative scenario with conventional gasifier technology has also been evaluated. This case considers the use of natural gas injection into the coal syngas as a means to achieve significantly higher syngas CH₄ content, resulting in additional plant performance improvements.

The design and cost bases for this evaluation have been largely extracted from “Cost and Performance Baseline for Fossil Energy Plants, Volume 1: Bituminous Coal and Natural Gas to Electricity,” published by NETL in 2010, so that these IGFC plant results can be directly compared to the baseline results for other fossil fuel power generation technologies.

Summaries of plant configurations and pathway parameters considered in this study are presented in Exhibit 1 and Exhibit 2. The baseline plant utilizes SOFC operating conditions and performance capabilities based on the current status of subscale testing.

Exhibit 1. Conventional Gasifier IGFC Pathway Description

Case	Pathway Parameter	Gasifier (methane %)	SOFC Pressure & Overpotential	Capacity Factor (%)	Cell Degradation (%/1000 h)	SOFC Stack Cost (\$/kW)	Inverter Eff. (%)
1	Baseline Atm-pressure	CoP (6%)	15.6 psia 140 mV	80	1.5	296	97
1-1	Degradation	CoP (6%)	15.6 psia 140 mV	80	0.2	296	97
1-2	Overpotential	CoP (6%)	15.6 psia 70 mV	80	0.2	296	97
1-3	Capacity Factor	CoP (6%)	15.6 psia 70 mV	85	0.2	296	97
1-4	Gasifier	Enhanced (10%)	15.6 psia 70mV	85	0.2	296	97
1-5	Capacity Factor	Enhanced (10%)	15.6 psia 70 mV	90	0.2	296	97
1-6	SOFC cost reduction)	Enhanced (10%)	15.6 psia 70 mV	90	0.2	268	97
1-7	Inverter Efficiency	Enhanced (10%)	15.6 psia 70 mV	90	0.2	268	98
2	Baseline Pressurized	Enhanced (11%)	285 psia 70 mV	85	0.2	442	98
2-1	Capacity Factor	Enhanced (11%)	285 psia 70 mV	90	0.2	442	98
2-2	SOFC cost reduction)	Enhanced (11%)	285 psia 70 mV	90	0.2	414	98

Exhibit 2. Catalytic Gasifier IGFC Pathway Description

Case	Pathway Parameter	SOFC Pressure & Overpotential	Capacity Factor (%)	Cell Degradation (%/1000 h)	SOFC Stack Cost (\$/kW)	Inverter Eff. (%)
3	Baseline Atm-pressure	15.6 140 mV	80	1.5	296	97
3-1	Degradation	15.6 140 mV	80	0.2	296	97
3-2	Overpotential	15.6 70 mV	80	0.2	296	97
3-3	Capacity Factor	15.6 70 mV	85	0.2	296	97
3-4	Capacity Factor	15.6 70 mV	90	0.2	296	97
3-5	SOFC cost reduction	15.6 70 mV	90	0.2	268	97
3-6	Inverter Efficiency	15.6 70 mV	90	0.2	296	98
4	Baseline Pressurized	285 psia 70 mV	85	0.2	442	98
4-1	Increased Capacity Factor	285 psia 70mV	90	0.2	442	98
4-2	SOFC cost reduction	285 psia 70 mV	90	0.2	414	98

Relationship to Program

This project will support important advances within the SOFC systems development and analysis focus of the NETL Fuel Cells Program. The benefits of the study include the following:

- Quantifies the performance and cost benefits for a series of projected gains made through the development of advanced technologies or improvements in plant operation and maintenance.
- Illustrates the potential future benefits of IGFC technology development.
- Helps to provide DOE with a basis to select the most appropriate development path for IGFC.
- Helps to measure and prioritize the contribution of the IGFC R&D program to future power system technologies.

Primary Project Goal

The overall goal of this project is to quantify the performance and economic benefit from the successful development of advances in IGFC plant configurations.

Objectives

The project has the following objectives:

1. Create a suitable design basis that can realistically step from currently available technologies through each advanced technology or improvement in plant operations and maintenance in a reasonable time frame.
2. Utilize ChemCAD simulations to complete performance estimates for each plant configuration outlined in the design basis document.
3. Complete capital cost estimates and cost of electricity estimates for each case utilizing consistent economic assumptions.
4. Document the results of the pathway analysis in a report that details the effects on plant performance and cost with each advanced technology.

04: FC26-04NT41837

Project Number	Project Title		
FC26-04NT41837	SECA Coal-Based Systems – FuelCell Energy		
Contacts	Name	Organization	Email
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<i>Partners</i>	Versa Power Systems, Inc., WorleyParsons Group, Inc., Pacific Northwest National Laboratory		
Stage of Development			
<input type="checkbox"/> Fundamental R&D	<input type="checkbox"/> Applied R&D	<input checked="" type="checkbox"/> Prototype Testing	<input type="checkbox"/> Proof of Concept
			<input type="checkbox"/> Demonstration

Technical Background

FuelCell Energy, Inc. (FCE) is a leading developer of high-temperature fuel cell systems for stationary power generation. FCE's ultraclean, high-efficiency Direct FuelCell® power plants are generating power at over 50 locations worldwide. The company's power plants have generated over 600 million kWh of power using a variety of fuels, including renewable wastewater gas, food and beverage waste, natural gas, and other hydrocarbon fuels. FCE has partnerships with major power plant developers and power companies around the world. The development of solid oxide fuel cell (SOFC) systems is a natural extension of the company's business development strategies for maintaining its position and competitiveness as an original equipment manufacturer of fuel cells. Along this vein, FCE has elected to pursue the development of planar anode-supported fuel cell technology because of its projected higher performance, long-term endurance, ease of fabrication, and low cost.

FCE has been engaged in a DOE-managed, Solid State Energy Conversion Alliance (SECA) program to develop a 3–10 kW SOFC power plant system since April 2003. In 2006, the FCE team was selected through a competitive process by DOE to participate in a new SECA multi-phase program aimed at the development of very efficient coal-to-electricity power plants. In September 2006, the 3–10 kW cost reduction program was merged with the coal-based multi-phase program for the development of very efficient large-scale (multi-megawatt) SOFC power plants with near-zero emissions.

FCE utilizes cell and stack technology of its partner Versa Power Systems, Inc. (VPS) in the design of leading-edge fuel cell stack modules. VPS has developed high power density, cost-effective, anode-supported planar SOFC technology that forms the basis for the next generation of power plants. This technology is suitable for a gamut of applications that range from small distributed generation to large multi-megawatt-scale coal-based power stations. One of VPS' most significant achievements is its success in scaling up its manufacturing process to cell sizes of 1,000 cm². Performance repeatability of scaled-up cells has been validated with several repeat single cell and stack tests, using the current baseline with 625 cm² components (550 cm² active area). When combined with the existence of infrastructure for fuel cell manufacturing and packaging, FCE's experience in the development of MW-scale fuel cell products and its multitude of internationally located power plants are unique assets to the SECA program. To be cost competitive with other power generating technologies of similar capacity without the need for incentive funding programs, significant SOFC stack and system cost reduction must occur

from the current low-volume development level to high-volume, mass-produced prices. FCE/VPS, working with Pacific Northwest National Laboratory, are currently involved in the cost reduction efforts using a multipronged approach consisting of thermo-mechanical modeling of fuel cell stacks, utilizing less expensive and more durable materials for cell components, exploring simpler routes for manufacturing, and developing the technologies with higher power density.

FCE also collaborates with WorleyParsons Group, Inc., one of the largest multi-national engineering and construction firms in the world. WorleyParsons provides expertise in the design of large-scale stationary power plants, coal gasification islands, integrated gasification combined cycle plants, and carbon capture and sequestration systems. Besides the engineering know-how, WorleyParsons has a vast pool of cost data related to balance-of-plant equipment, electrical and grid connectivity, field work, and process piping and instrumentation—all of which are available to the project.

PROJECT APPROACH

FCE's SECA program is organized in three Phases. Phase I of the program, completed in December 2008, was focused on cell and stack development. This phase included the scale-up of SOFC cell area and stack size (number of cells), as well as performance and endurance improvements. Preliminary engineering design and analysis for multi-megawatt power plant systems were also conducted. The Phase I deliverable included the operation of a >10 kW SOFC stack building block unit that is representative of a MW-class module running on simulated coal synthesis gas (syngas). Test results met all DOE-specified metrics for performance (e.g., nominal power output and efficiency), endurance, reliability, and cost. The DOE-specified metric for the Phase I system factory cost was \$600/kWe or less.

In Phase II of the project, the FCE/VPS development work has been focused on key cell issues related to cost reduction, endurance improvement, and performance enhancement. The main technical approach has included extension of the operating temperature window, reduction of average operating temperature, thermo-mechanical strength improvement, and scaled-up cell and stack fabrication process development. The emphasis was placed on the development of a thin anode substrate with increased thermo-mechanical strength. Material solutions with enhanced electrochemical properties have been evaluated. Laboratory process and equipment retooling have been utilized to support the cell scale-up process development to 33 cm x 33 cm size. Various cell component design considerations, such as anode substrate thickness and porosity, have been evaluated to identify the optimum cell configuration for operation at high power density on coal syngas. Parameters such as performance (power, thermal management, and efficiency), design simplicity, technical risk, manufacturability, and cost have been considered in the design selection process.

Baseline power plant conceptual design has focused on evaluation of process alternatives that would increase power plant efficiency, meet carbon capture requirements, and minimize cost of the power plant's power island. The project team has conducted various process configuration analyses and parametric studies that consider voltage, current density, fuel utilization, stream recycle levels, and process components. The Phase II deliverable included a test demonstration of a SOFC stack module (> 25 kW peak power rating) in a relevant environment representative of MW-class modules of the future. Test results have met the specified metrics for performance (nominal power output and efficiency), endurance, reliability, and cost. This testing included the verification of system peak power performance that was used as the basis for cost. The DOE-specified metric for the Phase II system factory cost is less than \$400/kWe.

With achievements of cost, performance, and endurance targets for Phase II, FCE looks forward to commencing Phase III of the SECA project. FCE will leverage its fuel cell

commercialization experience and VPS' cell and stack manufacturing expertise to design, fabricate, assemble, commission, and test a 250 kW proof-of-concept module power plant during Phase III of the SECA program. The development of this plant will pave the way for future multi-megawatt power plant demonstration and commercialization opportunities. Phase III of the project spans from implementing fuel cell manufacturing production rates beyond 1 MW of stacks per year, to building and testing large-scale stack modules of 60 kW, 120 kW, and, ultimately, 250 kW. Research and development activities will focus on supporting improvements in stack fabrication for increased reliability, better construction materials, scaled-up cell manufacturing processes, and balance-of-plant equipment design.

RESULTS

Early in the Phase II program, a significant milestone was accomplished: FCE achieved continuous operation of two fuel cell stacks, each surpassing SECA's requirement of 5,000 hours of service. Subsequently, a more recent milestone was achieved through operation of a 120-cell stack for greater than 1,500 hours with a degradation of ~1% per 1,000 hours, half as much as targeted by DOE's minimum requirements. Furthermore, the stack verified a peak power operation of 25 kW at a power density of 382 MW/cm², about 25% higher than DOE's target for the SECA Phase II.

The broad project objectives of cost, life, and efficiency were pursued in Phase II through parallel technology development efforts. This approach has yielded a large number of potential cell, stack, and system improvements, which are detailed in the following paragraphs.

Performance Enhancement and Degradation Rate Reduction

The activities focused on developing higher-performance and more stable cells through material modifications and microstructure optimization. Cell performance was further enhanced through anode refinements. The newly developed cells can deliver a power density of 500 mW/cm² at an operating voltage of 0.8 V at 650°C, corresponding to a power density of 0.4 W/cm². This power density is more than double the power density provided by TSC-2 (Phase I baseline) cells at the same operating conditions. Furthermore, significant improvements were achieved in the long-term stability of the new cell technology. The ongoing endurance tests of the improved cathodes and modified anodes in single cells (81 cm² active area) continue to demonstrate very low performance degradation rates. A cell test has accumulated over 12,000 hours with an average performance degradation rate of less than 0.3%/1,000 hours (at 500 mA/cm²) operating at 750°C. To expand the operating temperature window (for stack implementation of the cell technology), the performance degradation rate at temperatures other than 750°C is also being reduced. The cell performance degradation rate has been reduced significantly at a high temperature of 800°C and at a low temperature of 650°C. The cell performance degradation rate at 800°C has been reduced to 0.46%/1,000 hours (at 500 mA/cm²), as demonstrated in a 5,000-hour test.

Thin Cell Development for Cost Reduction

A major advancement in the SOFC technology area was the development of thin anode substrate cells for cost reduction. The anode substrate represents more than 65% of the cell's material cost. By reducing the anode substrate thickness by 40%, the cell material cost can be reduced by more than 25%. Potential challenges in utilizing thin cells in stacks were identified through testing and modeling. Improving intrinsic anode substrate strength is one of the key strategies for implementing thinner cells in a stack. A cell with higher biaxial strength is expected to be stronger and less likely to fracture during fabrication and operation. Anode substrates showing more than 50% improvement in biaxial strength compared to the standard anode substrates were developed. Scaled-up thin cells incorporating reduced anode substrate thickness and 25 cm x 25 cm cell size were produced and tested in a 16-cell stack.

Performance validation in fuel utilization tests (50%–80% utilization range) indicated that the cells were structurally intact.

Cell Scale-up

Fabrication processes for incorporating the new improved cathodes and thin anode substrates were implemented for large 25 cm x 25 cm cell sizes (550 cm² active area) using a third-generation tape casting/screen printing/co-firing process (TSC-3). An overall performance gain of ~8%, with ~2% points derived from anode substrate thickness reduction, has been observed by the large area TSC-3 cells as compared to the standard thickness TSC-2 cells. A 32-cell stack using TSC-3 cell technology has operated nearly for one year with a degradation of less than 1%/1,000 hours. Additionally, the capabilities for production of cells with ~1,000 cm² active area (almost double the size of the baseline cells) were demonstrated by fabrication and testing of cells with dimensions of 33 cm x 33 cm (1,000 cm² active area). A 33 cm x 33 cm cell with the new improved cathode was tested for 1,900 hours with a degradation rate of 1.3%/1,000 hours (at 520 mA/cm²). During initial performance testing, the cell produced a peak power of 880 W (915 mW/cm²) at 1,200 A. The 33 cm x 33 cm cells have also been tested in 10-cell stacks with excellent performance that was equivalent to smaller cell sizes. This achievement shows a path to future scale-up of the SOFC technology.

Cell Manufacturing Process Development

Cell manufacturing process standardization was completed for the initial Phase II stack design. A total of 780 cells, 25 cm x 25 cm in cell size, were produced in eight trials. An excellent material yield of 95% was achieved, which completed a key milestone for the project. Further effort in cell manufacturing process development was focused on 25 cm x 25 cm thin scaled-up cells. Over 1,000 thin cells were fabricated. Further improvement is expected as the advanced thin cell technology is moved from the research and development stage to the pilot manufacturing stage. The completion of final cell manufacturing process development and pilot trials of the thin cells has led to a new baseline cell platform, TSC-3, for the Phase II deliverable stack.

Stack Development

Early in the project, the 10 kW metric tests from Phase I were continued into Phase II with two 64-cell stacks composed of the baseline cells with 550 cm² active area. Both 10 kW stacks successfully met DOE's minimum requirements for 5,000-hour endurance. The stacks exhibited an overall degradation of only 1.7% and 2.6% per 1,000 hours, which was much less than the SECA's interim (2008) target of 4% per 1,000 hours. In an effort to push the boundaries, one of the 10 kW stacks successfully ran for over 9,000 hours. Additionally, a potential for stack cost reduction was demonstrated by fabrication of a 10-cell stack using super-sized 1,000 cm² active area cells. The stack performed very well, even under a high fuel utilization of 80%, achieving an average cell voltage of 800 mV at 388 mA/cm². Concurrently, the baseline stack building block was scaled up from 64 to 92 cell count. Three 92-cell stacks, representing early Phase II stack technology, were built and performance tested to validate the stack design. Performances of all three stacks were quite comparable. The direct current (DC) output of the 92-cell stack block was ~18 kW nominally, reaching a peak power of 19.87 kW and a power density of 0.393 W/cm². Two of the 92-cell stack blocks were later utilized to assemble a stack tower. The stack tower accumulated over 1,000 hours of hot tests, achieving a DC power output of 30.2 kW at 210 A (382 mA/cm²). The tower was tested in a module enclosure environment, with fuel compositions representative of the system (simulated baseline power plant fuel gas). The tower tests verified the building block approach (i.e., using factory stack blocks to assemble large arrays of towers in MW-scale modules).

SOFC Module Development

The SOFC module concept development focused on the design of a >250 kW module. It is based on a stack tower array of eight towers (in vertical orientation), each containing two 96-cell (550 cm² cell active area) stack blocks. The towers are arranged in two groups, with each 4-tower group assembled on a single fixed-end base (quad). Computational fluid dynamics (CFD) modeling was performed throughout the design activities to ensure sound thermal and flow profiles. Finite element analysis (FEA) was also used to safeguard the mechanical robustness of the hardware despite the thermal stresses and long-term material creep.

Module Demonstration Unit (MDU)

The conceptual process design of a ≥250kW SOFC proof-of-concept power plant, verifying the module design operation in an actual environment, was completed. The MDU will serve as a system platform for the proof-of-concept module (PCM) tests required in Phase III of the SECA program. Several system configuration options were developed and system simulations were carried out to guide the 250 kW MDU conceptual design. The configurations considered included anode recycle, cathode recycle, and fuel humidifier options. A configuration was downselected based on the system performance comparison and a preliminary cost analysis. The system offers an electrical efficiency of >61% based on the lower heating value (LHV) of natural gas.

End-of-Phase II Metric Test

A 120-cell stack, using the latest TSC-3 cell technology (550 cm² active area), was built for Phase II metric tests. Over a 22-hour peak power test period, the stack generated 25.2 kW, which corresponded to an average cell voltage of 831 mV at 459 mA/cm² and a power density of 381 mW/cm². The Phase II metric of achieving 25 kW peak power was satisfied. Following the peak power test, normal operating conditions (NOC) were established for the long-term steady-state test. The stack performance at NOC corresponded to an average cell voltage of 835 mV at 367 mA/cm² and a direct current power of 20.2 kW. The 120-cell stack metric test successfully met DOE's requirement of completing 1,500 hours of testing before the end of Phase II. The steady-state average power degradation rate of the stack is 0.9%/1,000 hours, which is well below the Phase II DOE requirement of ≤ 2%/1,000 hours.

Baseline System Conceptual Design and Factory Cost

Advanced Baseline System configuration development and analysis resulted in a highly efficient coal-based power plant. The system employs catalytic gasification and warm gas cleanup to provide syngas fuel for the SOFC. The system also employs oxycombustion of the anode exhaust for carbon dioxide (CO₂) capture using a portion of the oxygen from the air separation unit at the gasification site. A comprehensive system optimization effort, including modification of subsystem operating conditions and updates of equipment performance parameters and specifications, was carried out. The improvements resulted in a system electrical efficiency of 58.7% based on the higher heating value (HHV) of coal, while capturing > 99% of carbon (in the syngas) as CO₂. Water balances were generated to analyze the baseline power plant system water usage. The SOFC system consumes 75% less water compared to pulverized coal combustion plants (using scrubbing technology for carbon capture). A Phase II factory cost analysis for the fuel cell stack and the Baseline SOFC power island was performed. The SOFC stack cost estimate is \$85/kW and the power island (integrated gasification fuel cell [IGFC] plant) factory equipment cost is \$372/kW (\$287 balance-of-plant cost). The cost numbers are based on a peak power output of 671,819 kW net alternating current and assume an annual production level of two 671.8 MW size baseline power plants per year, which requires the production of 43,008 stacks (stack building blocks) per year. The factory cost estimates are less than the SECA goals of \$100/kW and \$400/kW for stack and power island costs, respectively.

Relationship to Program

This project will support important advances within the SOFC systems development and analysis focus of the NETL Fuel Cells Program. The development of SOFC technology will significantly advance the nation's energy security and independence interests, address pollution and greenhouse gases concerns, and help enhance the nation's economic growth. Specific benefits to advancing SOFC technology for large-scale, coal-based power generation include the following:

- Makes use of coal, the largest natural fuel source in the United States, with an estimated 250 years of reserves
- Provides high power plant efficiency with low cost of electricity
- Has lowest pollution emissions (e.g., nitrogen oxides [NO_x] and sulfur oxides [SO_x]) compared to conventional power generation technologies
- Addresses greenhouse gas concerns; enables simple power plant system design for carbon capture leading to sequestration
- Enables power plant fuel tolerance to varying coal gasifier syngas compositions (hydrogen [H₂], methane [CH₄], carbon monoxide [CO], and CO₂)
- Enhances the nation's economic growth with domestic job creation and factory/equipment investment. The technologies developed under this DOE cooperative agreement require substantial manufacturing in the United States, thereby contributing to economic competitiveness

Primary Project Goal

The overarching goal of this project is to develop low-cost, high-performance SOFC technology to support multi-megawatt coal-fueled central power systems. The project has the following supporting objectives:

- Advance SOFC core technology to support program goals.
- Increase fuel cell performance and long-term stability of SOFC systems.
- Resolve barrier issues concerning larger-size SOFCs and demonstrate an SOFC building block for multi-megawatt applications.
- Develop and optimize a design for a large-scale (>100 MWe) baseline IGFC power plant, incorporating an SOFC that will produce electrical power from coal. The system will have the following characteristics:
 - Highly efficient (>50% coal HHV)
 - Environmentally friendly (>90% carbon capture as CO₂ from coal-derived syngas)
 - Cost-effective (<\$400/kWe [2000 U.S. dollar], exclusive of coal gasification and CO₂ separation subsystems)
 - Reduced water consumption (as compared to alternative coal-fueled technologies)
- Design, manufacture, and test a proof-of-concept system derived from the IGFC design.

Objectives

This Phase II project is focused on SOFC technology advancement, cell and stack size scale-up, stack manufacturing capacity development, large-scale SOFC stack module design, and

development of a baseline power plant fueled by syngas from a coal gasifier. The objectives of Phase II address the primary goal of the SECA program of designing a baseline IGFC system that meets cost, performance (efficiency), and carbon capture targets. One of the main project objectives is centered on the core research and development activities related to improvements in SOFC cell components to enhance cell performance, lower performance degradation rate, and decrease cost. The recognized improvements are to be incorporated in fabrication of scaled-up cells and stacks. Additionally, the project objectives include improvements in both materials as well as fuel cell structure leading to a significant reduction of the fuel cell cost. Also, the project objectives include design, fabrication, and testing of SOFC stacks, which will be the building blocks of the larger multi-megawatt fuel cell modules applicable to large coal-based systems. Furthermore, the Phase II project encompasses the development of a >250 kilowatt-class stack module and module demonstration unit design concept suitable for validation (in Phase III of the project) of the SOFC module performance and endurance.

The culmination of the project's research and development objectives is to manifest operation of a fuel cell stack with a peak power of a ≥ 25 kW SOFC that is representative of a MW-class module on simulated coal syngas. The stack shall be tested and evaluated in accordance with the guidance provided in the DOE-approved test plan and the SECA minimum requirements. The cell repeat unit size (in terms of active area) shall be sufficient to form the basis of fuel cell stacks that are technically and economically viable for aggregation into a ≥ 250 kW fuel cell module, which in turn would serve as the building block for a ≥ 100 MWe IGFC system. Test results must meet all DOE-specified metrics for performance (nominal power output and efficiency), endurance, reliability, and cost.

05: FC26-08NT0004 | I 3

Project Number	Project Title		
FC26-08NT0004113	Validation of Novel Planar Cell Design for Megawatt-Scale SOFC Power Systems		
Contacts	Name	Organization	Email
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<i>Partners</i>	The Ohio State University, Department of Mechanical Engineering		
Stage of Development			
<input type="checkbox"/> Fundamental R&D	<input checked="" type="checkbox"/> Applied R&D	<input type="checkbox"/> Prototype Testing	<input type="checkbox"/> Proof of Concept
			<input type="checkbox"/> Demonstration

Technical Background

In mid-2005, NexTech initiated development of solid oxide fuel cell (SOFC) and stack technology based on its novel FlexCell membrane design. The FlexCell is a patent-pending, electrolyte-supported planar SOFC cell design based on a two-layer structure comprising a thin electrolyte membrane layer that is mechanically supported by a “honeycomb” mesh layer of electrolyte material. With the FlexCell, more than 60% of the electrolyte membrane within the active area is thin (<40 microns), and the periphery of the cell is dense. After the bi-layer electrolyte element is sintered, electrode (anode and cathode) layers are separately deposited onto the major faces to define the active cell region. In conjunction with NexTech’s parallel development efforts on SOFC materials, the project team has achieved several demonstrations of the truly unique attributes of SOFCs based on NexTech’s FlexCell platform. These attributes are further detailed in the following paragraphs.

HIGH-EFFICIENCY OPERATION

Gas diffusion is greatly enhanced in the FlexCell, which allows high performance to be achieved at high fuel utilization. Thus, high performance and high efficiency are obtained simultaneously. This combination is difficult to achieve with contemporary anode-supported cells without employing complex anode exhaust recycling schemes.

MATERIALS-INDEPENDENT CELL DESIGN

Since electrode layers in NexTech’s FlexCell are deposited in separate steps, it is straightforward to incorporate new and improved electrode materials, including sulfur-tolerant anodes and chrome-resistant cathodes. NexTech has demonstrated high performance and exceptional long-term stability in a single-cell test with manifolds made of a high-chrome alloy. The cathode material used in this test is based on zinc-doped lanthanum strontium ferrite (LSZF), a material developed in a previous DOE-funded project and subsequently patented by NexTech.

SULFUR TOLERANCE

NexTech has demonstrated anodes that are immune to high levels of sulfur at temperatures of 800°C and above. This capability has enormous implications for the design of SOFCs operating on sulfur-containing fuel gas derived from coal. NexTech recently demonstrated sulfur tolerance of a three-cell stack made with YSZ-based FlexCells. This first-of-its kind demonstration of an SOFC stack operating at high utilization with reformat fuel containing 50 ppm hydrogen sulfide (H₂S) makes NexTech’s FlexCell technology truly enabling for many military fuel cell system applications. NexTech is continuing development of these sulfur-tolerant anodes in an ongoing project funded by the Air Force.

EASE OF SEALING

The dense electrolyte periphery, intrinsic to the FlexCell design, greatly reduces the challenges associated with achieving hermetic seals because both surfaces to be sealed are dense. This density increases the scope of seal materials and design options.

MECHANICAL STRENGTH AND FLEXIBILITY

The FlexCell is made of a high-strength ceramic electrolyte material, which results in a unique combination of flexibility and mechanical strength. This material composition enables development of stacks with high durability and ruggedness.

SCALABILITY

Increasing cell area is extremely pertinent to this proposed project. With the FlexCell, the thin membrane layer is made of the same material as the frame that supports it. Thus, thermal expansion mismatch is eliminated, making it much easier to maintain planarity when cell areas increase. NexTech routinely manufactures FlexCells with a total area of approximately 300 cm² for its 2 kW stack development efforts.

Relationship to Program

This project will support important electrodes advances within the component research and development focus of the NETL Fuel Cells Program. The overall goal of DOE's Solid State Energy Conversion Alliance (SECA) program is to develop SOFC technology for use in central generation power plant facilities that are fueled by synthesis gas (syngas) derived from coal gasification processes. Compared to existing coal-based power plants, SOFC-based power plants offer higher electrical efficiency, lower electrical production cost, and relative ease of carbon dioxide sequestration. NexTech's FlexCell technology offers an alternative SOFC cell design for stacks and meets the demanding requirements of SECA's targeted coal-based SOFC power systems. Specific to coal-based power systems, the primary technical benefits of NexTech's FlexCell technology include scalability to large cell areas, ability to operate at high fuel utilization without performance compromises, tolerance of anodes to sulfur impurities in fuel, and stability of cathodes in the presence of gaseous chromium species that evolve from metallic interconnects.

Primary Project Goal

The overall goals of this project are to validate a new planar cell design, termed the FlexCell, for use in coal-based SOFC power systems and to introduce this technology to SECA's industry teams. In order to be considered for future use in SOFC stacks and systems being developed by SECA's industry teams, the project team needs to prove that the FlexCell has potential to meet SECA's requirements of stable operation on syngas typical of gasified coal after cleanup; scalability to large cell active areas required for MW-scale SOFC systems; and potential for low-cost manufacturing of cells and stacks.

Objectives

The specific technical objectives of Phase I included the following:

- Demonstrate high performance of FlexCells made with low-cost yttrium partially stabilized zirconia (YSZ) as the electrolyte material.
This objective will be met by fabricating YSZ-based FlexCells with active areas of 28 cm² and a total cell area of 100 cm². The project team will perform comprehensive single-cell SOFC tests that target a power density of 300 mW/cm² at 800°C (>0.70 volts and 70% fuel utilization).

- *Demonstrate the potential for achieving stack-manufacturing costs of less than \$100/kW using YSZ-based FlexCells.*
This objective will be met by performing a comprehensive manufacturing and cost analysis and confirming that cell costs will be less than \$50/kW at full-scale production levels (250 MW/year).
- *Demonstrate that FlexCells have sufficient mechanical robustness for SOFC applications.*
This objective will be met by establishing a finite element analysis model of the FlexCell design and using this model to optimize the FlexCell geometry with respect to support geometry, membrane thickness, and inclusion of support ribs within the active cell area. Mechanical robustness of FlexCells will be assessed at Ohio State University.

The objectives of Phase II include the following:

- *Demonstrate scalability of the FlexCell design by fabricating FlexCells having a total area of at least 500 cm² and an active cell area of at least 350 cm².*
This objective will be met by fabricating a minimum of 20 large-area cells and achieving a production yield of greater than 80%.
- *Demonstrate that high performance can be achieved in large-area FlexCells.*
This objective will be met by fabricating YSZ-based FlexCells with active areas of 350 cm² and a total cell area of 500 cm². Comprehensive single-cell SOFC tests will be performed targeting a power density of 300 mW/cm² at 800°C (>0.7 volts and 70% fuel utilization).
- *Demonstrate the potential for achieving stack-manufacturing costs of less than \$100/kW using YSZ-based FlexCells.*
This objective will be met by updating the manufacturing and cost analysis completed for large-area cells in Phase I and confirming that cell costs will be less than \$50/kW at full-scale production levels (250 MW/year).

06: FC26-08NT0005177

Project Number	Project Title			
FC26-08NT0005177	Viscous Glass/Composite SOFC Sealants			
Contacts	Name	Organization	Email	
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<i>Principal Investigator</i>	Scott Misture	Alfred University	misture@alfred.edu	
<i>Partners</i>				
Stage of Development				
<input checked="" type="checkbox"/> Fundamental R&D	<input type="checkbox"/> Applied R&D	<input type="checkbox"/> Prototype Testing	<input type="checkbox"/> Proof of Concept	<input type="checkbox"/> Demonstration

Technical Background

This project centers on developing new viscous oxide glass sealants that will flow at the system operating temperature to reduce mechanical stresses between components while also maintaining the required hermeticity in the solid oxide fuel cell (SOFC) stack. Traditional glass sealants are rigid and thus must have thermal expansion that matches the other cell components, which limits possible glass compositions. The project differs from most previous work on glass sealants because the goal is to create viscous rather than rigid seals, thus moving into new compositional space. The ideal viscous glass sealant will have limited chemical interaction with the SOFC components and will facilitate relief of mechanical stresses over the lifetime of the SOFC.

The use of composite sealants appears possible with both glass systems being pursued by the project team. Gallio-silicate and germano-silicate glasses remain amorphous at interfaces with 8YSZ (yttria-stabilized zirconia) substrates. The dissolution of yttrium (Y) and zirconium (Zr) ions affects nucleation behavior of the studied glasses and inhibits crystallization. A composite sealant of the developed glasses with 8YSZ fiber may result in a totally amorphous glass in contact with the fiber, which may provide benefits beyond the partially crystallized glasses.

To develop these new viscous oxide glass sealants, the project team has set the following milestones:

- Produce Candidate Glasses* (planned completion October 2009)
Initially, 15 types of glasses were melted to study crystallization behavior and sealing temperatures. These glasses crystallized extensively and required sealing temperatures above 850°C. Gallio- and germano-silicate glasses were downselected for further compositional modification. Three additional iterations of glass compositions with lower alkali content or substitutions of boron were studied. These glasses formed seals as low as ≈700°C with high coefficients of thermal expansion (CTE) and glass transition temperatures near 600°C.
- Thermophysical and Reactivity Data* (planned completion February 2010)
Many of the modified germano-silicate glasses remain ≈70% amorphous even after 1,500 hours at 850°C, with thermal cycling to room temperature every 500 hours. Reactions with YSZ and alumina range from undetectable to extensive, depending on the glass composition. For example, one composition exhibits a stable interface with 8YSZ electrolytes after 1,500 hours at 850°C, while another slowly dissolves the electrolyte. Contact with aluminized stainless steels results in interfaces rich in chromium, germanium, and alkaline earths, many of which are stable to 1,500 hours.

- *Thermomechanical and Stability Data* (planned completion October 2010)
Most of the glasses have thermal expansion coefficients that are above 8 parts per million per degree Kelvin (ppm/K), with some above 10 ppm/K. Nearly all glasses formed stable bonds with aluminized stainless steel or YSZ.
- *Long-Term Testing* (planned completion May 2011)
Approximately 40 glasses have been tested in contact with 8YSZ, alumina, or aluminized stainless steel for up to 1,500 hours at 850°C. Microstructure and interfacial analysis via scanning electron microscope and the microprobe allow assessment of the stability of the sealants. Several compositions exhibit interfaces that are stable for up to 1,500 hours.
- *Extend Glass Compositions* (planned completion January 2011)
A fourth iteration of compositional modification of the gallio-silicate glasses resulted in glass transition temperatures near 620°C and seal formation near 750°C, while at the same time limiting the boron and alkali content to below 10 molar percent (mol%). These glasses remain ≈60% amorphous after 500 hours at 850°C, and many remain fully amorphous after 500 hours at 650°C. The glasses react with 8YSZ to form stable interfaces at 850°C in most cases, yet exhibit minimal interaction at 650°C after 500 hours.
- *Documentation/Reporting* (planned completion September 2011)
All quarterly and yearly reports have been submitted to date.

Relationship to Program

This project will support important materials advances within the core technologies component research and development focus of the NETL Fuel Cells Program. Successful viscous sealants developed in the current project will allow vast flexibility and added reliability to the operation of SOFC stacks. The direct benefits include the following:

- Ideal viscous sealants will retain crack healing properties for the lifetime of the SOFC stack, thus eliminating failures from thermal cycling. Many developed compositions retain a high content of glass phase after long heat treatments to sustain this behavior.
- Some compositions appear to be applicable for a wide range of operating temperatures, between 650°C and 850°C. This characteristic would allow SOFC manufacturers the flexibility to use a single sealant composition even for vastly different designs or target operating temperatures.

A significant collateral benefit is the broad applicability of glass sealants in other energy technologies. Certainly applications that include lighting, high-temperature sensors (especially oxygen sensors), and some solar applications require reliable ceramic-to-metal sealants, and the project team envisions the applicability of the new sealants in some of these other technologies.

Primary Project Goal

The overall goal of the project is to develop new viscous glass sealants that have the potential for long-term stability in SOFC stacks. Any candidate material must maintain a partially or fully amorphous state at the operating temperature and exhibit sufficient flow behavior to prevent failure by cracking. Alternatively, a successful candidate sealant will allow any cracks that form during temperature cycling to heal, thus restoring the hermeticity of the seal. Sealant tolerance of both air and fuel streams is a critical parameter, as is sealant stability when in contact with the other SOFC components.

Objectives

The objective of Phase I of the project is to develop new viscous glass sealant materials needed to advance SOFC technologies. Phase I of the project will focus on identification of glass compositions that meet initial property requirements based upon screening measurements. An iterative approach will allow the project team to design improved viscous sealants as the Phase I project progresses.

In Phase II of the program, the project team will perform more detailed characterization with the goal of improving their fundamental understanding of these materials. Concurrent compositional work will then focus on improving the overall long-term performance of the sealants.

07: DE-FE0000982

Project Number	Project Title			
DE-FE0000982	Improved Flow Field Structures for Direct Methanol Fuel Cells			
Contacts	Name	Organization	Email	
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<i>Partners</i>				
Stage of Development				
<input type="checkbox"/> Fundamental R&D	<input checked="" type="checkbox"/> Applied R&D	<input type="checkbox"/> Prototype Testing	<input type="checkbox"/> Proof of Concept	<input type="checkbox"/> Demonstration

Technical Background

The underlying technology of the project is direct methanol fuel cells. Previously, direct methanol fuel cells (DMFC) were operated using dilute methanol solutions, which diminishes the energy density of the systems and renders them non-feasible. The systems that use concentrated methanol require external plant balancing, adding to the system size and therefore decreasing its energy density. The passive DMFC systems are all orientation dependent, which requires them to always operate in a fixed position. This project focuses on active DMFC technology that enables DMFC systems to operate on concentrated methanol and be orientation independent.

Relationship to Program

This project will support important advances within the solid oxide fuel cells (SOFCs) systems development and analysis focus of the NETL Fuel Cells Program. Specifically, this project will contribute the following benefits:

- System operation that is orientation independent
- High gross fuel energy density (GFED)
- Ability to apply to other fuel cell systems operating on the same principles (e.g., direct ethanol fuel cells and direct formic acid fuel cells)
- Cost reduction in the case of operation with alkaline membranes and non-noble catalysts

Primary Project Goal

The primary goal of this project is to demonstrate the operation of a short, research-grade DMFC stack that operates with concentrated methanol and is orientation independent.

Objectives

To achieve this goal, the project has the following objectives:

- Model the rate of permeation of various methanol solutions through the plate and the uniformity of liquid distribution within the plate (task accomplished).
- Develop porous plates at desired porosity and permeability (task accomplished).
- Mill the optimum flowfield that leads to the best distribution and permeation rate of liquid distribution through the plate (task accomplished).

- Integrate the plate in proper DMFC housing (task accomplished).
- Optimize the operating parameters of the DMFC so that maximum GFED (watt-hour/liter of fuel) is obtained (task accomplished and ongoing, with improving results).
- Build a research-grade DMFC stack that takes advantage of the technology (task in progress).

08: DE-FE0000303

Project Number	Project Title			
DE-FE0000303	SECA Coal-Based Systems - Rolls-Royce			
Contacts	Name	Organization	Email	
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<i>Partners</i>	Rolls-Royce Fuel Cell System Ltd (UK) University of Connecticut Case Western Reserve University Pacific Northwest National Laboratory Oak Ridge National Laboratory Matrix Innovations, Inc. VariTech			
Stage of Development				
<input type="checkbox"/> Fundamental R&D	<input checked="" type="checkbox"/> Applied R&D	<input type="checkbox"/> Prototype Testing	<input type="checkbox"/> Proof of Concept	<input type="checkbox"/> Demonstration

Technical Background

The Solid State Energy Conversion Alliance (SECA) program is focused on the development of solid oxide fuel cell (SOFC) technology for use in highly efficient, economically competitive integrated gasification fuel cell (IGFC) central generation power plant facilities fueled by coal synthesis gas (syngas). The development of this technology will significantly advance the nation's energy security and independence interests while simultaneously addressing environmental concerns, including greenhouse gas emissions and water usage. The multi-phase program incorporates the following supporting objectives:

- Reduce SOFC-based electrical power generation system cost to \$700/kWe or less for a >100 MW power plant, exclusive of coal gasification and carbon dioxide (CO₂) separation subsystem costs.
- Achieve an overall power plant efficiency of ≥50%, from coal (higher heating value [HHV]) to alternating current (AC) power (inclusive of coal gasification and carbon separation processes).
- Reduce the release of CO₂ to the environment to ≤ 10% of the carbon in the coal feedstock.
- Increase fuel cell reliability to achieve a design life of >40,000 hours.

HISTORICAL PERSPECTIVE ON ROLLS-ROYCE FUEL CELL SYSTEM SOFC PROGRAM

The Rolls-Royce Fuel Cell System (RRFCS) SOFC technology has been under development since 1985, initially as fundamental and applied research, but since roughly 2002 it has had an emphasis on prototype demonstration with proof-of-concept (POC) demonstrations for key subsystems including the fuel cell generator/power module, turbogenerator, power electronics, and fuel processing. The POC testing included 125 kW systems integrated tests. RRFCS installed a natural-gas-fueled 1 MW distributed energy system package in 2008 at a field demonstration site of American Electric Power, but that test and evaluation program was terminated to await improved generator module SOFC stack technology. Since 2009, RRFCS's internal development program has been focused on overcoming remaining technical challenges and establishing a system-relevant testing program at the 20–30 kW stack block size to validate

the technology prior to resuming the large-scale demonstration testing at the 250 kW–1 MW scale.

DESCRIPTION OF RRFCS SOFC TECHNOLOGY

The RRFCS technology is a pressurized system operating at ~6 bar_a (absolute) pressure and an average stack block temperature of 860°C. The system consists of well-integrated heat balancing through chemical recuperation, achieved by the internal reforming (internal to the pressured volume) and through separate anode and cathode loops with recycle. Pressure supplied by a turbogenerator is the motive force driving anode and cathode recycle by ejectors rather than relying on high-temperature blowers. This hybrid pressurized system produces approximately 95% of its power from the SOFC and 5% from the turbogenerator.

The RRFCS SOFC technology is termed integrated planar SOFC (IP-SOFC) and is based on thin planar cells, which are series-connected on a fuel-carrying porous ceramic support substrate. These active substrates are the elemental building blocks of the fuel cell stack and are grouped together to form a megawatt-scale IP-SOFC system. These cells are applied onto the substrates using well-established thick film screenprinting techniques. Contrary to other SOFC developers who seek ever larger single-cell active areas, RRFCS desires smaller cells to reduce current levels and achieve lower ohmic (I^2R) losses. RRFCS currently prints 60 cells of ~1.3 cm² on each side of the substrate. This represents a difference in design philosophy from a low-voltage, high-current fuel cell to a high-voltage, low-current approach. Substrates having the narrow 60-cell design (adopted pre-SECA) allow the use of lower conductivity and lower cost-basis materials to meet in-plane conductance requirements, which has been important for achieving the DOE cost targets of <\$700/kWe (in 2007 dollars). Further progression in the performance (area-specific resistance [ASR]) of the RRFCS technology has occurred over the past year and the focus of the program is now on validating the long-term durability under the system conditions selected for the RRFCS IP-SOFC power block module of the IGFC plant. The general system design approach being taken for the nearer-term 1 MW distributed energy product would be scaled to the IGFC application with detailed engineering design activities to define generator module sizing for the IGFC application, to be performed in subsequent SECA program phases. The distributed energy market is expected to serve as initial validation of the commercial readiness of SOFC technology prior to serving the IGFC centralized power generation application.

Relationship to Program

This project will support important advances within the SOFC Systems Development and Analysis focus of the NETL Fuel Cells Program. A successful RRFCS SECA Phase 1 project will result in the following benefits:

1. Validation that the epsilon stage RRFCS integrated planar cell technology and stack design achieves the area-specific resistance, fuel utilization, and electrochemical degradation trends to satisfy the system requirements set for nearer-term market entry distributed energy opportunities. The RRFCS 1 MW distributed energy system would be the product construct to gain market acceptance of IP-SOFC technology, and drive the manufacturing scale-up necessary to achieve cost reductions.
2. Demonstration of next generation zeta cell technology having improved performance levels, at lower costs, while meeting or exceeding degradation trends of the epsilon technology. Zeta technology satisfying IGFC system requirements would be further reduced to practice under subsequent SECA program funding.

3. Qualification of a new supplier of substrates, with substrates having optimized permeability characteristics while meeting strength specifications.
4. Qualification of a lower-cost manufacturing approach for ~70% of the dense ceramic fuel manifold components that compose the RRFCS ceramic stack technology.

Primary Project Goal

The primary goal of the RRFCS Phase I SECA project is to deliver a ~15 kW SOFC stack block (at normal system operating design point) incorporating the technology advancements and developments of the Phase I work. The stack will be tested in accordance with the guidance provided in the DOE-approved test plan and the SECA minimum requirements, and the performance and cost evaluated with respect to the key program metrics specified therein:

1. *Stack Performance and Costs*: Based on the peak power obtained for the stack block, achieve a stack cost of ~\$175/kW, which when input into a detailed Factory Cost Model for the power block module of the IGFC plant, achieves a cost of <\$700/kW.
2. *Stack Durability*: Achieve a stack degradation rate of <2%/1,000 hours operating at normal system operating design point for 1,500 hours during the Phase 1 program and extending to 5,000 hours during Phase 2.

The fundamental technology incorporated into the stack deliverable should be suitable for integration into a 250–1,000 kW fuel cell power module and a 5 MW POC system operating on coal syngas. A fully scaled stack, power module, and POC system will be designed, fabricated, and tested in subsequent project phases.

Objectives

The emphasis of the Phase 1 work is the development and qualification of lower-cost cell and stack materials, to include: stack manifold components, primary (cell-to-cell on substrate) and secondary interconnects (substrate-to-substrate), anode and anode current collectors, and cathode and cathode current collectors. Stack design optimization has been performed to achieve uniformity in fuel distribution to allow stacks to be run reliably at the high fuel utilization required to meet IGFC system efficiency targets. Subscale durability testing of key active cell materials and stack component changes are performed to validate the long-term performance of the RRFCS technology prior to commencing the ~15 kW stack block Phase 1 metric test. A summary of the objectives for the work breakdown structure is given below:

1.0 Program Management

- Meet all program reporting requirements.

2.0 Cost Modeling

- Develop detailed activity-based, high-volume Stack Cost Model (~\$175/kW target).
- Develop overall Factory Cost Model for a 100 MW SOFC power module of an IGFC (\$700/kW target).

3.0 Optimized Stack Designs

3.1 Stack Technology

- Establish supply of lower-cost pressed (versus injection-molded) stack fuel manifold components.

- Develop stack component redesign to achieve intra-bundle and bundle-to-bundle fuel distribution uniformity.
- Refine substrate specification to achieve required gaseous diffusivity for low ASR/high fuel utilization and thermal expansion matching to lower-cost active layers and stack manifold components.

3.2 Substrate Durability

- Establish more detailed mechanical property understanding and database of substrate material.
- Examine long-term stability of current sealant glass, evaluate alternate suppliers, and identify glass candidate for higher thermal expansion substrate ranges.

4.0 Cell Development

4.1 Primary Interconnect Development

- Select nearer-term precious metal via-based interconnect design that meets area-specific resistance target and contributes low cell degradation rate.
- Develop ceramic-based interconnect for further stack cost reduction.

4.2 Anode Development

- Identify primary anode degradation mechanisms and mitigation schemes.
- Develop and qualify a lowest-cost nickel cermet anode material set that meets degradation targets.

4.3 Cathode Development

- Investigate impact of moisture conditions on cathode performance and durability.
- Develop and qualify a lower area-specific resistance cathode materials set.

4.4 Secondary Interconnect Development

- Confirm long-term performance of selected secondary interconnect approaches.

5.0 Electrochemical Performance Testing

5.1 Subscale System Relevant Testing

- Perform durability tests of five-cell subscale and bundle (six substrates) at full system design point conditions (temperature, pressure, fuel utilization, current density) to verify durability of selected active cell materials selected for the Phase 1 metric test.

5.2 Stack Test Stand Preparation

- Modify the pressurized stack block test (funded outside of SECA) to supply a simulated coal syngas reformat.
- Perform final commissioning of the stack block test stand.
- Determine chromium species volatility from balance of plant components and mitigation schemes.

5.3 Phase 1 Stack Metric Testing

- Perform 15 kW stack metric test following approved test plan, satisfying the SECA program minimum reporting requirements.

09: DE-FE0000773

Project Number	Project Title		
DE-FE0000773	Rolls-Royce Solid Oxide Fuel Cell (SOFC) Model Development		
Contacts	Name	Organization	Email
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<i>Partners</i>	Dr. Ben Haberman – consultant to Rolls-Royce Fuel Cell Systems, Toronto, ON		
Stage of Development			
<input type="checkbox"/> Fundamental R&D	<input checked="" type="checkbox"/> Applied R&D	<input type="checkbox"/> Prototype Testing	<input type="checkbox"/> Proof of Concept
			<input type="checkbox"/> Demonstration

Technical Background

Rolls-Royce Fuel Cell Systems (RRFCS) requires computational performance evaluation and prediction tools to integrate into all of its solid oxide fuel cell (SOFC) design activities, from single-cell components to system-level analysis. Computational requirements include the following:

- Simulation of coupled processes:
 - Laminar and turbulent fluid flow
 - Mass transport in porous materials
 - Heat transfer by convection, conduction, and radiation
 - Current flow and ionic transport
 - Electrochemical kinetics
 - Chemical reactions
- Detailed geometric modeling using computer-aided design (CAD)-geometry capture of RRFCS integrated planar cell, bundle, strip, and stack block features including peripheral/boundary components
- Steady-state and transient analysis
- Ability to support other modeling efforts at RRFCS, including the following:
 - Finite element analysis (FEA), stress analysis, and CARES-based (Ceramics Analysis and Reliability Evaluation of Structures) methods for prediction of failure probability and reliability, which requires detailed temperature distributions within cell components and temperature evolution over time
 - System-level modeling, which requires detailed performance predictions for performance mapping

Fuel cell model development to date has proceeded using multiple and independent approaches, which have been developed within RRFCS and in conjunction with various universities (e.g., Imperial College, Genoa University, University of Cambridge). Each approach has focused on different computational aspects of the RRFCS fuel cell models and modeling capabilities. These are summarized in the following table.

Development Team	Type	Geometric Approach	Models Included	Platform
RRFCS	Steady-state analytical single-cell and tube model	1D and coarse 2D rectangular mesh	1D models for porous materials, analytical current flow model. Coarse 2D electrochemistry, heat transfer, and temperature for tube.	EXCEL
Genoa	Steady-state tube and bundle model	Coarse 2D rectangular mesh	1D heat and mass balances for gas flows, not coupled to current flow. Analytical 1D porous model. No radiation.	Fortran
Imperial/ Cambridge	Steady-state multi-physics simulation of cell/tube/bundles	3D fine rectangular meshes	Coupled fluid flow, porous flow, electrochemistry, chemical reaction, and heat transfer. No radiation	Fortran
RRFCS	CFD thermal simulation of tubes	3D unstructured fine mesh	Fluid flow modeling and heat released from cells under constant current operation. Radiation included.	FLUENT
Genoa	Steady-state single-cell simulation	2D unstructured fine mesh	Current flow only	COMSOL
RRFCS	Stack block simulation	3D coarse model	1D heat and mass balances for gas flows, not coupled to current flow. Analytical 1D porous models. No radiation.	MATLAB

The parallel development work has progressed in conjunction with validation against experimental data made available by RRFCS to its model development partners.

The individual models outlined in the above table do not meet the proposed project requirements due to either (1) a lack of geometric capability, (2) coupled physical modeling, or (3) both. In addition, sufficient radiation modeling and transient analysis capabilities are only present in commercially available codes. Therefore, further developments need to leverage the performance and flexibility of a commercial multi-physics platform with capabilities to integrate the important features of the latest RRFCS and industry/academic models, and provide a flexible platform for future model upgrades.

In this project, multi-physics code (MPC) platforms will be assessed according to their ability to meet several key criteria required for current and future RRFCS development needs:

- Existing simulation capability: emphasis on turbulent fluid flow and radiation heat transfer
- Geometric flexibility: generation of 3D unstructured meshes and compatibility with CAD software
- Development capability: suitability for inclusion of new features (user-defined code) not common to existing platforms such as electrochemistry and current flow

The chosen commercial MPC shall then be adapted to include the capabilities of existing RRFCS fuel cell models as delineated above (as appropriate) as well as new models. This

development exercise shall take place concurrently with code evaluation by RRFCS to ensure that performance, usability, and reliability are not compromised. The code shall be validated against experimental measurements made by RRFCS on single integrated planar cell segments, complete cells, and bundles throughout the performance of the work.

The project deliverable is a computational design tool that will provide improved accuracy of steady-state behavior predictions and detailed examination of transient behavior. Transient analysis capabilities will directly contribute to the credibility of failure mode and reliability analyses and also ensure safe system operation during start up, shut down and off-design transients. This code shall ultimately be integrated into the RRFCS design process and shall provide a platform for future model enhancement with state-of-the-art research.

Relationship to Program

This project will support important advances within the SOFC Systems Development and Analysis area of the NETL Fuel Cells Program. The project provides the following benefits:

- Consolidates RRFCS SOFC multi-physics analysis capabilities under a single commercial code
- Provides a user friendly graphical user interface from which engineers can perform design analyses without requiring the code developer's skills
- Analysis capability/details that will help optimize current and future fuel cell design
- Cost savings due to fewer tests and test rigs to acquire data needed for fuel cell development

Primary Project Goal

The primary goal of the project is to consolidate existing RRFCS SOFC modeling knowledge and enhance it, where needed, to provide a state-of-the-art computer code suitable to support the detailed performance modeling required to progress current and future SOFC product design needs.

Objectives

The program is developed around the following five major objectives.

OBJECTIVE 1: REVIEW EXISTING RRFCS MODELS AND STATE-OF-THE-ART SOFC RESEARCH

The RRFCS MPC development shall be initiated with a review of the existing modeling capabilities and research as well as feedback from internal RRFCS stakeholders. One requirement shall be suitability to accommodate anticipated future modeling needs, identified by discussing current research activities with academic partners and reviewing status of research being conducted elsewhere.

Objective Status: COMPLETE

Dr. Haberman led the review of current SOFC research and publications applicable to the program's modeling goals, and continues to follow modeling tasks in the literature. Initial review of the leading commercial MPCs was completed. This review and consultation exercise (Milestone 1) was successfully completed on schedule in 2009.

The MPC will be used in a wide variety of applications including simulating fuel cell behavior, analyzing fluid flow in peripheral components, and providing temperature distributions to reliability and lifetime prediction models. Typical fuel cell applications will range from simulating the behavior of a single cell to predicting the performance of a complete fuel cell bundle.

In order to make accurate fuel cell performance predictions, the MPC is required to model a wide range of physical phenomena that occur in SOFCs, including the following:

- *Fluid Flow (FF)*, which can be laminar or turbulent and steady state or transient, and describes the transport of fuel through manifolds and along internal tube channels and the flow of air over the outside of the tubes.
- *Porous Flows (PF)*, which describes the transport of gases through porous components such as the tube and the fuel cell electrodes.
- *Heat Transfer (HT)* by convection, conduction, and radiation, which determines the temperature distribution throughout the model.
- *Chemical reactions (CH)*, which are catalyzed by the fuel cell components and make significant contributions to fuel cell behavior.
- *Electrochemistry (EL)*, which governs the behavior of the charge transfer reactions occurring at the interfaces between the cell electrodes and the electrolyte.
- *Current Flow (CF)*, including the flow of electronic current through the fuel cell electrodes and the electrical connections between tubes, in addition to the ionic current flow in the electrolytes.
- *Degradation (DG)*, which reduces cell performance over time via physical and chemical processes.

In addition to the variety of physical models described above, accurate predictions also require powerful meshing tools that can interpret all the relevant model geometric features from CAD drawings and understand component interconnections. Geometric modeling is particularly challenging because of the large number of model components and their wide range of length scales (cell component thickness of ~10 μm ; bundle fuel flow path length of ~1 m).

Further to the physical and geometric modeling requirements outlined above, the MPC is also required to provide a degree of modeling flexibility to allow application-dependent model customization. For example, a one-dimensional isothermal model is sufficient for single-cell calculations, whereas three-dimensional thermal models are a necessity for making accurate bundle simulations. This requirement will be achieved by implementing interchangeable high- and low-fidelity versions of each physical model in the MPC, as shown in the following table.

High- and Low-Fidelity Models			
Physical Model		Interchangeable Fidelity Level	
		Low (1)	High (2)
Fluid Flow	FF	1D plug flows (steady-state, laminar)	CFD calculations
Porous Flow	PF	Darcy model	CPIM model
Heat Transfer	HT	Isothermal	Convection, conduction, and radiation
Chemistry	CH	Global one-step reactions	Multi-step reactions
Electrochemistry	EL	Uniform current density	Integrated with current flow simulation
Current Flow	CF	Analytical Ohmic loss model.	3D numerical model
Degradation	DG	Empirical models	Kinetic models

The details of the high- and low-fidelity models summarized above were assembled from an extensive review of published and in-house research. The table below summarizes the most suitable model combinations for the range of MPC fuel cell simulation applications.

Application-Dependent Model Selections (2 = high fidelity, 1 = low fidelity)						
Physical Model		Application				
		1D Single Cell	2D Single/Penta Cell	3D Penta Cell	3D Tube	3D Bundle
Fluid Flow	FF	2	2	2	2	1,2
Porous Flow	PF	2	2	2	2	1
Heat Transfer	HT	1	1	1	2	2
Chemistry	CH	1,2	1,2	1,2	1,2	1
Electro-chemistry	EL	1	2	2	2	1
Current Flow	CF	-	2	2	2	1
Degradation	DG	-	1,2	1,2	1	1

In addition to providing a detailed simulation capability for RRFCS, the MPC is also required to support other projects within the company. These interactions include the following:

- Supporting lifetime and reliability predictions, which will require detailed temperature distributions from tube and bundle simulations
- Providing accurate validated models of fuel cell processes, such as electrochemistry, in a format that is suitable for use by large-scale, less detailed models

OBJECTIVE 2: EVALUATE CANDIDATE MPCS

The evaluation process shall involve assessments of the capability and potential of each candidate MPC to meet the current and future requirements for RRFCS fuel cell applications:

- Discussions with candidate commercial code suppliers shall be conducted regarding the applicability of mesh generation and simulation capabilities to the RRFCS integrated planar cell and bundle geometry, with particular focus on radiation and transient modeling. Assessment criteria will include the following:
 - Accuracy
 - Convergence time
 - Computer requirements and multi-platform compatibility
 - Ease of use (pre- and post-processing)
- The ability of each code to incorporate new models/user-defined subroutines (e.g., advanced porous flow model)
- The compatibility of each code with current CAD and FEA software

RRFCS shall consult with the Pacific Northwest National Laboratory Solid State Energy Conversion Alliance (SECA) modeling team to understand the basis for their SOFC MPC selection and subsequent development.

Objective Status: COMPLETE

Three candidate codes were chosen for evaluation as potential MPCs: FLUENT (by ANSYS), STAR-CCM+ (by CD-adapco), and Marc (by MSC Software). A set of code evaluation criteria was created based on the MPC requirements and a series of tests was developed to measure the performance of each code against these criteria. These test questions were passed to each code vendor and two of the three vendors (ANSYS and CD-adapco) replied. The evaluation exercise was completed as scheduled at the end of November 2009.

OBJECTIVE 3: DOWNSELECT MPC

An RRFCS downselect panel shall discuss the findings of the evaluation process and select the MPC to take forward.

Objective Status: COMPLETE

The vendor test results and evaluation scores that were obtained during the evaluation exercise were reviewed within RRFCS during December 2009. The test scores indicated that STAR-CCM+ (by CD-adapco) was the preferred MPC for the RRFCS application. The overall findings of the evaluation and downselect exercises were presented to DOE and approved before the end of 2009, which lead to completion of Milestone 2 on January 1, 2010.

OBJECTIVE 4: ENHANCE MPC FOR THE RRFCS FUEL CELL INCLUDING MODEL IMPLEMENTATIONS AND RUN-TIME EFFICIENCY

A suitable methodology shall be developed to incorporate existing and new models into the chosen MPC. Models/capabilities/features shall then be implemented in stages. During each stage, the code will be retested against previous benchmarks to ensure code operation and performance have not been compromised.

Objective Status: Progressing on schedule and according to plan

Version 1 code release was completed on schedule. Version 2 code release is currently in progress with a year-end 2010 release expected. Version 3 is planned for 2011. The following discussion summarizes the overall plan for code version release and progress against that plan.

A code enhancement methodology was developed prior to the commencement of code release development to provide an effective and efficient means of implementing new models into STAR-CCM+. The principal features of this methodology are as follows:

- *Field Functions*, which provide a means to input user-defined calculations into STAR-CCM+ and are used for all MPC code enhancements such as setting material properties, boundary conditions, and source terms for conservation equations
- *Java Macro API*, which gives the user full access to the STAR-CCM+ source code and enables macros to be written to perform any task. Macros are used to automate all tasks performed within STAR-CCM+, including setting up existing model features, installing code enhancements, running simulations, post-processing, and providing feedback and error messaging to the user
- *Simulation spreadsheet*, which is used to store all user input required for initializing and running STAR-CCM+ models

Code Release 1

The primary focus of Code Release 1 is to establish basic fuel cell calculations and validate these on single-cell model geometry. The following code developments were delivered with Code Release 1:

- *FF2*: High-fidelity fluid flow modeling using the built-in CFD capabilities of STAR-CCM+
- *PF2 and PF1*: High- and low-fidelity porous flow models and validated empirical porous material data
- *HT1*: Low-fidelity thermal model, which enforces isothermal operation
- *CH2 and CH1*: High- and low-fidelity chemistry models and validated empirical kinetic data to describe fuel cell chemical reactions
- *EL1*: A generalized electrochemistry model that can work with CH1 or CH2 chemistry models using a prescribed uniform current density and validated empirical kinetic data to describe fuel cell electrochemical reactions

Code Release 1 also delivered a one-dimensional, single-cell model that was validated using the above models (PF2, HT1, CH1+2, EL1) against experimental single-cell performance measurements.

Code Release 2

The primary focus of Code Release 2 is to integrate current flow into the MPC and extend the validated models to two- and three-dimensional models up to the bundle scale. The following code developments are intended for delivery with Code Release 2:

- *HT2*: High-fidelity heat transfer calculations including convection, conduction, and radiation

- *CF2 and CF1*: High-fidelity numerical current flow model, a low-fidelity analytical current flow model, and a validated set of empirical cell component conductivity data
- *EL2*: High-fidelity electrochemistry model integrated with the CF2 current flow model

Code Release 2 is also scheduled to deliver the following validated models:

- Two-dimensional single- and penta-cell models utilizing FF2, PF2, HT1, CH1/2, EL2, and CF2 models.
- Three-dimensional penta-cell model utilizing FF2, PF2, HT1, CH1/2, EL2, CF2 models.
- Three-dimensional tube model utilizing FF2, PF2, HT1, CH1/2, EL1, CF1 models.

OBJECTIVE 5: VERIFY AND VALIDATE MPC ENHANCEMENTS

MPC validation shall be performed against existing RRFCS integrated planar cell segments, complete cells, and bundle experimental data sets. This work shall establish required empirical constants and the accuracy of the models. Following the success of this initial validation phase, validation will continue as new data is made available from ongoing tests.

Objective Status: Progressing on schedule and according to plan

The project plan includes a model verification and validation work program that runs in parallel to the code enhancement program outlined above. The activities that support Code Release 1 were completed on schedule at the end of May 2010 (Milestone 3) and the tasks undertaken in support of Code Release 2 are due for completion on schedule at the end of November 2010 (Milestone 4). Work tasks have also been planned in support of Code Releases 3 and 4.

10: FC26-08NT0004104

Project Number	Project Title			
FC26-08NT0004104	Solid Oxide Fuel Cell Cathodes: Unraveling the Relationship Between Structure, Surface Chemistry & Oxygen Reduction			
Contacts	Name	Organization	Email	
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<i>Partners</i>				
Stage of Development				
<input checked="" type="checkbox"/> Fundamental R&D	<input type="checkbox"/> Applied R&D	<input type="checkbox"/> Prototype Testing	<input type="checkbox"/> Proof of Concept	<input type="checkbox"/> Demonstration

Technical Background

Many of the specific details of the oxygen reduction reaction in a solid oxide fuel cell (SOFC) remain poorly understood. Surface chemistry directly influences the nature of oxygen reduction reaction pathways on the SOFC cathodes and the rates at which the individual processes proceed. From semi-empirical correlations between the chemistry and structure of oxide surfaces and their electrocatalytic performance, the true cause-and-effect relationships in the oxygen reduction processes at the cathode could be elucidated. This would provide valuable guidance in improving cathode performance.

This project aims to acquire such surface-specific chemical and structural data on heteroepitaxial thin films of $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_3$ (lanthanum strontium manganite [LSM]) and $\text{La}_{0.6}\text{Sr}_{0.4}\text{Co}_{0.2}\text{Fe}_{0.8}\text{O}_3$ (lanthanum strontium cobalt ferrite [LSCF]) cathodes on single-crystals of yttria-stabilized zirconia (YSZ) and YSZ coated with a barrier layer of rare-earth-doped ceria (e.g., yttrium oxide [Y_2O_3]-doped cerium oxide [CeO_2] or yttrium-doped ceria [YDC]) electrolytes. This will be accomplished using a combination of analytical spectroscopic techniques and transmission electron microscopy (TEM). The overall objective is to correlate the structural and surface chemical information with the oxygen reduction reactions.

In the first part of the project, the project team has decided to focus on LaAlO_3 (lanthanum aluminate [LAO]) substrates due to their wide availability and ease of deposition of epitaxial LSM thin films. The initial surface structure and surface chemistry measurements, and the in-situ electrochemical characterization experiments, will be performed on LSM thin films deposited on LAO. Later in the program, the project team plans to employ single-crystal substrates of YSZ and also incorporate other cathode materials in the LSCF family.

Relationship to Program

This project will support important advances within the Electrode Component Research and Development focus of the Core Technologies area of the NETL Fuel Cells Program. The following are benefits to the Solid State Energy Conversion Alliance (SECA) program arising from this project:

- Advanced understanding of cathode oxygen reduction process
- Advanced understanding of the key role played by the oxidation state of the transition metal cation

- Advanced understanding of changes occurring at the cathode surface during oxygen reduction and its relationship with the oxygen reduction kinetics at the cathode
- When all information is collated, a path toward designing high-performance cathode materials, which will lead to the achievement of the SECA cost targets

Primary Project Goal

The primary goal of this project is to understand the role of structure, surface chemistry, and electrocatalysis on the oxygen charge transfer and transport processes involved in the oxygen reduction reaction. Structure is defined as the crystalline and the electronic structures of the surface, interface, and the bulk. In particular, the structures of the cathode and cathode-electrolyte as well as the gas-cathode-electrolyte (triple-phase boundary [TPB]) interfaces are of particular interest. The role of the structural features of the TPBs, gas-exposed cathodic surface area, and cathode-electrolyte contact area on the oxygen charge transfer and transport processes will be investigated.

Objectives

Project objectives include the following:

- Determine if cathode surfaces and cathode/electrolyte interfaces reconstruct during pO_2 (partial pressure of oxygen) and temperature changes.
- Total reflection X-ray fluorescence (TRXF) data indicate that some surface segregation of strontium (Sr) occurs on the LSM surfaces when annealed under SOFC cathodic conditions, which is irreversible.
- Correlate surface/interface reconstructions to oxygen transport and exchange kinetics measured through electrochemical measurements.
- Electronic structure measurements show that the manganese (Mn) oxidation state can be tracked through soft X-ray spectroscopies.
- Determine if structural changes are sensitive to the direct current (DC) electric field (or DC polarization) and whether such changes are reversible.
- It has been determined that the Mn oxidation state changes with the applied DC polarization. This has been confirmed through X-ray emission spectroscopy (XES) and X-ray absorption spectroscopy (XAS).
- Determine the role of electronic structure on the electrocatalysis of oxygen reduction.
- The project team has been able to correlate the oxidation state of the Mn in LSM with the change in cathode polarization and, therefore, with the oxygen reduction catalysis. There is clear evidence of Mn going into an oxidation state of 4+ with time at constant DC polarization.

II: FC26-08NT0004105

Project Number	Project Title			
FC26-08NT0004105	Investigation of Cathode Electrocatalytic Activity using Surfaced Engineered Thin Film Samples and High Temperature Property Measurements			
Contacts	Name	Organization	Email	
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Stage of Development				
<input checked="" type="checkbox"/> Fundamental R&D	<input type="checkbox"/> Applied R&D	<input type="checkbox"/> Prototype Testing	<input type="checkbox"/> Proof of Concept	<input type="checkbox"/> Demonstration

Technical Background

Recent advances in both scientific investigations and industrial developments have helped DOE's Solid State Energy Conversion Alliance (SECA) meet its Phase I goals in industrial systems. Still, considerable more work is required to meet the overall goal of producing electricity at efficiencies of 45%–50%, for \$400/kW, in systems operating for >25,000 hours with degradation rates in system performance of no more than 0.2%/kWh. One approach to meet these goals is to reduce the losses in solid oxide fuel cells (SOFCs), which would increase their efficiency as long as cost and lifetime are not sacrificed. Reductions in losses (or overpotentials) are likely to be most beneficial if realized in the cathode, since cathode losses typically represent about half of the total electrochemical loss in the cell (which may be around 150 mV at a typical cell voltage of 0.7 V). A considerable amount of effort has been expended in correlating processing/microstructural features to cathode performance (such as porosity, interconnectivity, phases, and phase amounts), and typical microstructures are well engineered to maximize their overall performance. Yet there is relatively little information that correlates the fundamental surface chemistry and structure of oxide surfaces with electrochemical performance. Owing to the complexity of the actual microstructure of cathodes, model systems must be found in which specific microstructural features can be well controlled and tested for their influence on surface properties. In this work, the project team: generates well-defined epitaxial, textured, and polycrystalline films having controlled surface chemistries; and generates experimental data on surface properties that indicate how the electrocatalytic activity of SOFC cathodes can be optimized to yield improved cathodes. The aim is to provide support to industrial teams by describing the basic parameters that can be exploited for performance improvement.

Traditional surface science experiments rely heavily on the use of high-vacuum conditions as well as electron and ion probes that are well suited to such environments. Such techniques have been used to understand the surfaces of complex oxides, but their relevance to operational conditions of fuel cells and to optimizing the electrocatalytic activity in cathodes remains an open question. It is well known that surface activity and materials compositions are strongly dependent on temperature and pressure in SOFC materials, and there is a growing body of evidence that the surface composition is a function of operational conditions. The use of single-crystal surfaces has shown that orientation plays a major role in catalytic activity (at low temperatures). Characterizing the surface structure/composition is challenging because electron and ion probes are not useful in the high pressures appropriate for in-situ testing of SOFC

cathodes; this requires the use of synchrotron X-ray sources and appropriately modified beam-lines. What is unclear is precisely which surface features/properties can be correlated directly to performance. The project team will contribute to this understanding by making such samples and generating in-situ data of surface properties, ultimately aiming to isolate the important parameters that can be used to optimize SOFC cathode performance.

A comprehensive surface science study that isolates a correlation between controllable materials parameters and electrocatalytic activity of single-crystal cathode surfaces would include in-situ characterization of many features. These include: the surface structure/composition, a range of properties that probe the surface activity, the surface electronic states/structure, surface interactions with gas-phase/adsorbed chemical species, and a theory/computational component to isolate at least a phenomenological description of the basic physics that allow for predictions to be made for improvements. Prior work reported in disparate areas of the archival literature has demonstrated that such a comprehensive program could be successful, although it requires a considerable range of talents, equipment, and financial commitment. Many of the techniques used to measure surface and electronic properties are easily adapted to be carried out on thin films in operational conditions.

Relationship to Program

This project will support important advances within the Electrode Component Research and Development focus of the Core Technologies area of the NETL Fuel Cells Program. The expected results include: generation of surface-engineered SOFC cathode films, an understanding of surface chemistry and stability, a complete understanding of the electrocatalytic activity of surfaces, and a library of data to be shared with collaborators on DOE-SECA teams.

These investigations will provide experimental input for semi-empirical or theoretical correlations to be made between the chemistry and structure of oxide surfaces and their electrocatalytic performance. The benefits to DOE are that the outcomes of this work, which include surface-engineered samples of SOFC cathodes and their physical characterization, will provide valuable guidance to SOFC developers and SECA Industry Teams wishing to enhance cathode performance. Moreover, the project team will alter the surface chemistry and again determine the surface properties and outer layer stability, similar to infiltration methods being proposed for catalytic improvement in either cathodes or anodes. This data will also be provided to other SECA teams aimed at modeling or generating theoretical models that capture the phenomenological physics of oxygen reduction in SOFC cathodes. The project team's results already indicate that a significant improvement can be made above 800°C through strain engineering and that a significant improvement can be made below 800°C using extended defects.

Primary Project Goal

This primary goal of this project, which is a self-contained study inside of a broader effort, is to generate experimental correlations to make the link between surface chemistry/structure and electrocatalytic activity for the oxygen reduction reactions. A more specific description is to link chemistry, orientation, strain, dislocation content, and grain boundary content to oxygen exchange of SOFC cathodes.

Objectives

The overarching objectives of this work will be to generate a basic understanding of cathode surface chemistry by working with a group of experts capable of addressing an appropriate range of relevant parameters in SOFC operating conditions. The specific objectives of this project are to generate well-defined epitaxial, textured, and polycrystalline films of the four major

compositions of interest to SOFC cathodes that also have controlled surface chemistries; and generate experimental data on surface properties that indicate how the electrocatalytic activity of SOFC cathodes can be optimized to yield improved cathodes. Ultimately, the project team aims to identify the primary parameter associated with surface activity for the cathode materials and to use this to inform infiltration experiments.

A significant effort will be expended to provide samples (parts of Tasks 2 and 3) to collaborators at both Argonne National Laboratory (ANL) and Massachusetts Institute of Technology (MIT), on which complementary experiments and modeling will be carried out to determine composition, surface structure, electronic structure, thermodynamics of oxygen adsorption, and kinetics of oxygen exchange with the gas phase. At Carnegie Mellon, the project team will determine surface properties such as electronic states and kinetics of oxygen exchange with the gas phase using a combination of Kelvin probe spectroscopy (KPS) and electrical conductivity relaxation; and will characterize samples with a suite of structural techniques.

SCOPE OF WORK

The overall scope of work includes the preparation of high-quality samples (Tasks 2–3) and the physical and structural characterization of samples (Tasks 4–8). The project team will prepare dense thin film (reservoir) samples by pulsed laser deposition (PLD) or laser-molecular beam epitaxy (L-MBE), as well as, in Phase 2, surface active layers (gates) deposited on top of the dense reservoir layer. Reservoirs include: LaSrMnO_3 (lanthanum strontium manganite [LSM]) and LaSrCoFeO_3 (lanthanum strontium cobalt ferrite [LSCF]), the common cathode materials; and LaSrCoO_3 (lanthanum strontium cobaltite [LSC]) and LaSrFeO_3 (lanthanum strontium ferrite [LSF]), as necessary. In Phase 1, the project team focused on intrinsic gates (surfaces composed of material in the bulk); in Phase 2, the project team will include introduce gates (surfaces containing material not in the bulk) to engineer the surface and electrocatalytic properties of the cathodes, emulating infiltration investigations.

Two basic types of samples will be prepared. Type 1 samples are epitaxial single-crystal films on perovskite single-crystal substrates, in which microstructural traits are minimized. Type 2 samples are epitaxially textured films on fluorite electrolyte single-crystal substrates, in which variant/grain boundaries complicate the microstructure compared to that of Type 1 films. Type 2 films are more similar to real cathodes and can be electrochemically tested. Samples will be prepared as requested from collaborators. Sample preparation includes extensive structural and surface characterization to ensure the samples are high quality and similar, to enable comparisons between samples investigated with different techniques.

At Carnegie Mellon, surface electronic and kinetic properties will be measured using a combination of KPS and electrical conductivity (EC) measurements. KPS will be carried out in steady-state mode on select samples to isolate the effect of work functions (a basic feature of the electrochemical level of electrons in the cathode) on cathode performance. KPS will also be carried out in transient mode, or relaxation mode, to investigate the oxygen adsorption/uptake properties of engineered cathode films. Electrical conductivity will also be measured in relaxation (ECR) and steady-state modes to determine oxygen exchange kinetics and to compare the effects of work function change with overall conductivity change. Gravimetric measurements pursued in Phase 1 will be dropped in Phase 2, owing to issues with the attainment of appropriate equipment. To compare work done at ANL or MIT in determining surface compositions in-situ with ex-situ measurements and correlating surface or microstructural features with activity, the project team will use transmission electron microscopy (TEM). Finally, the project team will also explore mature models developed by Walt Harrison to describe the electrocatalytic properties of cathodes. In the description of tasks, the project team focuses on the experimental efforts to be performed and describes inside those tasks the scientific issues that will be addressed within each.

TASKS TO BE PERFORMED

Task 1.0 Project Management, Planning, and Reporting

The primary goal of this task is to ensure success to the project by appropriately managing the tasks and disseminating results in accordance with the Project Management Plan. The results and status of the risk management process shall be presented during project reviews and in Progress Reports with emphasis placed on the medium- and high-risk items.

Task 2.0 Thin Film Sample Preparation

The primary goal of this task is to generate samples at Carnegie Mellon University (CMU) using PLD. Films will be deposited using the two PLD systems, one of which was designed as a hybrid chamber to carry out a reflection high-energy electron diffraction (RHEED)-assisted L-MBE/MBE hybrid deposition. The deposition parameters will be optimized to generate ultraflat films having specific microstructural features and to allow for the outer surface layer. Targets of all compositions will be fabricated at CMU using standard ceramic procedures. Surface modifications will be made by depositing a thin layer of controlled thickness having a different composition to the bulk of the film. For example, a thin layer (one monolayer thick) of SrMnO₃ (strontium manganite), LaMnO₃ (lanthanum manganite), or LSCF will be deposited on LSM to directly control the outer surface chemistry of thin films. The outer surface chemistry will be investigated using Auger spectroscopy, X-ray photoelectron spectroscopy (XPS), and atomic force microscopy (AFM) to ensure that the thickness and contiguity of the outer surface layer is appropriate for controlling the outer surface chemistry.

Task 2.1 Thin Film Sample Preparation for ANL

Samples will be prepared for experiments to be performed at ANL using in-situ synchrotron x-rays at the Advanced Photon Source.

Task 2.2 Thin Film Sample Preparation for MIT/University of Nevada, Las Vegas

Samples will be prepared for experiments to be performed at MIT and University of Nevada, Las Vegas (UNLV) using in-situ Scanning Tunneling Microscope at Harvard and synchrotron x-rays at the Advanced Light Source at Stanford, as well as ex-situ experiments at UNLV and MIT and in-situ electrochemical testing at MIT.

Task 2.3 Thin Film Sample Preparation for CMU

Samples will be prepared for experiments to be performed at CMU.

Task 3.0 Structural Characterization

The primary goals of this task are to ensure that samples generated in Task 2 indeed have their targeted structural and microstructural characteristics and to determine what changes occur after characterizations are carried out in Tasks 4–7. The project team will ensure that the films are well-characterized before physical properties are measured upon them, especially because samples will be measured in multiple locations. All of these characterization techniques are well known and are used as common tools in solid-state and materials science of thin films. Samples will be measured again after physical properties are measured to explore the changes associated with exposure to high temperatures. X-ray reflectometry is also used to routinely measure the growth rate of the project team's ultraflat films. X-ray diffraction is carried out on several diffractometers to determine phase, strain, epitaxy, texture, orientation, lattice parameters, etc. AFM is used to characterize the surface morphology of thin films and substrates. Select samples will be characterized using RHEED in conjunction with AFM to determine the surface structure of the project team's materials both before and after physical property measurements.

Task 4.0 Kelvin Probe Measurements

The primary goal of this task is to determine the work function of thin film samples by measuring contact potential difference changes in both steady-state, relaxation (transient), and temperature-programmed modes and over a range of temperatures and pressures. KPS can be carried out on films at temperatures and pressures appropriate to SOFCs and, by combining that with ECR, one can identify both the Fermi level and surface dipoles, both of which affect electrocatalysis. The project team's goal in Phase 2 is to carry out KPS on LSM, LSCF, and surface-engineered samples to understand how one can modify the surface parameters to affect electrocatalysis.

Task 5.0 Electrical Conductivity Measurements

The primary goal of this task is to determine the surface properties of thin film samples by measuring electrical conductivity in steady-state and relaxation (transient) mode and, when appropriate, in temperature-programmed mode. High-temperature EC measurement apparatuses include the ability to measure ECR by either: (1) using a small volume rig that is inserted into the furnace and high-gas flows are passed through after having been mixed to a specific oxygen activity by combining gases of different compositions; or (2) using a low-pressure dynamic vacuum system of reasonable volume and lower flow rates of a single gas. Steady-state EC measurements will be made to correlate changes in electrical properties between KP (Task 4) and ECR (Task 5) to properly deconvolute parameters that contribute to each. Primary focus will be on unraveling the effects of orientation and surface composition for LSM, LSCF, and those surface-engineered samples.

Task 6.0 Gravimetric Measurements using Piezoelectric Microbalances

Owing to an unanticipated acquisition of the supplier of PCM heads, the necessary equipment required to continue this work beyond Phase 1 cannot be acquired. As a result, work will be discontinued on this task in Phase 2, except to finalize the measurements and to publish a paper on LNO responses.

Task 7.0 Transmission Electron Microscopy

The primary goal of this task is to identify local structural defects, such as surface segregation or extended defect segregation at surfaces. The project team has provided such support in the past to SECA through a separate contract. In Phase 2, the project team will use TEM measurements and methods developed in other SECA programs to quantify the distributions of cations in thin films using focused-ion-beam preparation, electron energy-loss spectroscopy (EELS), and a newly installed Titan microscope.

Task 8.0 Connections to Theoretical Components

The primary goal of this task is to compare results obtained from theory to those generated by the three experimental techniques described in the previous tasks. The project lead is in contact with Walt Harrison on a DOE-funded project in which tight-binding models are being developed to generate theoretical descriptions of fuel cell cathodes. The project lead also interacts with other researchers at MIT and CMU on theory of cathode activity. Ultimately, the project team's investigations will be coupled to that theoretical work to determine the surface sensitive parameter that dictates electrocatalytic activity of fuel cells.

DELIVERABLES

At the end of the project, the project team will deliver a report describing the effect of a variety of parameters on the surface-sensitive property of relevance to commercial fuel cells. Combined results from each task will be presented at various conferences, including SECA conferences, and will be published in archival journals. Other reports will mainly include short presentations given to the program manager from time to time as requested, as well as presentations to the broader community at conferences and publications in the archival literature. Thin film samples will be delivered to collaborators at ANL and MIT for complementary experiments to be carried out at those institutions.

12: FWP-40552 (Task 1)

Project Number	Project Title		
FWP-40552 (Task 1)	SECA Core Technology Program: Task 1 – SOFC Component Development		
Contacts	Name	Organization	Email
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<i>Partners</i>			
Stage of Development			
<input checked="" type="checkbox"/> Fundamental R&D	<input type="checkbox"/> Applied R&D	<input type="checkbox"/> Prototype Testing	<input type="checkbox"/> Proof of Concept
			<input type="checkbox"/> Demonstration

Technical Background

Solid oxide fuel cells (SOFCs) place severe demands on cell and stack designs and materials due to their operating temperatures (typically $\geq 650^{\circ}\text{C}$), the presence of large thermal gradients (150°C – 200°C), and their complex exposure environments (multi-constituent fuels and oxidants). Although significant progress in improving the electrical performance and performance stability of the cells and stacks at reduced temperatures (650°C – 850°C) has been achieved, significant challenges remain to be overcome, particularly in terms of degradation and reliability.

Pacific Northwest National Laboratory (PNNL) is addressing these challenges on behalf of the Solid State Energy Conversion Alliance (SECA) Core Technology Program. Research and development activities covered by this project are primarily focused on developing, optimizing, and validating advanced cell and stack component materials, and improving understanding and mitigation of cell/stack degradation mechanisms. Specific task areas have been defined within the overall Component Development Task. The first four tasks are directed toward finding solutions of specific materials challenges faced by SOFC developers; the fifth task provides testing/validation of new materials and fabrication processes under stack-like conditions.

TASK 1.1: SOFC INTERCONNECTS AND COATINGS

Alloy Interconnects

SOFC interconnects physically separate the fuel in the anode chamber from the oxidant in the cathode chamber and also provide cell-to-cell series electrical connection in cell stacks. In recent years, progress in materials and fabrication techniques have allowed for a reduction in SOFC operating temperatures to a range (e.g., 650°C – 850°C) at which alloys can be considered as replacement materials for the ceramic interconnect materials used in high-temperature (900°C – $1,000^{\circ}\text{C}$) SOFC stacks. Compared to ceramic materials, the high-temperature, oxidation-resistant alloys can offer advantages such as improved manufacturability, higher thermal conductivity, and lower raw material and fabrication costs. However, to demonstrate durability and performance as interconnects, the metallic alloys must satisfy a set of stringent material requirements, including oxidation resistance, appropriate coefficients of thermal expansion (CTE), high electrical conductivity (bulk and oxide scale), chemical compatibility, and low cost.

Overall, selected ferritic stainless steels are the most promising alloy candidates, in terms of cost, thermal expansion, ease of fabrication, oxidation resistance, and formation of an electronically conductive oxide scale. In recent years, PNNL's studies have focused on AISI

441, a low-cost, commercially available, ferritic stainless steel that contains minor alloy additions that suppress the formation of an insulating silica layer at the alloy/scale interface. However, as is the case for all chromia-forming interconnect steels, 441 exhibits limitations in terms of chromium (Cr) volatility and long-term oxidation resistance at SOFC operating temperatures, indicating the need for protective surface modification. Promising results (e.g., improved oxidation resistance and low area-specific resistance [ASR]) have been obtained through application of $(\text{Mn,Co})_3\text{O}_4$ spinel (manganese cobalt [MC]) coatings onto ferritic stainless steels. The conductive spinel coating acts as a mass barrier to both Cr outward and oxygen inward diffusion, thus improving interconnect surface stability and mitigating Cr poisoning. More recently, to address scale adhesion issues, cerium (Ce)-modified MC (Ce-MC) coatings were developed, which add the advantages of rare earth (RE) surface treatment to the other established benefits of the MC spinel coating.

Ceramic Interconnects

For SOFC operating at relatively high temperatures (e.g., $>900^\circ\text{C}$), ceramic interconnects are expected to perform better than alloy-based interconnects. The standard ceramic interconnect material is alkaline earth-doped lanthanum chromite (LC), but recent studies at PNNL indicate that yttrium chromite, suitably doped with calcium on the A-site and transition metals on the B-site of the perovskite structure, can offer lower sintering temperatures and lower chemical expansion than conventional LC materials, while still exhibiting adequate electrical conductivity and thermal expansion match.

TASK 1.2: INTERCONNECT/ELECTRODE CONTACT MATERIALS

A complete solution to interconnect challenges must take into account not only optimization of the interconnect alloy and protective coating, but also the electrode/interconnect interfaces. Thus, it is necessary to develop a complete materials system, which includes not only the interconnect itself, but also stable, high-performance contact materials for electrode/interconnect interfaces. (Seal/interconnect interfaces are also of concern, and are also addressed in this project.) There are several basic requirements for contact materials in order to obtain low, stable contact resistance:

- High electrical conductivity to minimize the resistance of the contact layer and the contact interfaces
- Chemical compatibility with the interconnect and the electrodes. If reaction occurs, the resulting reaction products should be stable and conductive
- Appropriate thermal expansion behavior and high thermo-chemical and structural stability in the SOFC operating environment
- Appropriate bond-forming ability or sintering activity for increased contact area and decreased contact resistance, as well as improved interfacial structural stability
- Low cost

Finding suitable materials for electrical contact layers at the cathode interface can be especially challenging, particularly in intermediate temperature (650°C – 850°C) SOFCs, due to the relatively low stack sealing temperature (typically 825°C – $1,000^\circ\text{C}$). This low temperature provides limited thermal energy for sintering and bonding of the contact material (typically a conductive perovskite oxide), resulting in high porosity and limited contact strength and conductivity.

TASK I.3: SEALS FOR SOFC STACKS

Planar SOFC stacks require seals to prevent mixing of the oxidant and fuel gases within the stack, and leakage of the gases from the stack. Several different approaches to sealing SOFC stacks are available, including rigid, bonded seals (e.g., devitrifying glass), compliant seals (e.g., non-devitrifying glass), and compressive seals (e.g., mica-based gaskets).

Devitrifying glass-based seals

Many sealing approaches rely on a glass that will soften and “glue together” the adjacent stack components during stack fabrication (at a temperature above the operating temperature), but then become rigid and immobile (to avoid excessive flow or creep), typically due to devitrification, when cooled to the operating temperature. Glass-based seals represent a relatively easy means of sealing an SOFC stack, but they face challenges in meeting the stringent SOFC requirements. Their brittle nature makes the seals vulnerable to crack formation due to thermal stresses, so the CTE must be similar to that of the other components. Most SOFC sealing glasses are designed for relatively low sealing temperatures, close to stack operating conditions. For example, PNNL’s G18 sealing glass was developed for sealing at $\leq 850^\circ\text{C}$ for stacks operating at $\sim 700^\circ\text{C}$ – 800°C . After sealing, the glass undergoes substantial crystallization but still contains an appreciable amount of residual glass, which tends to be more reactive than the crystalline phases. Also, the CTE of the G18 decreases during long-term operation. In response to these issues, “refractory” glass seals, which are sealed at higher temperatures (e.g., $>900^\circ\text{C}$), were developed at PNNL. Refractory sealing glasses offer improved thermomechanical and chemical stability compared to standard sealing glasses. Another advantage of higher sealing temperatures lies in the fact that higher stack fabrication temperatures may result in increased strength and electrical conductivity for cathode/interconnect contact zones.

Compliant glass-based seals

Seals incorporating a glass which is compliant at SOFC operating temperatures potentially offer advantages that include the minimization of thermal stresses and the self-healing of cracks generated during thermal cycling. Challenges related to this type of seal include containment of the relatively mobile glass, devitrification over operating lifetime, and reactivity with other cell/stack components.

Compressive seals

These seals typically utilize materials such as sheet-structure silicates that do not bond adjacent SOFC components; instead, the sealing material acts as a gasket, and gas-tightness is achieved by applying a compressive force to the stack. Both compliant and compressive seals potentially improve the ability of the stack to tolerate thermal expansion mismatch between the various stack components.

Prevention of seal interactions

Alkaline earth aluminosilicate glasses generally adhere well to yttria-stabilized zirconia (YSZ) with little chemical interaction, but tend to react with steel interconnects to form barium or strontium chromate with very high CTE that can result in reduced interfacial strength. To improve interfacial stability, PNNL has developed a slurry-based aluminization process, which is effective in preventing the interaction between sealing glass and steel, which leads to chromate formation.

TASK I.4: ELECTRODE MATERIALS AND INTERACTIONS

Minimization of electrode polarization (especially cathodic polarization) represents one of the greatest challenges in obtaining high, stable power densities from SOFCs. Cathodic polarization exhibits high activation energy, so the need to improve cathode performance becomes

increasingly important as the SOFC operating temperature is reduced. Cathode materials must be stable at the SOFC operating temperature in air and must have high electronic conductivity, catalytic activity for oxygen dissociation and reduction, and appropriate thermal expansion. Chemical interactions with other cell/stack components must be minimal. In addition, the cathode material must have a porous microstructure that remains stable during SOFC operation over the lifetime of the cell.

For high-temperature SOFCs operating above $\sim 800^{\circ}\text{C}$, the preferred cathode material is doped LM, which offers relatively high electrical conductivity and electrocatalytic activity, reasonable thermal expansion match to YSZ, and stability in the SOFC cathode operating environment. Composite approaches (e.g., LM/YSZ mixtures) can be used to further reduce cathodic polarization. For SOFCs operating at lower temperatures, alternative cathode materials may be required. Alternative perovskite compositions—typically containing lanthanum on the A-site, and transition metals such as Co, iron, and/or nickel on the B-site—are potential replacement candidates. In general, they offer higher oxygen ion diffusion rates and exhibit faster oxygen reduction kinetics than LM-based cathodes. Promising results using these materials have been widely reported, but challenges remain, particularly in regard to long-term stability. Some non-perovskite compositions, such as Pr_2NiO_4 (praseodymium nickel oxide), have also shown promise as intermediate-temperature SOFC cathode materials.

TASK I.5: SOFC STACK FIXTURE TESTS

PNNL has a wide range of characterization techniques (e.g., X-ray diffraction [XRD], scanning electron microscopy [SEM], energy-dispersive X-ray spectroscopy [EDS], transmission electron microscopy [TEM], X-ray photoelectron spectroscopy [XPS], thermogravimetric analysis [TGA], differential scanning calorimetry [DSC], pressure swing adsorption [PSA], dilatometry, conductivity, single & dual atmosphere oxidation) and multi-component performance tests (e.g., button cell, interconnect/electrode ASR, seal/interconnect interfacial stability, and seal leak tests) available for evaluation of SOFC component materials. However, given the complexity and variety of materials utilized in SOFC stacks, it is important to test the performance of various components in a representative stack environment. Such tests can help bridge the gap between small-scale tests, such as button cells, and the full-size cells and stacks under development by industrial developers. In response to this need, PNNL is developing and implementing a stack test fixture that will allow for evaluation and validation testing of newly developed SOFC materials, processes, and design concepts. During FY10, a “2nd generation” stack fixture design was optimized for single- and three-cell tests.

Relationship to Program

This project will support important advances within the core technologies focus of the NETL Fuel Cells Program. Successful development and transfer to SECA industry teams of improved understanding of degradation mechanisms and optimized materials technology to minimize/eliminate performance degradation will accelerate the commercialization and deployment of SOFC-based power systems. Some specific benefits are summarized below.

Interconnects

Alloy-based interconnects show great promise for IT-SOFC applications in terms of cost and ease of fabrication. However, cathode-side protection layers are required to minimize Cr volatility and oxidation rate. Development of an optimized alloy/coating combination will help enable the design and manufacture of cost-effective SOFC stacks offering stable electrical performance over the system lifetime.

Contact Materials

Contact materials, especially at the cathode/interconnect interface, are typically a “weak link” in the stack in terms of mechanical strength and durability due to the limited sintering and bonding that occurs during stack fabrication. Development of optimized contact materials and/or fabrication processes will result in increased strength at that interface without compromising electrical performance, leading to improved thermal cycle stability of the stacks.

Seals

Sealing of planar SOFC stacks is generally acknowledged to be a significant challenge facing SOFC developers. In addition to preventing leakage of gases from the stack, and mixing of oxidant and fuel gases within the stack, the seals must also allow the stack to be thermally cycled between ambient conditions and relatively high operating temperatures (e.g., 800°C). Development of inexpensive, reliable stack sealing technology will assist SECA industrial developers in designing and manufacturing SOFC stacks which meet the SECA cost and performance targets.

Cathodes

The use of more active cathodes results in higher initial cell performance, but the higher performance is generally accompanied by a higher rate of performance degradation. An improved understanding of specific mechanisms responsible for higher degradation rates (including effects of volatile species from upstream components), and optimization of state-of-the-art cathode materials to minimize degradation rates, will allow for increased, stable power density in SOFC stacks, which will assist developers in meeting the SECA cost and performance targets.

Primary Project Goal

The goal of this task is to develop, test, and optimize high-performance, reliable cell and stack component materials and fabrication techniques for low-cost, reliable SOFC stacks, and to transfer developed technology to the SECA industry teams for performance validation and implementation.

Objectives

The primary objectives of this project are to identify, develop, test, characterize, and optimize cost-effective cell and stack component materials and fabrication techniques; and develop an improved understanding of cell/stack degradation mechanisms. Knowledge gained in regard to degradation mechanisms helps to guide materials and fabrication technique development activities intended to reduce/eliminate cell and stack performance degradation. Specific objectives and approaches for each of the task areas are described below.

TASK 1.1: SOFC INTERCONNECTS AND COATINGS

Task 1.1.1: Alloy-based Interconnects for SOFC

Global objectives:

- Investigate and develop advanced, cost-effective metallic interconnects and interconnect coatings that demonstrate long-term chemical, electrical, and structural stability.
- Evaluate and understand behavior of high-temperature oxidation-resistant alloys in SOFC environments, and assess the impact of that behavior on long-term SOFC interconnect performance.

Specific objectives for FY11:

- Improved understanding and quantification of long-term oxidation behavior and oxide scale growth/adhesion/spallation of AISI 441 with Ce-modified MnCo (Ce-MC) spinel coatings.
- Determine the effects of pre-coating surface treatments to the steel on oxidation behavior and scale adhesion.
- Develop and optimize slurry-based ultrasonic spray fabrication techniques for PNNL's Ce-MC spinel coatings.

Task 1.1.2: Ceramic Interconnects for SOFC

Global objectives:

- Develop ceramic interconnect materials that demonstrate long-term chemical, electrical, and structural stability in dual (i.e., oxidizing and reducing) environments.
- Investigate processing and composition options for fabrication of ceramic interconnects via co-sintering or constrained sintering with other SOFC components.

Specific objective for FY11:

- Investigate approaches for improving densification behavior of doped yttrium chromite layers under constrained sintering and co-sintering conditions.

TASK 1.2: INTERCONNECT/ELECTRODE CONTACT MATERIALS

Task 1.2.1 Cathode/interconnect contact materials

Global objective:

- Investigate and develop cost-effective cathode/interconnect contact materials and processing techniques that demonstrate long-term chemical stability, low electrical resistance, and improved sintering activity and bond strength.

Specific objective for FY11:

- Develop reaction-sintering approaches to enhance sintering/bonding of candidate cathode contact materials.

Task 1.2.2 Anode/interconnect contact materials

Global objective:

- Investigate and develop cost-effective anode/interconnect contact materials and processing techniques.

Specific objective for FY11:

- Investigate effects of contact material properties (e.g., phase/composition, particle size, solids loading, and viscosity) and processing conditions (e.g., thickness, drying condition, and applied load) on interfacial strength.

TASK 1.3: SEALS FOR SOFC STACKS

Global objective:

- Develop glass-based seals and seal/component interfaces with stable thermal, mechanical, electrical, and chemical properties for long-term operation in SOFC environments.

Specific objective for FY11:

- Develop and evaluate compliant glass-based seals, i.e., seals based on a glass that has minimum tendency to crystallize and relatively low viscosity at IT-SOFC operating temperatures.

TASK 1.4: ELECTRODE MATERIALS AND INTERACTIONS

Global objectives:

- Develop SOFC electrodes offering low polarization losses and long-term stability at intermediate SOFC operating temperatures (650°C–850°C).
- Investigate and mitigate effects of gas stream contaminants on electrode performance and stability.

Specific objectives for FY11:

- Investigate a series of LSCF-6428 cathode materials with varying levels of A-site cation deficiency to determine relationships between composition and performance. Lanthanum strontium cobalt ferrite (LSCF)/doped ceria composite cathode materials will also be investigated.
- Refine methodology for performing in-situ high-temperature XRD analysis on working cathodes.
- Improve the density of screen-printed samarium-doped ceria interlayers, and determine the effect of improved density on cell performance and stability.

TASK I.5: SOFC STACK FIXTURE TESTS

Global objectives:

- Develop and implement SOFC stack test fixtures to evaluate/validate the performance of materials, processes, and design concepts developed by PNNL and other Core Technology Program participants.
- Share the fixture designs and test results with SECA Core Technology Program and SECA industry team participants.

Specific objectives for FY11:

- Perform stack fixture tests to evaluate/validate the performance of selected SOFC component materials, fabrication processes, and design concepts developed by PNNL and other SECA Core Technology Program team members.
- Modify fabrication/design of test fixture components to minimize machining time and cost.
- Assist NETL in implementation of stack fixture testing at their test facility in Morgantown, WV.

13: FY10.MSE.1610248.621

Project Number	Project Title			
FY10.MSE.1610248.621	Solid Oxide Fuel Cell Research and Development: Impact of Minor Species from Coal Syngas on SOFC Performance			
Contacts	Name	Organization	Email	
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<i>Partners</i>				
Stage of Development				
<input type="checkbox"/> Fundamental R&D	<input checked="" type="checkbox"/> Applied R&D	<input type="checkbox"/> Prototype Testing	<input type="checkbox"/> Proof of Concept	<input type="checkbox"/> Demonstration

Technical Background

Solid oxide fuel cell (SOFC) systems that provide utility-scale power will be fueled with synthesis gas (carbon monoxide [CO] and hydrogen [H₂]) derived from coal gasification. Although a fuel cell / gasification system is expected to demonstrate high efficiency, the coal gasification process may volatilize some of the naturally occurring trace materials found in the coal. These trace species may react with the nickel-based materials constituting the SOFC anode, thus producing deleterious impacts that include accelerated SOFC performance degradation. The SOFC trace material exposure thresholds must be evaluated for common gas constituents, trace materials, and process chemicals. Exposure data collected can be used to inform the design of synthesis gas (syngas) cleanup systems required to meet the programmatic SOFC degradation target of <1% per 1,000 hours (40+ kilowatt-hour lifetime).

The trace elemental concentrations and species to which the SOFC is subjected depend on operating conditions of the gasifier and the post-gasification cleanup system. In general, trace materials negatively impact performance by blocking active reaction sites within the anode or reacting with the anode to produce undesirable secondary phases. The key technology gap for all trace material interaction characterizations is an absence of well controlled, long-term (500+ hour) test data for the trace materials of interest. Steady control of all test parameters through a 500-hour experiment is difficult to maintain, and comparison to repeatable baseline cell results is necessary. This project leverages mature test systems that have been operated and refined over years of SOFC research. The developed maturity of available test systems is critical to the evaluation of cell degradation, which is often subtle even over the course of a 500-hour test.

Relationship to Program

This project will support important advances within the SOFC systems development and analysis focus of the NETL Fuel Cells Program. If the project is successful, the following benefits will result:

- Clear identification of all relevant trace materials to be removed by the cleanup system (theoretical calculations confirmed by experimental results)
- Clear identification of cleanup targets for primary contaminants, including naphthalene, benzene, ethylene, and Selexol. Cleanup targets will be delivered for assumed power

density, base degradation rate, and cell lifetime estimates. Cleanup targets will be sufficiently generalized to permit application to a range of SOFC technology configurations.

- Sufficient information will be provided to design an integrated cleanup system that meets process needs and is potentially cost optimized.
- Development of a method by which trace metals can be identified and quantified rapidly in a gas phase process. This method is widely applicable to all research in fossil energy conversion processes (e.g., refining, chemicals production, catalysts, sorbents, membranes, and filters).

Primary Project Goal

For nickel-based SOFC anodes fueled with coal-derived syngas, the primary goal of this project is to identify threshold trace material exposure concentrations (especially for higher-order hydrocarbons) and concomitant syngas cleaning and reforming targets that prevent cell degradation rates exceeding Solid State Energy Conversion Alliance (SECA) targets (<1%/1,000 hours).

Objectives

This project addresses trace material exposure limitations in four complementary efforts:

- Theoretical evaluation of trace material exposure
- Controlled trace material exposure experiments (laboratory)
- Uncontrolled direct trace material exposure testing (field)
- Reporting of results and transfer of information

Thermodynamic evaluations are used to guide the selection of trace materials for experimental evaluation. Controlled laboratory experiments individually test the most relevant trace materials identified in the theoretical analyses. Field experiments validate the laboratory tests and screen for trace material exposures that were not predicted in the theoretical analysis. The comprehensive results from all phases of study are communicated to industrial teams, cleanup system designers, and process modelers to inform efforts to develop a strategy for trace material removal that meets programmatic degradation goals while achieving system cost targets.

Thermodynamic analyses were completed for two primary process configurations, the operating parameters that represent boundaries for contemporary and future cleanup systems. The analyses evaluate the trace metal content of syngas streams generated from a survey of gasification system designs. Syngas loaded with a standardized load of trace material is equilibrated at a set thermodynamic condition (temperature, pressure, etc). The selected conditions represent conventional low-temperature cleanup based on the Selexol process, and future cleanup systems based on high-temperature (300°C–500°C) gas filtration and sorbent technology. The trace materials passing through the gas cleanup system are assumed to reach the SOFC anode. Typical trace materials predicted to reach the SOFC, as determined through thermodynamic analyses, include trace metals such as mercury, selenium, and arsenic. The list of thermodynamically predicted trace materials is expanded further to include trace hydrocarbons such as benzene, naphthalene, and ethylene, and process chemicals such as polyethylene-glycol-dimethyl-ether and zinc. Hydrocarbons, in particular, are important for consideration, as they are expected to be generated in greater quantities in the higher-pressure, lower-temperature methane-producing gasifiers envisioned in the SECA systems.

Carefully controlled laboratory experiments were completed for individual trace species exposure in which SOFC anodes are exposed to simulated and direct coal syngas containing trace materials; performance was recorded through an extended duration test (typically 500 hours). The interaction of low concentration and trace contaminant materials (especially hydrocarbons) is investigated. Temporal electrochemical performance data are collected as a function of contaminant exposure (e.g., naphthalene, ethylene, dimethyl ether, and selenium), and predictions of trace material exposure tolerance are generated. Electrochemical performance, microstructural evolution, and chemical reaction information are compiled to quantify the threshold of trace material exposure. The typical mechanisms of low concentration and trace material interaction are explored to quantify the time scales over which degradation may be expected to occur.

Field testing of SOFC on direct syngas was conducted by interfacing a mobile test unit with a slipstream of syngas generated by the National Carbon Capture Center's (NCCC) coal gasifier. Located in Wilsonville, Alabama, the NCCC includes an engineering-scale demonstration of key advanced power system components, including a KBR transport reactor, high-temperature particulate filter, dry coal feed systems, and dry ash removal systems. The NCCC is a unique test facility because it is large enough to produce commercially representative data from the major components required for a commercial plant, while remaining small enough for economic operation.

The mobile SOFC testing platform known as the Multi-Cell Array (MCA) was designed specifically to interface with remote sources of syngas (such as the NCCC) for direct exposure testing. The MCA features a 12-cell, parallel testing array facilitating simultaneous cell performance evaluation for independent specimen. Cells are fueled from a common syngas supply, but cells are electrochemically tested by independently loading the individual cells. A solid cell performance baseline has been established through a statistically significant number of test operations; this baseline permits the project team to compare results obtained in direct field tests to the baseline for clear evaluation of cell performance.

Finally, data and analysis generated in this project have been published to inform SECA developers of required gas cleanup efforts, and further guide programmatic research priorities. The research output of these studies, while not directly patentable itself, is necessary to facilitate the generation of designs applicable to the integrated commercial power production facilities. The research reports are publicly reported to encourage system innovations by the core program participants and by third-party collaborators with the SECA program.

I4: FC26-08NT0006557

Project Number	Project Title		
FC26-08NT0006557	Theory, Investigation and Stability of Cathode Electrocatalytic Activity		
Contacts	Name	Organization	Email
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<i>Partners</i>			
Stage of Development			
<input checked="" type="checkbox"/> Fundamental R&D	<input type="checkbox"/> Applied R&D	<input type="checkbox"/> Prototype Testing	<input type="checkbox"/> Proof of Concept
			<input type="checkbox"/> Demonstration

Technical Background

The cathode is an important area of solid oxide fuel cell (SOFC) development because the energy efficiency of each cell is dominated by cathode polarization, which is even more evident at lower operating temperatures. Georgia Tech Research Corporation's novel cathode consists of a porous backbone of high ionic and electronic conductivity, such as $\text{La}_{0.6}\text{Sr}_{0.4}\text{Co}_{0.2}\text{Fe}_{0.8}\text{O}_{3-\delta}$ (lanthanum strontium cobalt ferrite [LSCF]), and a thin coating of a catalyst with high stability and catalytic activity toward oxygen (O_2) reduction, such as $\text{La}_x\text{Sr}_{1-x}\text{Mn O}_{3-\delta}$ (lanthanum strontium manganite [LSM]) and $\text{Ce}_{0.8}\text{Sm}_{0.2}\text{O}_3$ (samaria-doped ceria [SDC]). The uniqueness of this approach makes effective use of the best properties of two different materials: the high ionic and electronic conductivity of LSCF and the long-term stability and catalytic activity of a catalyst (e.g., LSM).

The challenge of this approach is achieving a rational design with the desired architecture and microstructure of each component and cost effectively fabricating the cathode with reduced polarization and enhanced stability. While the higher ionic and electronic conductivity of LSCF, in comparison to LSM cathodes, significantly extends the active sites beyond the triple-phase boundaries, there is sufficient evidence that the catalytic activity of a stand-alone LSCF cathode is likely to be limited by the surface catalytic property. Further, the surface properties of LSCF cathodes often change during cell operation, leading to degradation in performance. Thus, the project team has developed a cost-effective infiltration process and demonstrated the enhanced activity and stability of LSCF with a continuous or discontinuous layer of catalyst through infiltration. The project team plans to perfect the model for optimization of the electrode design and to demonstrate its benefits in commercial cells.

KEY PROGRESS TO DATE

2.1. A unique test cell platform

A test cell platform with a new electrode structure or architecture has been carefully designed to determine the intrinsic surface catalytic properties of cathode materials. The project team has also developed a model to evaluate sheet resistance in thin-film working electrodes for the exploration of fundamental properties of the mixed ionic electronic conductors of interest.

2.2. Development of the infiltration process

Ideally, the project team hopes to create a uniform coating of catalyst on the surface of a porous LSCF. The coating could be a porous layer of discrete catalyst particles or a dense thin film of catalyst. A porous layer of particles would be more appropriate for ionic conductors such as SDC, which have been successfully deposited on an LSCF surface by infiltration of aqueous nitrates solutions. In contrast, a dense thin film is better suited to mixed conductors such as LSM, which have been prepared using non-aqueous solutions as described below.

In order to produce dense LSM films (rather than LSM particles), the project team used 2-methoxyethanol and acetic acid to replace water as solvents, and strontium acetate and manganese acetate as metal organic precursors to replace nitrate precursors. The non-aqueous LSM sol showed improved wettability on the LSCF surface. The project team successfully fabricated dense LSM films with desired structure, composition, morphology, and thickness on the LSCF surface. The LSM film had been annealed at 900°C for 1 hour to develop the desired perovskite phase. Images taken of these films suggest that the LSM film assumes an epitaxial relationship with respect to the underlying LSCF grains due to the structural similarity between LSM and LSCF. The project team has carefully examined the microscopic features of these LSM films before and after long-term annealing under conditions similar to SOFC operating conditions in order to correlate them with the observed electrochemical performance.

Further, the project team has also investigated the sol-gel LSM solution infiltration into porous LSCF cathode in order to confirm the performance enhancement in actual cells. Blank LSCF and LSCF cathodes infiltrated with different concentrations of LSM sol after annealing at 900°C for 1 hour similarly appear to be epitaxial to the LSCF grains. The thickness of the films can be controlled by the amount and concentration of the LSM solutions.

2.3. Electrochemical performance of cells with catalyst-infiltrated LSCF cathodes

2.3.1. LSM-infiltrated LSCF cathodes

To demonstrate the long-term stability of the LSM coating, the performances of the anode-supported fuel cells with LSM-coated LSCF cathodes were tested for longer periods of time. The LSM coatings were fabricated with two processing techniques—solution infiltration and gas phase deposition—both of which resulted in performance and stability improvements. The performance improvement was immediate with gas-phase deposition but was delayed for about 100 hours with infiltration. Current densities of cells with LSM-modification eventually became 200 milliamperes (mA)/cm² higher than that of the cell with blank LSCF after 500 hours of testing. In the case of electrocatalytic activation of the LSM-coated LSCF electrode, the impedance of a blank LSCF cathode is directly compared with those infiltrated with 0.05 M and 0.3 M LSM sol, demonstrating reduced electrode polarization under fuel cell operating conditions.

The project team used LSM sol infiltration with 0.05 M, 0.1 M, and 0.3 M in symmetrical cells, using platinum mesh as current collector, to study the effect of LSM concentration. Comparisons of a blank LSCF and an LSM-infiltrated LSCF cathode with different concentrations of LSM solutions measured at different current densities showed that interfacial polarization resistance (R_p) of all infiltrated LSCF cathodes is larger than that of the blank LSCF under the open circuit voltage condition, and it increases with solution concentration. When there is a cathodic current passing through the cell, R_p decreased in all cases. The higher the infiltration solution concentration, the larger the decreasing rate. As the current density is high enough (i.e., 1 A cm⁻²), the R_p is similar for all infiltrated LSCF and visibly lower than that of a blank LSCF cathode under the same conditions. Accordingly, it seems there is a compromise between performance

improvement and solution concentration under different operation conditions. When comparing the O_2 partial pressure (pO_2) dependence of R_p of blank and LSM-coated sputtered cells, the LSM-coated film shows little dependence upon pO_2 , reflecting the relative ease of adsorption on the LSM surface. This may be one of the reasons that LSM-infiltrated LSCF cathode has improved performance.

2.3.2 Cells Infiltrated with Other Catalysts (e.g., SDC, calcium-doped lanthanum chromites, and solid carbonate-ceria composite)

The project team has also explored some other catalytically active materials as infiltration species into LSCF porous cathode. The performance improvement of these cells is significant when the amount of catalyst is appropriate and the particle sizes are relatively small. The performance can be reduced if the amount of catalyst is excessive, increasing the impedance to gas transport through the pores.

2.4. Continuum modeling and simulation

A possible explanation for the kinetic response of uncoated and LSM-coated LSCF under cathodic polarization lies in the solid-state defect chemistry of the two materials. The project team simulated a response of the polarization resistance of LSCF and LSM under bias, normalized to the open circuit voltage (OCV) value and assuming no bulk transport losses, using a micro-kinetic modeling technique that links steady-state defect concentrations to oxygen reduction rate on the surface. In this particular simulation, the oxygen reduction rate was set to be directly proportional to the steady-state surface oxygen vacancy concentration to the value at equilibrium. The trend of LSCF polarization resistance has reasonable qualitative agreement with experimental data for blank LSCF films. The trend for LSM is suggestive of the experimental observation of the LSM-coated LSCF thin-film working electrode; the polarization resistance drops very quickly with increasingly negative cathodic overpotential compared to LSCF and does not increase once large cathodic overpotentials are reached. Therefore, a surface with an LSM coating may have a larger polarization resistance under OCV but be more highly activated under bias, resulting in a lower net polarization resistance at operating voltage. This micro-kinetic technique, along with consideration of transport, can be applied onto porous microstructures. Simulations of the distribution of oxygen vacancies under a small cathodic bias in a porous LSCF structure can be used to better understand the response of porous electrodes, connect experimental results of LSM-infiltrated cathodes to theory, and help design novel porous structures.

2.5 Microanalysis of structure, composition, and morphology of surface and interface

Water-free sol-gel LSM was spin-coated on an LSCF pellet, producing an LSM film with thickness ranging from 42 nm to 50 nm. Compositions of the derived LSM films were determined to be $La_{0.60}Sr_{0.41}Mn_{0.20}$, which yields an A/B ratio of ~ 1.0 . The sol-gel LSM on LSCF pellet was subsequently annealed at 850°C for 900 hours. Transmission electron microscope (TEM) and Z-contrast images of the film demonstrate a film thickness of 48 nm and a comparable thickness prior to annealing. The observation is critical as it pertains to mass-stability of the LSM. Nonetheless, the LSM film has lost long-range order of atomic arrangement, except at its bottom portion up to about 10 nm thick. Structure coherence of perovskite lattices of both phases are maintained, and profiles of elemental concentration and atomic percent show that the concentration of cobalt (Co) is nearly constant within the bottom portion of the LSM film and tapers off near the film surface. The fastest Co diffusion observed is consistent with the high Co diffusion rate in LSM. In neither the as-deposited nor the annealed LSM is the surface strontium (Sr)-enrichment seen. The Sr-enrichment has been widely accepted as the major cause of LSCF cathodes instability and performance degradation.

After annealing at 850°C for 900 hours, the detailed microstructure, composition, and morphology of an LSCF grain in an LSM-infiltrated porous LSCF cathode was examined by TEM analysis. The LSCF grain maintains the perovskite structure, as evident by the lattice fringes deep in the bulk and at the edge of the LSCF grain. The surface layer contains all the cations of LSCF and LSM, and lacks long-range order of atomic arrangement as shown in the electron diffraction. Thickness of the surface layer ranges from 2 nm to 23 nm. Profiles of elemental concentration and atomic percent show peaks of manganese (Mn) at the grain boundary and the grain surface. The profiles similarly do not show any surface-enrichment of Sr. TEM observations suggest that the thickness of the LSM films derived from a sol-gel process on an LSCF pellet was largely preserved during annealing at 850°C for 900 hours. However, it appears that Mn migration along the LSCF grain surface, combined with evolution of LSM on the LSCF grain, led to the formation of a thin layer of LSM that contained some Co. The degree of regularity of atom arrangement is also reduced (from long to short range order), which favors oxygen ion conductivity. On the other hand, the LSM layer is very thin, ranging from 2 nm to 23 nm. The small thickness is expected to ease transport of the oxygen ions to the LSCF.

Relationship to Program

This project will support important electrode advances within the core technologies component research and development focus of the NETL Fuel Cells Program. The project will contribute the following benefits to the program:

- Develop a cost-effective process for surface modification to enhance SOFC cathode activity and stability. The simple solution infiltration process is also amenable to high-volume manufacturing.
- Offer new approaches to more efficient cathodes through new architectures and new materials.
- Reduce capital costs for cells, stacks, and coal-based integrated gasification fuel cell power plants.
- Improve system and power plant efficiencies due to lower losses both intrinsically and from parasitic cathode air blower requirements.

Primary Project Goal

The primary project goal is to correlate the electrochemical performance with the local structure, composition, and morphology of surfaces and interfaces of a catalyst-infiltrated LSCF cathode, aiming at establishing the scientific basis for rational design of better cathodes with enhanced stability and activity for oxygen reduction.

Objectives

The project has the following objectives:

- Fabricate and test catalyst-infiltrated LSCF cathodes for better performance and stability.
- Characterize local structure, composition, and morphology of surface and interface systematically.
- Develop models for test cell design, data interpretation, and rational design of better electrodes.
- Demonstrate performance and stability improvement in commercial cells.

15: FEAA066

Project Number	Project Title			
FEAA066	Reliability of Materials and Components for Solid Oxide Fuel Cells			
Contacts	Name	Organization	Email	
<i>DOE/NETL Project Mgr.</i>	Rin Burke	NETL – Power Systems Division	Patcharin.Burke@netl.doe.gov	
<i>Principal Investigator</i>	Edgar Lara-Curzio	Oak Ridge National Laboratory	laracurzioe@ornl.gov	
<i>Partners</i>	Pacific Northwest National Laboratory Delphi Rolls Royce Fuel Cells (US) Inc			
Stage of Development				
<input type="checkbox"/> Fundamental R&D	<input checked="" type="checkbox"/> Applied R&D	<input type="checkbox"/> Prototype Testing	<input type="checkbox"/> Proof of Concept	<input type="checkbox"/> Demonstration

Technical Background

One of the primary aims of the Solid State Energy Conversion Alliance (SECA) program is to reduce the cost of manufacturing and operating solid oxide fuel cells (SOFCs). Because the SOFC stack is a complex system, reducing the overall manufacturing costs requires the application of predictive modeling tools. Models are, however, only as good as the experimental data that is fed into them. Since becoming involved in the SECA program, Oak Ridge National Laboratory (ORNL) has developed and implemented test methods to generate experimental data that is used to support the development of reliability and durability models of materials and components for SOFCs. While many projects within the SECA umbrella focus on the electrochemical reliability of SOFC components, the ORNL project is one of the few that focus on the mechanical reliability of SOFC materials and components. The ORNL team has characterized the mechanical reliability of most SOFC components, including anodes, cathodes, electrolytes, interconnects, and the interfaces between them. For the first five years, the program focused on characterizing the anode and electrolyte materials; the following three years, the program focused on the cathode and cathode side interfaces. In the last couple of years, the focus has been on developing and characterizing reliable glass seals.

Relationship to Program

This project will support important materials advances within the core technologies component research and development focus of the NETL Fuel Cells Program. The success of the proposed tests and studies will lead to the following contributions:

- Development of more reliable glass seal materials and concepts that can increase the overall reliability of the system
- A methodology to predict the adhesion strength of the oxide scale on the interconnect
- Experimental data to support the development of models to predict the thermal and mechanical performance of SOFCs
- More reliable and durable SOFCs
- Training of researchers and scientists in the area of sustainable fossil energy generation

Primary Project Goal

The primary goal of this project is to identify and characterize the mechanisms that are responsible for the failure of SOFC materials, components, and stacks. In particular, this project

focuses on the multilayer anode/electrolyte/cathode/interconnect assemblies, which constitute the building blocks of these systems.

Objectives

For the performance periods associated with fiscal year 2010 (FY2010) and FY2011, the ORNL SECA program objectives include the following:

- *The characterization of specific commercial glasses in the SECA Core Technology Program for potential use as SOFC seal materials.*
Progress – The project team has characterized two commercially available glasses and the change in their microstructure with up to 10,000 hours of SOFC environment exposure.
- *The development and design of engineered glass sealing concepts.*
Progress – Several concepts have been developed. Information on the concepts is proprietary.
- *The characterization of the various interfaces within the SOFC assembly, in particular the interfaces between metallic interconnects, their thermally grown oxide layer, and protective coatings applied to metallic interconnects.*
Progress – A test methodology based on the Brazilian disk geometry has been developed to characterize the adhesion of oxide scales on the metallic interconnects.
- *The support of the SECA Industry Teams and other core technology partners like Pacific Northwest National Laboratory (PNNL).*
Progress – Cooperative development projects have been executed with Delphi Corporation and Rolls Royce Fuel Cells (United States). The ORNL team closely partners with PNNL in various areas such as seal leakage testing.
- *The continued development of the ASME Design Basis Guide.*
Progress – Contributed to the preparation of the ASME Design Basis Guide to design cost-effective, structurally reliable, and durable SOFC stacks.

16: FC26-08NT0004 | 17

Project Number	Project Title		
FC26-08NT0004117	Chemistry of SOFC Cathode Surfaces: Fundamental Investigation and Tailoring of Electronic Behavior		
Contacts	Name	Organization	Email
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Stage of Development			
<input checked="" type="checkbox"/> Fundamental R&D	<input type="checkbox"/> Applied R&D	<input type="checkbox"/> Prototype Testing	<input type="checkbox"/> Proof of Concept
			<input type="checkbox"/> Demonstration

Technical Background

The electricity as well as the chemical/fuel products in a reversible operation from solid oxide fuel cells (SOFCs) can directly benefit a wide range of energy industries. However, key barriers to widespread use of SOFCs thus far are the materials degradation at the high operating temperatures, and poor performance of the cathode at lower temperatures. The conventional cathode catalyst, doped lanthanum manganite, generally dominates the overall cell resistance and presently prohibits the use of SOFCs at temperatures below 750°C. Major contributors to the cathode performance limitations at low temperatures are the slow kinetics of oxygen reduction reaction (ORR) at the air-cathode interface and the slow transfer of the oxygen ions through the cathode bulk.

The design of inexpensive, stable, and catalytically active materials for the ORR in SOFCs will require fundamental breakthroughs. An opportunity to provide these advances can arise from the ability to tune the molecular- and atomic-level structural, chemical, and electron transfer properties of the SOFC cathode surfaces. Realization of this opportunity requires first obtaining a fundamental understanding of the electrocatalytic activity on materials using the most advanced scientific tools that are available. This knowledge has been largely missing for the SOFC cathode. Only with such understanding can electrocatalyst interfaces begin to be tailored on the basis of fundamental insight. This can be especially important for the design of infiltrated cathode compositions and microstructures, where both the solid-gas and solid-solid interfaces play an important role for its activity and stability.

The findings of this project advanced the project team's understanding of how the SOFC cathode surface cation chemistry and electron transfer properties, related to oxygen reduction activity, change with temperature, oxygen pressure, material microstructure, and lattice strain. While the temperature and pressure are determined by the functional operational conditions of SOFC, the material microstructure and lattice strain can be controlled to enable more active cathodes, especially in the form of thin films. These findings benefit the development of SOFC cathode chemistries rationally. Furthermore, the capabilities developed in this project—including the in-situ assessment of surface structure, chemistry, and electron transfer properties—are transferable to investigating other materials and structures of interest to SOFC development in harsh conditions of high temperatures and reactive gasses. Below is a summary of the project team's major findings that benefit the understanding and further development of active cathode materials, all demonstrated on the model system $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ (lanthanum strontium manganite

[LSM]), first in the form of textured polycrystalline films (in A), and then in the form of epitaxial films (in B):

- For the LSM films that were crystallographically highly textured on yttria-stabilized zirconia (YSZ), with evident grain boundaries (but not single crystal, epitaxial), the three important findings are as follows:
- The project team identified that the surface chemistry and electronic structure (band-gap) depended on the film thickness. The thin LSM films (10–50 nm) exhibit higher A/B = (La+Sr)/Mn ratio on LSM surface compared to thicker films (100 nm) when deposited at the same conditions. The electron transfer favors the thicker films, with a smaller band gap, and larger presence of manganese (Mn) on the surface. Electrochemically, too, the thinner films are limited by surface reaction kinetics. These observations together suggest that Mn-terminated surfaces on LSM cathodes could be possible to attain for thicker films (>~100 nm), and such a surface chemistry would favor the electron transfer kinetics in the ORR.
- At high temperatures, the project team identified Sr enrichment, and La and Mn depletion, which resulted in an increase in the A/B = (La+Sr)/Mn ratio on LSM surface above 500°C. An accompanying decrease in the electron tunneling conductance was observed. This indicates that the A-site cation rich surfaces are catalytically less active than Mn-terminated surfaces. As in Finding 1 above, the findings here, too, suggest that enabling Mn-terminated surfaces on LSM cathode would be beneficial for the electron transfer kinetics in the oxygen reduction.
- A broad distribution of the electronic structure, in particular the band gap, was observed on the surface of the LSM films on YSZ substrates, even when the films were highly textured in one crystallographic direction and smooth. This was an intriguing observation, implying the presence of a variety of local chemistry and structures prevailing the inhomogeneous spatial distribution of electronic structure on LSM surface. Specifically, a higher electron transfer rate at select grain boundaries compared to bulk surfaces was found. This higher activity at grain boundaries could be explained by an altered non-stoichiometry, leading to the presence of desirable charged defects at the grain boundaries. This suggests that select grain boundaries can serve as fast oxygen incorporation sites, due to their local structure and chemistry, and further investigation is needed for further understanding and incorporating this to SOFC cathode microstructure design.
- Probing the reasons and the correlations discussed above in more detail (to confirm and explain) at the atomic scale requires the use of single-crystal LSM films epitaxially grown on different perovskite substrates. Epitaxial films minimize/avoid uncertainties arising from extended structural inhomogeneities such as grain boundaries, and allows a more precise atomic scale interrogation of the surface. These films also allow for better control of surface structural and chemical quality to enable a more reliable coordination and comparison between the results acquired by the University of Nevada–Las Vegas (UNLV) and the Massachusetts Institute of Technology (MIT). Epitaxial films in various oxygen pressures evolved dynamically with temperature, and correlated with distinct electron tunneling rates. These changes were probed with scanning tunneling microscopy and spectroscopy, both ex situ (at room temperature posterior to the high-temperature treatment of the surfaces) and in situ under the temperature and oxygen environment subjected to the films. The differences in topological and electronic structure of the surface are tentatively attributed to partial oxidation and reconstruction of the surfaces. High-resolution scanning tunneling microscopy and spectroscopy (STM/STS) and X-ray photoelectron spectroscopy (XPS)/ultraviolet photoelectron spectroscopy (UPS) investigations to probe the atomic scale explanation for these correlations are ongoing. The project team expects that high-resolution identification of the structure and chemical correlations to electron transfer properties between the surface and oxygen, for LSM as well as for lanthanum strontium cobalt ferrite (LSCF) in the

continuation of this work will provide insights useful for designing cathode surfaces with high activities in oxygen reduction.

- An important finding on epitaxial LSM films is the role of lattice strain in driving the oxygen reduction activity on oxide cathodes by influencing the surface chemistry and electronic structure. The project team demonstrated and mechanistically interpreted the effects of epitaxial strain on the surface cation chemistry, in particular the segregation of Sr, and the electronic structure on $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ (LSM) as a model system. The project team's results show that the epitaxial LSM thin film surfaces are layered and exhibit strain-dependent nanoscale lateral structures. XPS shows a larger Sr enrichment for the tensile strained LSM surface (in good agreement with the first principles-based calculations in another project, which predict lower Sr segregation energy on the tensile strained LSM surface). The electronic structure, measured by tunneling microscopy and spectroscopy, shows that the tensile strained LSM exhibits a larger band gap at room temperature, yet a higher tunneling conductance than the compressively strained LSM at elevated temperatures in oxygen. The project team's findings demonstrate the importance of lattice strain as a key parameter to tune the surface chemistry for facilitating oxygen reduction kinetics on transition metal perovskite cathode surfaces for SOFCs.
- An important set of capabilities is the measurements of the band structure combining UPS (valence band) and inverse photoemission spectroscopy (IPES; conduction band) to identify the electronic band gap laterally averaged on the surface; and the temperature-dependent probing of surface chemistry using XPS. The combined UPS-IPES measurements identified a smallest prevailing band gap of 1.25 (+/- 0.20) electron volts (eV). This value is consistent with the findings by tunneling spectroscopy, and strengthens the complementary findings from the MIT and UNLV teams discussed above. The temperature-dependent XPS measurements in vacuum showed that the surface chemical environment changes irreversibly at high temperatures, even though the oxygen is not lost from the surface on LSM. These are important observations and capabilities that allow the project team to establish comparisons of surface state at ex-situ or semi-in-situ conditions, which were previously not accessible.

Relationship to Program

This project will support important advances within the Electrode Component Research and Development focus of the Core Technologies area of the NETL Fuel Cells Program. The findings of this project advanced the project team's understanding of how the SOFC cathode surface cation chemistry and electron transfer properties, related to oxygen reduction activity, change with temperature, oxygen pressure, material microstructure, and lattice strain. These findings benefit the development of SOFC cathode chemistries rationally. Furthermore, the capabilities developed in this project—including the in-situ assessment of surface structure, chemistry, and electron transfer properties—are transferable to investigating other materials and structures of interest to SOFC development in harsh conditions of high temperatures and reactive gasses.

Primary Project Goal

The project team's ultimate technological goal is to enhance the electrochemical performance of cathodes to enable a reduction of the SOFC module cost to below \$400/kW (Solid State Energy Conversion Alliance [SECA] goal, in 2002 dollars). Realization of this objective requires new scientific knowledge and an optimal tailoring of the atomic- and molecular-level properties associated with the cathode surfaces. The primary driver of the project's specific research objectives is the hypothesis that near-term progress in the SOFC cathode activity can be achieved *through incorporation of active catalyst structures or layers onto existing backbones*

structures. Hence, in the investigation, the project team: considers thin film cathodes; controls their surface chemistry by synthesis conditions, grain boundary structures, and by strain states; and relates its findings to the activity of the cathode materials as they may exist in infiltrated structures.

Objectives

The project team's specific research objectives include (1) obtain a fundamental understanding of the key correlations between the stable structural (solid-state atomic, crystallographic), compositional, chemical and electronic properties and the oxygen electrocatalytic activity at SOFC cathode surfaces; (2) demonstrate enhanced electrocatalytic activity on favorable prototype cathode structures, based on the fundamental structure-chemistry relations to be identified for the cathode surfaces; and (3) provide an essential library of data that theorists can use to develop models for rational design of cathode chemistries based on first principles.

The project team's research to achieve these objectives combines: utilizing model reproducible cathodes fabricated using advanced techniques that allow atomic-level control of the composition profile and crystallography at nanoscale surfaces; determining the chemical and electronic structure of the surfaces using surface-sensitive techniques, including soft X-ray/electron spectroscopy, scanning tunneling microscopy, and spectroscopy; quantitatively correlating surface properties to the cathode activity through electrochemical characterization; and collaborating closely with theorists and other X-ray physicists studying the surfaces of cathodes in the SECA program. For thermodynamic and kinetic reasons, the cathode surfaces' chemical and electronic state depends on the temperature, oxygen partial pressure, and electrical potential. Therefore, the project team aim includes capturing the surface properties in as realistic conditions of temperature and oxygen pressure as possible, and also establishing comparisons of the surface states in realistic conditions and in high-vacuum and room-temperature conditions. The capability to characterize the surface chemical and electronic structure in situ, and the comparison of the in-situ and ex-situ results, can significantly contribute to the project team's scientific understanding of the electrocatalytic activity of cathode surfaces.

17: DE-FE0005132

Project Number	Project Title		
DE-FE0005132	Small Scale SOFC Demonstration using Bio-based and Fossil Fuels		
Contacts	Name	Organization	Email
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<i>Principal Investigator</i>	Robert Ruhl	Technology Management, Inc.	ruhl@stratos.net
<i>Partners</i>			
Stage of Development			
<input type="checkbox"/> Fundamental R&D	<input type="checkbox"/> Applied R&D	<input type="checkbox"/> Prototype Testing	<input checked="" type="checkbox"/> Proof of Concept
		<input type="checkbox"/> Demonstration	

Technical Background

Technology Management, Inc. (TMI) proposes to develop and demonstrate a residential-scale prototype fuel cell system that will provide the basis for a new paradigm power production and integration to utility smart grids: massively distributed generation. These small-scale systems would operate 24/7, producing electric power for on-site use and grid export with the option for recovered heat for cogeneration, thereby transforming today's residential power grid. Small on-site generation provides a critical missing component to the smart grid equation: intelligent on-site power generation that can adapt to user loads, including electric and plug-in hybrid vehicles. The systems would operate on both conventional and renewable biofuels, providing cost effective, uninterruptible, whole-house power with major environmental and reliability advantages.

The critical component to point-of-use distributed power generation is the unique TMI solid oxide fuel cell (SOFC) integrated module, which would operate on whichever fuel is used for an adjacent furnace. Most residential systems would use multiple 1 kW modules to provide continuous 24/7 electric power needs, including power to charge plug-in hybrid and electric vehicles, and fulfill hot water needs of the home plus a significant fraction of its space heating. Excess power would be available to be exported to the grid whenever necessary or economically prudent, thus providing the equivalent of massively distributed power storage. During grid outages, the system would continue to provide uninterruptible power for an unlimited number of times, with a battery bank supplying surge power needs.

TMI SOFC SYSTEMS AND TECHNOLOGY

The basis of TMI's solid oxide systems was initially conceived by BP/Sohio in the late 1980s, and the technology was acquired by TMI in 1990. Since that time, approximately \$25 million in development funding (primarily through private, institutional, state, and federal grants/contracts) has taken the technology from initial cell feasibility to the current engineering prototype stage.

TMI has engineered unique features into its basic system platform to enable the development of competitive products in multiple market sectors. These features include: the ability to operate on multiple fuels, including both fossil fuels and renewable biofuels, which may be more available in rural and remote markets; a multi-module, redundant configuration designed for changing end-user demands and reliability; a simple planar cell and stack design that lends itself to automated mass production and allows straightforward thermal integration with air, exhaust, and fuel processing subsystems—necessary to produce a low-cost system module; and a system design that can be manufactured, operated, and maintained at low costs.

Each 1 kW system can be installed without any modifications as either a complete free-standing system, designed either for use individually, or as a “module,” which can be connected in parallel (in any number) for increased power—an approach which has the added benefits of redundancy. This “mass customization” approach reflects TMI’s overarching design philosophy: to engineer fuel cell systems that are simple to make, use, and maintain. A second benefit of designed simplicity is low capital and operating costs, as well as the ability to use existing regional infrastructure such as different fuel supply and common carriers for overnight delivery.

By using ordinary and simple—instead of custom and unique—component and subassembly designs, TMI has de-emphasized the need for invention necessary to implement inventions, a cost and technical conundrum faced by a number of other fuel cell developers. By maintaining simplicity and focusing on low cost from inception, TMI has not only expanded the range of viable component and systems options, but has left open the opportunity for multiple business collaborations.

Low manufacturing costs can be influenced by both product design and manufacturing processes. Over time, continued attention to these two factors guided by simplicity and lean manufacturing philosophies can result in reduced product costs and improved product quality.

PRODUCT DESIGN

Product design emphasizes simplicity and minimization. TMI module design concepts are already believed to be simpler than other known SOFC systems. An overall systems approach ensures costs are balanced with electrical, thermal, mechanical, manufacturing, control, and operational trade-offs. Throughout the product development process, emphasis is placed on: using a systems approach to design; stressing design simplicity and manufacturability; lowering costs through mechanized and automated module manufacturing; and maintaining high module fuel efficiency and low maintenance costs.

Radial Flow Single-Cell Design

Simplicity starts with the cell and stack designs. In the TMI SOFC stack design, fuel and oxidant are supplied through holes in the center of the cell and flow radially outward through the porous electrode pathways. Internal manifolding minimizes the seal perimeter area between the fuel and oxidant. At the circumference of the stack, the remaining fuel and excess oxidant react completely before exiting as exhaust. TMI’s cell, at a 56 mm diameter, is full commercial scale. These planar cells are stacked to achieve higher voltage and power. Multiple stacks can be used as power requirements increase. No precious materials are used.

Impurity Tolerance

The simple cell design, uniform symmetry, and unconstrained perimeter have also allowed the incorporation of a variety of novel and improved materials, such as sulfur-tolerant anodes, that are not feasible in many other designs. Under a Defense Advanced Research Projects Agency-sponsored program in 1994, TMI was one of the first companies to operate a complete sulfur-tolerant system (integrated reformer and stack) demonstrating operation of a total SOFC system without sulfur removal or fuel pretreatment. In addition, the TMI system is completely tolerant to ammonia contamination, as demonstrated under a recent U.S. Department of Agriculture project. Results from these and other previous TMI development programs indicate that the range of tested sulfur and ammonia tolerance will prevail over operating conditions that are required by the TMI SOFC system operating on many conventional and bio-based fuels.

MANUFACTURING PROCESSES

All manufacturing processes for parts and modules employed by TMI at commercial production volumes are expected to be highly automated and will utilize lean manufacturing techniques.

Automation, particularly in the fabrication of cell components and stacks, is necessary to produce consistent high quality and low costs. The small size of the components and the relatively simple nature of the required manufacturing steps will also minimize both the utility and capital usage requirements for manufacturing.

Relationship to Program

This project will support important advances within the SOFC Systems Development and Analysis area of the NETL Fuel Cells Program. Benefits from this project include the following:

- **Reduction of energy imports:** Each million systems will produce 17.5 billion kWh of electric power per year, primarily displacing power from natural gas turbines (used for marginal generation), which have an approximate average delivered residential efficiency of 30% lower heating value (LHV). The new systems, when integrated with cogeneration systems, will have an average energy efficiency of 90%. In 2006, natural gas imports were 16% of U.S. consumption. All of the resulting savings could reduce imports: a calculated total of 144 billion standard cubic feet/year (\$864 million/year at \$6.00/thousand cubic feet) per million fuel cell systems installed.
- **Reductions of energy emissions and greenhouse gases:** Major reductions in fossil carbon dioxide (CO₂) and nitrogen oxide (NO_x) emissions will result from deployment of the proposed systems. The cited reduction in natural gas consumption will reduce fossil CO₂ emissions by 7.6 million metric tons/year per million systems. The new systems will emit zero NO_x emissions, unlike gas turbines (average NO_x emissions rate from utility power generation is 0.98 g/kWh or 17,150 metric tons/year in the example).
- **Improvement of energy efficiency:** The projected annual average energy efficiency of the cogeneration systems is approximately 90% (LHV basis). The average efficiency of delivered grid power from coal and natural gas is close to 30%. The new systems offer much higher potential efficiency.
- **Technology leadership:** At the present time, major efforts are under way in Europe, Japan, and Australia to commercialize residential fuel cell cogeneration systems. TMI believes its technology can be more cost effective than other systems and become the world leader, with eventual manufacturing plants around the world. In the absence of a strong U.S. commitment, an expected market worth tens of billions of dollars per year will default to other countries.

Primary Project Goal

The primary goal of this project is to demonstrate a small-scale SOFC system outside TMI's laboratory that is capable of operating on multiple conventional and bio-based fuels. The test will provide a benchmark for the level of commercial readiness of the technology, particularly as related to use by America's rural end users and individuals who want more control over their power production and consumption.

Objectives

This program supports TMI's engineering development of a residential-scale prototype SOFC, capable of producing high-quality electricity from a wide range of carbonaceous fuels including both bio-based and traditional fossil fuels such as natural gas or clean coal gas. TMI estimates that the proposed system can reduce fuel consumption by approximately 50% compared to conventional reciprocating engine systems and proposes to validate these savings by empirical data. In addition, use of this technology operating on bio-based fuels can eliminate carbon emissions to the atmosphere associated with the power produced (equivalent to approximately 9.6 metric tons CO₂/kW/year as compared with power produced from a coal-fired power plant).

This demonstration is noteworthy because today there are essentially no practical alternatives for ordinary consumers to obtain their home electric energy from biofuel, a potentially attractive feature to some environmentally conscious consumers.

The project includes five tasks:

TASK 1 – PROJECT MANAGEMENT, PLANNING, AND REPORTING

TMI will maintain a Project Management Plan in accordance with the requirements of the DOE NETL. TMI shall coordinate and plan the project. TMI will submit all required documentation and work toward approval according to DOE guidelines.

TASK 2 – SITE SELECTION

A candidate test site will be selected based upon: owner/operator co-participation in the site preparation and demonstration of system; secured access to the site by TMI and other interested parties for test monitoring and public relations activities; and cooperation of local political entities regarding any necessary site permits or inspections. TMI will attempt to minimize any negative impact of the fuel cell and may ultimately select a secured site that is controlled but representative of a consumer residence. The focus is on demonstrating a unique value and proof of concept. To help identify these potential sites, TMI will engage various entities including consultants, advisors, and advocacy groups, particularly the Ohio Soybean Council and the Ohio Farm Bureau Foundation, with whom TMI has successfully interacted in the past.

TASK 3 – SYSTEM DESIGN AND FABRICATION

Two 1 kW systems will be fabricated based upon site selection and pre-existing engineering designs and options. The systems will accommodate both fossil and bio-based fuel operation. Two systems will provide redundancy and back up to ensure successful demonstration for the duration of the test.

Subtask 3.1 – System Engineering: The demonstration will inform engineering. For instance, electrically, the system may have to accommodate interfaces to the existing electrical system or specialized loads. Safety and security for the system, the host site and personnel, and the public utility will be paramount considerations. Grid parallel operation (isolated loads that do not automatically interconnect with the utility grid) is the operating mode of choice and minimizes the potential for unsafe operation. Mounting and system protections (filters, circuit breakers, etc.) will be considered. Fuel availability and storage must be determined and systems designed to accommodate operations.

Subtask 3.2 – System Fabrication/Assembly/Pre-Testing: Once designs have been determined, two TMI systems will be fabricated with the appropriate design changes. Changes may include alternative/replacement balance of plant components, including pumps, fans, compressors, and electronics; hot subassembly modifications; and overall packaging subsystems. Remote monitoring and control hardware will be added to the system to allow 24-hour monitoring for safety and engineering.

Subtask 3.3 – Testing on Site: The two test systems will be operated with electrical loads used to determine the performance and efficiency over a range of operating conditions. Set point testing will be conducted at 25%, 50%, 75%, and 100% of rated power. A user-defined load profile or simulated equivalent—such as those provided by the National Renewable Energy Laboratory In-My-Backyard tool—may also be used for evaluation. Control will be demonstrated via remote access. Extensive testing at TMI is expected to reduce risk to the final demonstration and will provide baseline data for further analysis.

TASK 4 – STACK FABRICATION

Approximately 12 kW equivalent of SOFC components and stacks will be produced for engineering studies, system development, and the demonstration. The stacks will represent the best technology at the time of construction and will ideally be suited for unattended operation and operation on multiple fuels.

TASK 5 – DEMONSTRATION

The testing period is expected to be approximately 30–90 days located at the site selected in Task 1. Upon test completion, after systems are decommissioned and removed, site reparations will be made as necessary to ensure return of the end-user facility to safe conditions.

Subtask 5.1 – Site Preparation: The demonstration site will be prepared to receive test systems. All changes will be made according to any local, state, or federal codes or standards. Any changes will be temporary so that they can be removed post test with minimal disruption.

Subtask 5.2 – Installation and Testing: Once the site has been prepared, the systems will be installed. Operation will begin and remote monitoring will be used to measure performance over time. Several conditions will be selected for test and changes will be made to simulate potential user electrical loads. Several fuels will be tested including biofuels and hydrocarbon fuels. Actual electrical loads will be connected and removed to simulate end-user activities.

Subtask 5.3 – Decommission and Reporting: After testing is complete, the system will be shut down and removed. The site will be returned to original conditions as agreed upon by the participants. Summaries will be provided to the funding organization as required by the program.

APPENDIX F: LIST OF ACRONYMS AND ABBREVIATIONS

Acronym or Abbreviation	Definition
°C	Degrees Celsius
A	ampere
AC	alternating current
AFM	atomic force microscopy
Ag	silver
ANL	Argonne National Laboratory
A&WMA	Air & Waste Management Association
Ar	argon
ASME	American Society of Mechanical Engineers
ASR	area-specific resistance
ASU	air separation unit
BRTD	ASME Board on Research and Technology Development
CAD	computer-aided design
CARES	Ceramics Analysis and Reliability Evaluation of Structures
CCC	Copyright Clearance Center
CCPI	Clean Coal Power Initiative
CCS	carbon capture and sequestration
Ce	cerium
CeO ₂	cerium oxide
CF	current flow
CFD	computational fluid dynamics
CH	chemical reactions
CH ₄	methane
cm	centimeter
CMU	Carnegie Mellon University
Co	cobalt
CO	carbon monoxide
CO ₂	carbon dioxide
COE	cost of electricity
Cr	chromium
CRTD	ASME Center for Research and Technology Development
CTE	coefficients of thermal expansion
DC	direct current
DCFC	direct carbon fuel cell
DG	degradation
DMFC	direct methanol fuel cells
DOE	U.S. Department of Energy
DSC	differential scanning calorimetry
EC	electrical conductivity
ECR	electrical conductivity relaxation
EDS	energy-dispersive X-ray spectroscopy

Acronym or Abbreviation	Definition
EIS	electrochemical impedance spectroscopy
EL	electrochemistry
EPRI	Electric Power Research Institute
eV	electron volt
FCE	FuelCell Energy, Inc.
FE	Office of Fossil Energy
FEA	finite element analysis
FF	fluid flow
FY	fiscal year
GC	gas chromatograph
Gen 3	Generation 3
Gen 3.2	Generation 3.2
Gen 4	Generation 4
GFED	gross fuel energy density
GT	gas turbine
H ₂	hydrogen
H ₂ O	water
H ₂ S	hydrogen sulfide
HHV	higher heating value
HID	helium ionization
HPC	high-performance cathode
HT	heat transfer
IGCC	integrated gasification combined cycle
IGFC	integrated gasification fuel cell
IPES	inverse photoemission spectroscopy
IP-SOFC	integrated planar solid oxide fuel cell
J	joules
K	Kelvin
kW	kilowatt
KPS	Kelvin probe spectroscopy
kWe	kilowatt-electric
kWh	kilowatt-hour
LaMnO ₃	lanthanum manganite
LAO	lanthanum aluminate
LC	lanthanum chromite
LHV	lower heating value
L-MBE	laser-molecular beam epitaxy
LNO	lanthanum nickel oxide
LSC	lanthanum strontium cobaltite
LSCF	lanthanum strontium cobalt ferrite
LSM	lanthanum strontium manganite
LSZF	zinc-doped lanthanum strontium ferrite
LTI	Leonardo Technologies, Inc.

Acronym or Abbreviation	Definition
M	molarity
mA	milliampere
MC	manganese cobalt
MCA	multi-cell array
MDU	module demonstration unit
m/e	mass/electron
MIT	Massachusetts Institute of Technology
Mn	manganese
mol	molar percent
MPC	multi-physics code
MPCA	Minnesota Pollution Control Agency
MS	mass spectrometer
mV	millivolt
MW	megawatt
MWe	megawatt-electric
NCCC	National Carbon Capture Center
NETL	National Energy Technology Laboratory
nm	nanometer
N ₂	nitrogen
NOC	normal operating conditions
NO _x	nitrogen oxides
NRC	National Research Council
O ₂	oxygen
OCC	Office of Clean Coal
OCV	open circuit voltage
OMB	Office of Management and Budget
ORNL	Oak Ridge National Laboratory
ORR	oxygen reduction reaction
PCM	proof-of-concept module
PF	porous flow
PI	principal investigator
PLD	pulsed laser deposition
PNNL	Pacific Northwest National Laboratory
pO ₂	partial pressure of oxygen
POC	proof of concept
ppm	parts per million
Pr ₂ NiO ₄	praseodymium nickel oxide
PSA	pressure swing adsorption
R&D	research and development
RD&D	research, development, and demonstration
RE	rare earth
RHEED	reflection high-energy electron diffraction
R _p	polarization resistance

Acronym or Abbreviation	Definition
RRFCS	Rolls-Royce Fuel Cell System
SDC	samarium-doped ceria
SECA	Solid State Energy Conversion Alliance
SEM	scanning electron microscopy
SOFC	solid oxide fuel cell
SOFC/GT/ST	solid oxide fuel cell / gas turbine / steam turbine
SO _x	sulfur oxides
Sr	strontium
SrMnO ₃	strontium manganite
ST	steam turbine
STM	scanning tunneling microscopy
STS	scanning tunneling spectroscopy
syngas	synthesis gas
TEM	transmission electron microscope/microscopy
TGA	thermogravimetric analysis
TMI	Technology Management, Inc.
TPB	triple-phase boundary
TRXF	total reflection X-ray fluorescence
TSC	tape casting / screen printing / co-firing process
UNLV	University of Nevada, Las Vegas
UPS	ultraviolet photoelectron spectroscopy
V	volts
VPS	Versa Power Systems, Inc.
W	watt
XAS	X-ray absorption spectroscopy
XES	X-ray emission spectroscopy
XPS	X-ray photoelectron spectroscopy
XRD	X-ray diffraction
XRF	X-ray fluorescence
Y	yttrium
Y ₂ O ₃	yttrium-oxide
YDC	yttrium-doped ceria
YSZ	yttria-stabilized zirconia
Zr	zirconium