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Final Report
Strategic Center for Coal
Advanced Fuels
FY2011 Peer Review Meeting

Meeting Summary and Recommendations Report

Morgantown, West Virginia
October 18–22, 2010

U.S. DEPARTMENT OF ENERGY
OFFICE OF FOSSIL ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY

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FINAL REPORT
STRATEGIC CENTER FOR COAL ADVANCED FUELS FY 2011 PEER REVIEW MEETING

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MEETING SUMMARY AND RECOMMENDATIONS REPORT

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MEETING SUMMARY AND RECOMMENDATIONS REPORT

EXECUTIVE SUMMARY

The mission of the U.S. Department of Energy's (DOE) Office of Clean Coal (OCC) is to ensure the availability of ultra-clean, 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 Advanced Fuels Technology Program—is the subject of this report.

The Advanced Fuels Program consists of a portfolio of laboratory and field research, development, and demonstration projects focused on technologies that will advance the production of power, hydrogen, synthetic fuels, and chemicals produced primarily from coal. The program was redirected in fiscal year 2010 (FY 2010) to address co-production/polygeneration and to pursue potential benefits for power applications that include the reduced cost of electricity, improved efficiency, and reduced cost of carbon capture and storage. The existing project portfolio incorporates projects that focus on power, hydrogen, and fuels production as well as projects related to alternate production, utilization, and delivery that were implemented prior to the current program direction.

The Advanced Fuels Program goals include the following:

- Prove the feasibility of a 40 percent efficient, near-zero emissions power facility that uses membrane separation technology as well as other advanced technologies to reduce the cost of electricity by at least 35 percent (relative to a base case integrated gasification and combined cycle plant [IGCC] with carbon capture and storage [CCS] using currently available technologies).
- Develop hydrogen production and processing technologies that will contribute approximately 2.9 percent in improved efficiency and 12 percent reduction in cost of electricity to the 40 percent efficient near-zero emissions power facility.

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 FY 2011 Advanced Fuels 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 seven leading academic and industry experts on October 18–22, 2010, to conduct a five-day Peer Review of selected Advanced Fuels Program research projects supported by NETL.

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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.

Overview of Office of Fossil Energy Advanced Fuels Program Research Funding

The total funding of the 19 projects reviewed, over the duration of the projects, is $85,300,962. Of this amount, $65,063,111 (76.3%) is funded by DOE, while the remaining $20,237,851 (23.7%) is funded by project partner cost sharing.

The 19 projects that were the subject of this Peer Review are summarized in Table ES-1 and in Section II of this report.

TABLE ES-1 ADVANCED FUELS PROJECTS REVIEWED

Reference Number	Project No.	Title	Lead Organization	Principal Investigator	Total Funding*		Project Duration*	
					DOE	Cost Share	From	To
01	DE-FE0004001.410.01.22	Analysis of Coal to Hydrogen Systems	NETL Office of Systems, Analyses, and Planning-Systems Division	Larry Rath	$570,000	$0	10/30/2007	10/31/2010
02	FC26-05NT42469	Scale-Up of Hydrogen Transport Membranes for IGCC and FutureGen Plants	Eltron Research & Development Inc.	Carl Evenson	$11,170,312	$2,792,588	10/1/2005	6/30/2012
03	DE-FE0004908	Advanced Hydrogen Transport Membranes for Coal Gasification	Praxair	Joseph Schwartz	$1,500,722	$643,167	9/15/2010	12/15/2011
04	FC26-07NT43058	Composite Pd and Alloy Porous Stainless Steel Membranes for Hydrogen Production and Process Intensification	Worcester Polytechnic Institute	Yi Hua Ma	$1,756,444	$472,406	5/7/2007	5/6/2011
05	DE-FE0004967	Advanced Palladium Membrane Scale-Up for Hydrogen Separation	United Technologies Research Center	Sean Emerson	$1,492,188	$373,047	9/1/2010	11/30/2011
06	FY10.MSE.1610884.663	Coal & Biomass Derived Fuels	NETL Office of Research and Development – Chemistry & Surface Science Division	Bryan Morreale	$1,989,000	$0	10/1/2010	9/30/2011
07	FWP-49601	Development of Dense Ceramic Membranes for Hydrogen Separation	Argonne National Laboratory	U. (Balu) Balachandran	$400,000	$0	10/1/2009	9/30/2010
08	DE-FE0000507	Demonstration of Pressurizing Coal/Biomass Mixtures Using Posimetric Solids Pump Technology	GE Global Research	Tiffany Westendorf	$622,316	$485,993	8/7/2009	8/6/2011
09	FC26-05NT42465 DE-FC0003466	National Center for Hydrogen Technology	University of North Dakota	Michael Holmes	$15,984,970	$7,558,338	6/23/2005	5/31/2011
10	DE-FE0001009	Nanoporous, Metal Carbide, Surface Diffusion Membranes for High Temperature Hydrogen Separations	Colorado School of Mines	J. Douglas Way	$998,543	$250,628	10/1/2009	9/30/2012
11	DE-FE0001293	Integrated Water Gas Shift Membrane Reactor Utilizing Novel, Non-Precious Metal Mixed Matrix Membranes	The University of Texas at Dallas	John Ferraris	$1,000,000	$250,000	9/30/2009	9/30/2012
12	FC26-05NT42456	Production and Storage of Hydrogen from Coal Using C1 Chemistry	University of Kentucky – Consortium for Fossil Fuel Science	Gerald Huffman	$6,087,605	$1,522,020	6/2/2005	9/30/2011

Reference Number	Project No.	Title	Lead Organization	Principal Investigator	Total Funding*		Project Duration*	
					DOE	Cost Share	From	To
13	DE-FE0001248	Yeager Airport Hydrogen Vehicle Test Project	West Virginia University Research Corporation	William Davis	$812,960	$406,692	10/1/2009	9/30/2012
14	FC26-08NT0005988	Design and Construction of Early Lead Mini Fischer-Tropsch Refinery	University of Kentucky – Center for Applied Energy Research	Rodney Andrews	$4,568,940	$1,166,067	8/06/2008	3/10/2013
15	FC26-06NT42449	Production of High-Hydrogen Content Coal-Derived Liquids	Integrated Concepts and Research Corporation	Steve Bergin	$2,779,168	$698,326	3/30/2006	3/30/2011
16	FC26-06NT42761	Enhanced Hydrogen Economics Via Co-Production of Fuels and Carbon Products	West Virginia University	Elliot Kennel	$2,633,728	$890,644	4/1/2006	12/31/2010
17	DE-FE0000435	Methanol Economy	University of Southern California	George Olah	$1,826,970	$456,743	9/30/2009	9/30/2012
18	DE-FC26-05NT42457 DE-FE0000699	Continuation of Crosscutting Technology Development of CAST	Virginia Polytechnic Institute and State University and University of Kentucky Research Foundation	Roe-Hoan Yoon and Rick Honaker	$5,710,524	$1,427,631	5/12/2005	9/30/2011
19	FC26-06NT42804	Long-Term Environmental and Economic Impacts of Coal Liquefaction in China	West Virginia University	Jerald J. Fletcher	$3,158,721	$843,561	8/15/2006	12/31/2012
				TOTALS	$65,063,111	$20,237,851		

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

NETL ADVANCED FUELS PROGRAM OVERVIEW

A primary focus of the Advanced Fuels Program is to reduce technology barriers for the reliable, efficient, and environmentally friendly conversion of coal to hydrogen for utilization in advanced IGCC systems. Hydrogen has the potential to play a significant role in the nation's energy future, particularly for the production of clean electric power from coal. Production and use of hydrogen in a gasification combined cycle system for stationary power applications will complement the development of next-generation hydrogen turbine technology that enables the plant to achieve near-zero pollutant emissions and increased plant efficiency.

Efforts for hydrogen production focus on generation at the plant for large-scale, central power applications. A major research and development element of the program is the development and demonstration of hydrogen separation membranes which simultaneously produce a high-purity hydrogen product and isolate a high-pressure, high-purity CO_2 stream. Recent systems analyses at NETL have indicated that hydrogen separation membranes, when coupled with warm gas cleanup, have the potential to significantly increase power production efficiency in advanced coal gasification based power generation with carbon capture and storage.[1]

The goals of the Advanced Fuels Program research, development, and demonstration activities include the following:

- Prove the feasibility of a 40 percent efficient, near-zero emissions power facility that uses membrane separation technology as well as other advanced technologies to reduce the cost of electricity by at least 35 percent (relative to a base case IGCC plant with CCS using currently available technologies).
- Develop hydrogen production and processing technologies that will contribute approximately 2.9 percent in improved efficiency and 12 percent reduction in cost of electricity to the 40 percent efficient near-zero emissions power facility.[2]

The redirected Advanced Fuels Program is focused on the development of the following technologies:

- **Hydrogen from Coal Research** – This element of the portfolio focuses on technologies to facilitate separation and purification of ultra-high-purity hydrogen derived from coal for stationary electric power applications. When combined with CCS, these next-generation power plants will achieve significant reductions in greenhouse gas emissions with lower electricity costs compared to current technologies.
- **Coal and Biomass to Liquids Research** – This element of the program addresses advanced and novel technologies that ensure the use of our nation's abundant coal (and biomass) resources to co-produce affordable power, fuels, and chemicals in a safe and environmentally clean manner. The program sponsors research and development projects that address key challenges related to the utilization of coal-biomass mixtures.

In FY 2011, the Advanced Fuels Program continues to support bench-scale development of hydrogen separation technologies that are capable of performing multiple reactions and separation processes (process intensification)—including non-precious metal hydrogen separation membranes—along with the computational science and systems analysis to support technology development. The Advanced Fuels Program also continues to address key technology issues in co-feeding of coal and biomass mixtures in co-production concepts. Current activities in the coal/biomass area are fully funded with FY 2010 and prior year funds; ongoing research activities in prior related areas will be completed.

Efforts are focused on the research and development required to provide technologies for hydrogen production and for co-production of electricity and fuels from coal and biomass. The following challenges must be overcome to achieve each element's objectives and program goals: (1) reduce capital and operating costs; (2) address scale-up concerns; (3) intensify processes; and (4) overcome impurities.

1. Kristin Gerdes, David Gray, and others, National Energy Technology Laboratory and Noblis, Current and Future Technologies for Gasification-Based Power Generation, Volume 2: A Pathway Study Focused on Carbon Capture Advanced Power Systems R&D Using Bituminous Coal, Revision 1, (Washington, D.C.: U.S. Department of Energy, November 2010).

2. U.S. Department of Energy, Office of Fossil Energy, National Energy Technology Laboratory, *Hydrogen from Coal Program Research, Development, and Demonstration Plan*, (Washington, D.C.: U.S. Department of Energy, September 2010), http://www.netl.doe.gov/technologies/hydrogen_clean_fuels/refshelf/pubs/20100908_Draft_H2fromCoal%20RDD_final.pdf.

Overview of the Peer Review Process

NETL requested that ASME assemble an Advanced Fuels 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 60-minute PowerPoint presentation that was followed by a 30-minute question-and-answer session with the Panel. After the principal investigator and project team left the room, the Panel had a 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 contract support staff.

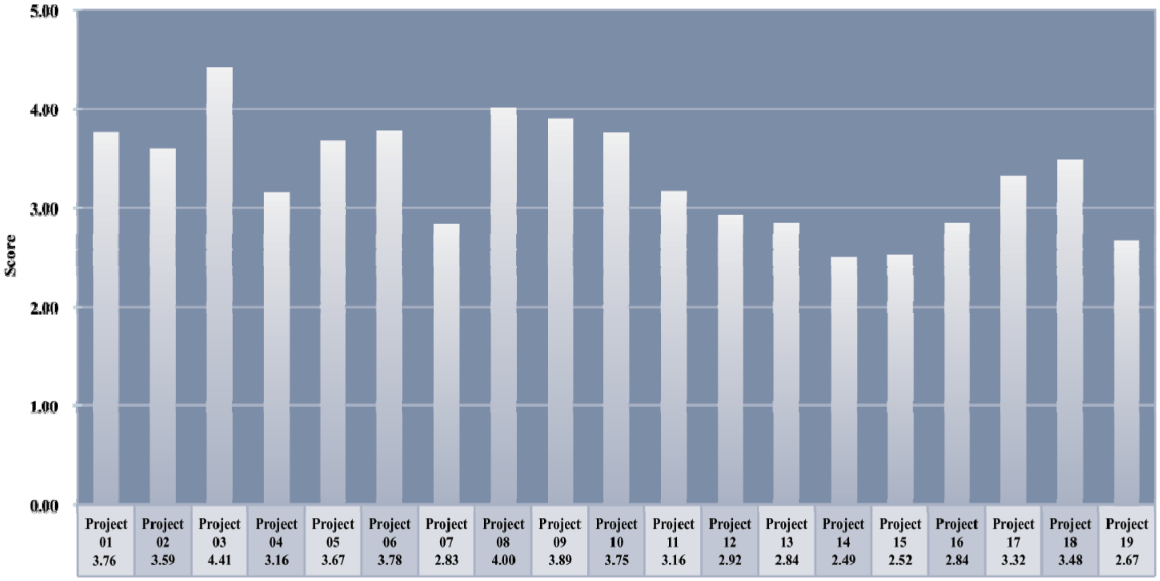
After the group discussions, each Panel member individually evaluated the 19 projects, providing written comments based on a predetermined set of review criteria. For each of the nine review criteria, the individual reviewer was asked to score the project as one of the following:

- 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 19 projects.

FIGURE ES-2 **AVERAGE SCORING, BY PROJECT**



The “Project Average” in Table ES-3 shows the score for each criterion averaged across all 19 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 ES-3 AVERAGE SCORING, BY REVIEW CRITERION

Criterion	Project Average	Highest Project Rating*	Lowest Project Rating
1. Scientific and Technical Merit	3.5	4.6	2.4
2. Existence of Clear, Measurable Milestones	3.4	4.7	2.6
3. Utilization of Government Resources	3.5	4.4	2.3
4. Technical Approach	3.4	4.7	2.1
5. Rate of Progress	3.4	4.0	2.4
6. Potential Technology Risks Considered	3.2	4.4	2.4
7. Performance and Economic Factors	2.9	4.3	2.0
8. Anticipated Benefits, if Successful	3.5	4.4	2.4
9. Technology Development Pathways	3.2	4.6	2.3

* 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 Path 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 **not applicable in this peer review*	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.

I. INTRODUCTION

In fiscal year 2011, the American Society of Mechanical Engineers (ASME) was requested to provide an independent, unbiased, and timely peer review of selected projects within the U.S. Department of Energy (DOE) Office of Fossil Energy Advanced Fuels Program (administered by the Office of Fossil Energy's National Energy Technology Laboratory [NETL]). On October 18–22, 2010, ASME convened a panel of seven leading academic and industry experts to conduct a five-day peer review of selected Advanced Fuels 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 Advanced Fuels 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 Advanced Fuels 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 19 Advanced Fuels Program projects. ASME performed this project review work as a subcontractor to prime NETL contractor Leonardo Technologies, Inc. NETL selected the 19 projects, while ASME organized an independent review panel of seven leading academic and industry experts. Prior to the meeting, project PIs submitted an 11-page written summary (Project Information Form) of their project's purpose, objectives, and progress. The PI's also submitted their PowerPoint presentations to the Panel prior to the meeting. 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 60-minute oral presentation, followed by a 30-minute question-and-answer (Q&A) session with the Panel and a 40-minute Panel discussion of each project. The length of the presentation and Q&A session was primarily a function of the perceived time requirement 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 Advanced Fuels Program research, ASME decided that both the PI presentations and Q&A sessions with the Panel for the Advanced Fuels Peer Review were to be 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. Each member of the Panel individually evaluated the project and provided written comments based on a predetermined set of review criteria. Panel members were also instructed to hold the discussions that took place during the Q&A session as confidential.

This publically available document, prepared by ASME, provides a general overview of the Advanced Fuels 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 Advanced Fuels Peer Review Meeting, organized as follows:

II. *Summary of Projects Reviewed in FY2011 Advanced Fuels Peer Review*:

A list of the 19 projects reviewed and the selection criteria

III. *An Overview of the Evaluation Scores*:

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 ADVANCED FUELS PEER REVIEW

NETL selected key projects within the Advanced Fuels 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: DE-FE0004001.410.01.22
Analysis of Coal to Hydrogen Systems
NETL Office of Systems, Analyses, and Planning-Systems Division

02: FC26-05NT42469
Scale-Up of Hydrogen Transport Membranes for IGCC and FutureGen Plants
Eltron Research & Development Inc.

03: DE-FE0004908
Advanced Hydrogen Transport Membranes for Coal Gasification
Praxair

04: FC26-07NT43058
Composite Pd and Alloy Porous Stainless Steel Membranes for Hydrogen Production and Process Intensification
Worcester Polytechnic Institute

05: DE-FE0004967
Advanced Palladium Membrane Scale-Up for Hydrogen Separation
United Technologies Research Center

06: FY10.MSE.1610884.663
Coal & Biomass Derived Fuels
NETL Office of Research and Development – Chemistry & Surface Science Division

07: FWP-49601
Development of Dense Ceramic Membranes for Hydrogen Separation
Argonne National Laboratory

08: DE-FE0000507
Demonstration of Pressurizing Coal/Biomass Mixtures Using Posimetric Solids Pump Technology
GE Global Research

09: FC26-05NT42465, DE-FC0003466
National Center for Hydrogen Technology
University of North Dakota

10: DE-FE0001009
Nanoporous, Metal Carbide, Surface Diffusion Membranes for High Temperature Hydrogen Separations
Colorado School of Mines

11: DE-FE0001293
Integrated Water Gas Shift Membrane Reactor Utilizing Novel, Non-Precious Metal Mixed Matrix Membranes
The University of Texas at Dallas

12: FC26-05NT42456
Production and Storage of Hydrogen from Coal Using C1 Chemistry
University of Kentucky – Consortium for Fossil Fuel Science

13: DE-FE0001248
Yeager Airport Hydrogen Vehicle Project
West Virginia University Research Corporation

14: FC26-08NT0005988
Design and Construction of Early Lead Mini Fischer-Tropsch Refinery
University of Kentucky – Center for Applied Energy Research

15: FC26-06NT42449
Production of High-Hydrogen Content Coal-Derived Liquids
Integrated Concepts and Research Corporation, Subsidiary of VSE Corp.

16: FC26-06NT42761
Enhanced Hydrogen Economics Via Co-Production of Fuels and Carbon Products
West Virginia University

17: DE-FE0000435
Methanol Economy
University of Southern California

18: DE-FC26-05NT42457, DE-FE0000699
Continuation of Crosscutting Technology Development of CAST
Virginia Polytechnic Institute and State University, University of Kentucky Research Foundation

19: FC26-06NT42804
Long-Term Environmental and Economic Impacts of Coal Liquefaction in China
West Virginia University

III. AN OVERVIEW OF THE EVALUATION SCORES FOR THE ADVANCED FUELS PROGRAM

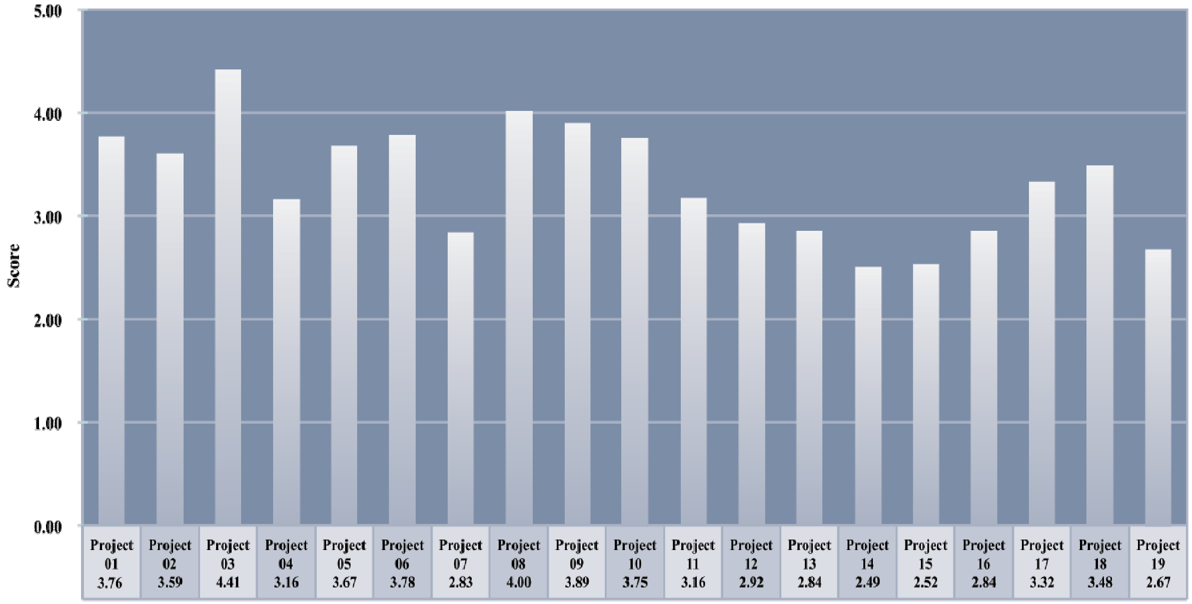
For each of the nine review criteria, individual reviewers were asked to score the project as one of the following:

- 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 Advanced Fuels 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 advanced fuels industry.

Figure 1 shows the average project scores, combining the average of the nine review criteria for each of the 19 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. Twelve of the nineteen projects reviewed from the Advanced Fuels 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. Seven of the nineteen projects fit within this category.

FIGURE 1 **AVERAGE SCORING, BY PROJECT**



General conclusions about the Advanced Fuels Program can also be drawn by looking at the average scores for each of the nine review criteria, which are shown in Table 1. All of the criteria received average scores between 2.9 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 Performance and Economic Factors, indicating that several projects did not provide sufficient cost estimates directed toward achieving DOE's technology cost goals. The highest-ranking review criteria, Scientific and Technical Merit, Utilization of Government Resources, and Anticipated Benefits, if Successful, earned average scores across all projects of 3.5, 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.

TABLE 1 AVERAGE SCORING, BY REVIEW CRITERION

Criterion	Project Average	Highest Project Rating*	Lowest Project Rating
1. Scientific and Technical Merit	3.5	4.6	2.4
2. Existence of Clear, Measurable Milestones	3.4	4.7	2.6
3. Utilization of Government Resources	3.5	4.4	2.3
4. Technical Approach	3.4	4.7	2.1
5. Rate of Progress	3.4	4.0	2.4
6. Potential Technology Risks Considered	3.2	4.4	2.4
7. Performance and Economic Factors	2.9	4.3	2.0
8. Anticipated Benefits, if Successful	3.5	4.4	2.4
9. Technology Development Pathways	3.2	4.6	2.3

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

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 19 projects evaluated at the Advanced Fuels Peer Review.

General Project Strengths

The Panel indicated that almost two-thirds of projects were sound, commending DOE for presenting a high-quality, diverse portfolio of projects with ambitious objectives and significant potential to advance hydrogen and clean fuels technology. Table I reflects the spread of average scores across all 19 projects among the nine criteria. All of the criteria received averages ranging from 3.2 to 3.5, except for Performance and Economic Factors, which received an average of 2.9. This indicates that, overall, the Advanced Fuels Program projects that were reviewed ranked above “adequate” in all but one criterion area, but did not receive outstanding ratings in any particular criterion.

As mentioned in Section III, the Program projects reviewed were rated the highest in the Scientific and Technical Merit, Utilization of Government Resources, and Anticipated Benefits, if Successful criteria, which earned average scores across all projects of 3.5. This reflects the Panel’s perception that, overall, the projects were based on sound science and adequately leveraged available resources to take on relevant R&D initiatives that, if successful, could contribute to achieving DOE objectives.

In general, the Panel was impressed with the breadth of the projects and the expertise of the researchers in the Advanced Fuels Program. In particular, the Panel commended the excellent in-house resources of DOE/NETL. The Panel also commended the work on hydrogen transport membranes, the expertise and quality of the people working on the projects in this area, and the relevance of such projects to DOE goals.

The highest-rated project was Project 3, “Advanced Hydrogen Transport Membranes for Coal Gasification,” conducted by Praxair, which received an average rating across the nine criteria of 4.4 out of 5.0. Project 8, “Demonstration of Pressurizing Coal/Biomass Mixtures Using Posimetric Solids Pumps”, conducted by GE Global Energy, ranked second, receiving an average rating of 4.0. These projects were commended by the Panel for the progress they have made toward advancing technology with respect to hydrogen membranes and coal/biomass fuels, which was largely attributed to strong principal investigators and project teams. These projects were also praised for effectively maintaining focus on activities and technology development pathways that are aligned with industry needs and NETL program objectives.

Project 6, “Coal & Biomass Derived Fuels”, conducted by NETL’s Office of R&D Chemistry and Surface Division; Project 9, “National Center for Hydrogen Technology” conducted by University of North Dakota; and Project 10, “Nanoporous, Metal Carbide, Surface Diffusion Membranes for High Temperature Hydrogen Separation,” conducted by the Colorado School of Mines, received scores close to 4.0 (3.8, 3.9 and 3.8 respectively). The Panel also cited the principal investigators and project teams and sound technical approaches as strengths of these projects.

General Project Weaknesses

The projects evaluated in the Advanced Fuels Program underperformed in Performance and Economic Factors, which averaged 2.9 across all the projects and was the lowest-scoring criterion. Two other criteria, Potential Technology Risks and Technology Development Pathways received scores of 3.2. The scores in these three areas indicate that the Panel found that the project teams of the Advanced Fuels Program did not sufficiently identify and consider the economics, risks, and commercial viability of their technologies.

The Panel noted that the issues related to the three criteria above may be due to many of the projects being in the fundamental and applied research stages of technology development. Accordingly, some project teams had difficulty addressing more practical considerations such as cost, risk, and commercial feasibility that become increasingly important as research progresses to prototype testing and proof-of-concept efforts.

Another recurring issue that arose during the Advanced Fuels Peer Review was the lack of attention paid to conducting tests under conditions that could advance technologies toward achieving DOE Program goals. For example, one project tested its technology using natural gas, when the DOE Program is focused on advancements in hydrogen production from coal. Most of the projects did not consider the DOE cost and performance goals related to carbon dioxide (CO_2) capture, which is intricately tied to the hydrogen production process, and failed to set targets for CO_2 purity in process streams. While the Advanced Fuels Program is not a formal CO_2 mitigation program, researchers should consider the need to reduce CO_2 and other emissions to address environmental concerns.

Lastly, the Panel found that multiple projects did not adequately define milestones and project goals; and the project goals often did not correspond to NETL's cost performance goals in the Advanced Fuels Program. The Panel observed that some of the projects had too broad a scope and/or tasks that were unrelated to each other; these projects did not clearly direct tasks toward helping DOE to achieve its program objectives. In such cases, this approach spread resources too thin when greater benefit would be achieved by focusing only on key tasks that had the most potential for success and which were aligned with DOE objectives.

Issues for Future Consideration

While many 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 first relates to the operating conditions of the tests that project teams performed, which sometimes did not seem relevant to DOE goals. The Panel emphasized the importance of understanding and, to the extent possible, testing under experimental and commercial conditions that will advance DOE Program goals of achieving a 40 percent efficient, near-zero emissions power facility. The Panel noted that several projects failed to consider the applicability of the project technology to CO_2 capture, an important DOE goal related to hydrogen production. Other projects did not test nor had plans to test their technologies under real-world conditions (i.e., gas streams with trace contaminants that are likely to be present in coal-based systems). NETL has recognized this issue as it relates to testing of hydrogen separation membranes, and has developed and published a "Hydrogen Separation Membrane Test Protocol" that defines test conditions and objectives that are directly relevant to syngas derived from coal gasification. NETL's intent is to have all contractors developing separation processes use this protocol, and has incorporated the protocol in the requirements for solicitations released in FY 2010.[2] While the Panel acknowledged that some of the more fundamental and applied research projects were making innovative technological advancements, they also indicated that the project teams should put greater emphasis on how their efforts will help DOE achieve its cost targets (35% cost of electricity reduction and 40% plant efficiency in an IGCC facility with CO_2 capture) and the specific benefits the technology would provide toward achieving the targets. NETL systems analysis reports are intended to provide this guidance and a framework for project analyses.[3]

Secondly, project teams, even those that are conducting more fundamental research, should devote more effort to practical considerations surrounding the cost of hydrogen production and technology risks. Teams need to perform analyses that assess the economic performance of a project in comparison to other technologies to ultimately determine the technology development pathways that have the strongest potential for success.

Lastly, as noted above, the Panel recommends that projects clearly distinguish project activities from project objectives and that the tasks be integrated and aligned with overall Program goals. Project teams should describe project objectives in terms of their relationship with and contribution to cost performance goals in NETL's Advanced Fuels Program.

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[2] National Energy Technology Laboratory, *NETL Test Protocol – Testing of Hydrogen Separation Membranes*, DOE/NETL 2008/1335, (Washington, D.C.: U.S. Department of Energy, October 2008), http://www.netl.doe.gov/technologies/hydrogen_clean_fuels/refshelf/pubs/Membrane%20test%20protocol%20v10_2008_final10092008.pdf.

[3] Kristin Gerdes, David Gray, and others, National Energy Technology Laboratory and Noblis, Current and Future Technologies for Gasification-Based Power Generation, Volume 2: A Pathway Study Focused on Carbon Capture Advanced Power Systems R&D Using Bituminous Coal, Revision 1, (Washington, D.C.: U.S. Department of Energy, November 2010).

V. PROCESS CONSIDERATIONS FOR FUTURE PEER REVIEWS

The Panel and DOE/NETL managers involved in the Advanced Fuels 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 requires little or no modification to remain effective. There was high praise for the facilitation and organization of the meeting and the setup of the room, particularly the size of the reviewers' table. The Panel members appreciated the early availability of the project requirements on the SharePoint site, as it gave them ample time prior to the Peer Review Meeting to read the project information documents. The Panel members also found the reminders that were sent out when new documents were uploaded to the site to be helpful. The Panel 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.

The Panel was impressed by the breadth and quality of activities and technologies included in the selected projects. They saw the detailed level of answers to their questions to presenters as a positive reflection of the improved level of principal investigator (PI) involvement in the projects. 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 them to provide more accurate feedback on a specific project. To create even greater context, the Panel suggested that if prior reviews have been conducted on the projects under review, it would be helpful for the PI to provide the results of that review and indicate the progress that has been made since then.

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 and hurting the process. Some reviewers found the 15-minute break between projects to be too short; they preferred to record their comments when the presentation is still fresh in their minds, but also needed time to take an actual break. The Panel suggested lengthening the breaks to 20 minutes between projects as a way to address this issue, while accepting that this might mean they would need to begin the day slightly earlier or finish slightly later, with a preference toward starting earlier.

The Panel also commented on the order of the projects, noting that they would have preferred the congressionally-directed projects (CDPs) to be spread out, rather than lumped together at the end of the meeting. The reviewers found that these projects often contained many distinct components, making the presentations lengthier and more complex. As a result, the Panel recommended that these projects be spread throughout the week of the meeting, so that the reviewers can provide as much useful feedback as possible.

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 number of slides was deemed manageable overall, but 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 make a clear statement of the project's contributions to the state of the art and DOE program goals in order to help the Panel better evaluate the ambitiousness of the project.

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 noted that the inclusion of the block flow diagram that showed the project's technology as part of a larger plant system was particularly helpful when provided and that it should be included in all presentations in the future. In addition, the Panel recommended that DOE/NETL impress upon presenters that they need to communicate how their project is addressing CO_2 capture, and that the presenter of a more technologically comprehensive fundamental research project should understand the commercial application for the research.

In addition to improving communication with the PIs, the Panel also recommended that DOE/NETL ensure that CDP presentations focus more on the areas where the Panel's recommendations can make a difference. Some reviewers also suggested that DOE/NETL provide a brief three- to five-minute description of the project in the context of the program before each presentation to provide clarifying background information on the project from the beginning.

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 led to differences in ratings among Panel members. The ability to view preliminary project ratings during the Panel discussion session was cited as helpful for identifying and mitigating these differences in criteria interpretation among individual Panel members. The Panel also found it difficult to assess certain CDPs and provide useful recommendations, due to the projects' complexity and the fact that the direction of many aspects of these projects had already been determined.

One potential improvement to the evaluation process suggested by the Panel is including a way to assess how projects are leveraging other NETL activities in the Office of Clean Coal, which increases the project's value to the Advanced Fuels Program. The Panel also had suggestions for improving the wording of the criteria itself. Instead of "Existence of Clear, Measurable Milestones," the Panel would like to rename the category "Clear, Measurable, and Appropriate Milestones" as an added measure to ensure that the project's milestones are useful in determining progress rather than simply activity for the project. Also, the Panel recommended changing “Potential Technology Risks Considered” to “Potential Technology Challenges Considered” to avoid differing interpretations of the term “risk.”

Review Panel

The Panel noticed that the diverse areas of the Panel members’ expertise offered other members needed insight on various topics during discussion, providing more accurate and comprehensive ratings and comments that will help NETL obtain the maximum value possible from the projects. The Panel enjoyed the learning experience and camaraderie of collaborating with their colleagues in the advanced fuels field and thanked ASME and DOE for the opportunity to participate in this Peer Review.

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 U.S. Department of Energy (DOE)/National Energy Technology Laboratory (NETL) FY 2011 Advanced Fuels 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 effectively plan and manage ASME's collaborative research activities 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.

Advanced Fuels 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 FY 2011 Advanced Fuels 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.

Advanced Fuels Peer Review Panel

The Advanced Fuels Peer Review Executive Committee accepted résumés for proposed Advanced Fuels 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 a seven-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 objectives, 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 Advanced Fuels Peer Review Meeting, presenters were held to a specific time limit (ranging from 45 to 60 minutes) to allow sufficient time for all presentations within the five-day meeting period. After each presentation, the project team participated in a 30-minute question-and-answer session with the Panel.

The Panel then spent 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:

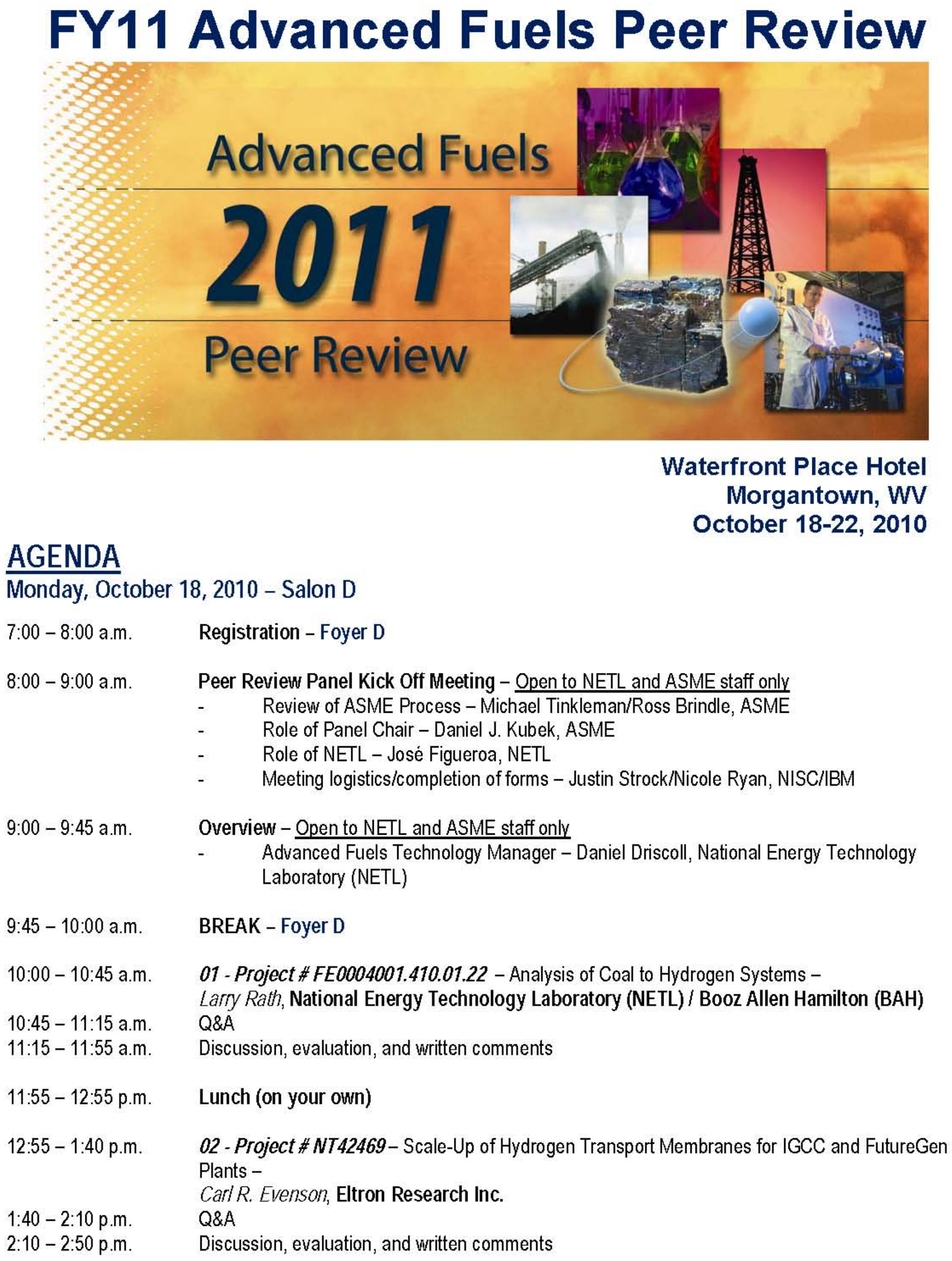
- Scientific and Technical Merit
- Existence of Clear, Measurable Milestones
- Utilization of Government Resources
- Technical Approach
- Rate of Progress
- Potential Technology Risks Considered
- Performance and Economic Factors
- Anticipated Benefits if Successful
- Technology Development Pathways

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 Advanced Fuels Peer Review

Waterfront Place Hotel
Morgantown, WV
October 18-22, 2010

AGENDA

Monday, October 18, 2010 – Salon D

7:00 – 8:00 a.m.	**Registration – Foyer D**
8:00 – 9:00 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 – Daniel J. Kubek, ASME - Role of NETL – José Figueroa, NETL - Meeting logistics/completion of forms – Justin Strock/Nicole Ryan, NISC/IBM
9:00 – 9:45 a.m.	**Overview –** Open to NETL and ASME staff only - Advanced Fuels Technology Manager – Daniel Driscoll, National Energy Technology Laboratory (NETL)
9:45 – 10:00 a.m.	**BREAK – Foyer D**
10:00 – 10:45 a.m.	***01 - Project # FE0004001.410.01.22*** – Analysis of Coal to Hydrogen Systems – *Larry Rath*, **National Energy Technology Laboratory (NETL) / Booz Allen Hamilton (BAH)**
10:45 – 11:15 a.m.	Q&A
11:15 – 11:55 a.m.	Discussion, evaluation, and written comments
11:55 – 12:55 p.m.	**Lunch (on your own)**
12:55 – 1:40 p.m.	***02 - Project # NT42469*** – Scale-Up of Hydrogen Transport Membranes for IGCC and FutureGen Plants – *Carl R. Evenson*, **Eltron Research Inc.**
1:40 – 2:10 p.m.	Q&A
2:10 – 2:50 p.m.	Discussion, evaluation, and written comments

Monday, October 18, 2010 – Salon D

2:50 – 3:05 p.m.	**BREAK** – **Foyer D**
3:05 – 3:50 p.m.	***03 - Project # FE0004908*** – Advanced Hydrogen Transport Membranes for Coal Gasification – *Joseph Schwartz*, **Praxair**
3:50 – 4:20 p.m.	Q&A
4:20 – 5:00 p.m.	Discussion, evaluation, and written comments
5:00 – 5:15 p.m.	**BREAK** – **Foyer D**
5:15 – 6:00 p.m.	***04 - Project # NT43058*** – Composite Pd and Alloy Porous Stainless Steel Membranes for Hydrogen Production and Process Intensification – *Yi Hua Ma*, **Worcester Polytechnic Institute (WPI)**
6:00 – 6:30 p.m.	Q&A
6:30 – 7:10 p.m.	Discussion, evaluation, and written comments

Tuesday, October 19, 2010 – Salon D

7:00 – 8:00 a.m.	**Registration** – **Foyer D**
8:00 – 8:45 a.m.	***05 - Project # FE0004967*** – Advanced Palladium Membrane Scale-up for Hydrogen Separation – *Sean C. Emerson*, **United Technologies Research Center (UTRC)**
8:45 – 9:15 a.m.	Q&A
9:15 – 9:55 a.m.	Discussion, evaluation, and written comments
9:55 – 10:10 a.m.	**BREAK** – **Foyer D**
10:10 – 10:55 a.m.	***06 - Project # FY10.MSE.1610884.663*** – Coal & Biomass Derived Fuels – *Charles E. Taylor*, **National Energy Technology Laboratory (NETL)**
10:55 – 11:25 a.m.	Q&A
11:25 – 12:05 p.m.	Discussion, evaluation, and written comments
12:05 – 1:05 p.m.	**Lunch (on your own)**
1:05 – 1:50 p.m.	***07 - Project # FWP-49601*** – Development of Dense Ceramic Membranes for Hydrogen Separation – *U. (Balu) Balachandran*, **Argonne National Laboratory (ANL)**
1:50 – 2:20 p.m.	Q&A
2:20 – 3:00 p.m.	Discussion, evaluation, and written comments
3:00 – 3:15 p.m.	**BREAK** – **Foyer D**
3:15 – 4:00 p.m.	***08 - Project # FE0000507*** – Demonstration of Pressurizing Coal/Biomass Mixtures Using Posimetric Solids Pump Technology – *Tiffany E. Westendorf*, **GE Global Research**
4:00 – 4:30 p.m.	Q&A
4:30 – 5:10 p.m.	Discussion, evaluation, and written comments

Wednesday, October 20, 2010 – Salon D

7:00 – 8:00 a.m.	**Registration – Foyer D**
8:00 – 8:45 a.m.	***09 - Project # NT42465*** – National Center for Hydrogen Technology – *Michael J. Holmes and Josh Stanislowski*, **University of North Dakota (UNDEERC)**
8:45 – 9:15 a.m.	Q&A
9:15 – 9:55 a.m.	Discussion, evaluation, and written comments
9:55 – 10:10 a.m.	**BREAK – Foyer D**
10:10 – 10:55 a.m.	***10 - Project # FE0001009*** – Nanoporous, Metal Carbide, Surface Diffusion Membranes for High Temperature Hydrogen Separations – *J. Douglas Way*, **Colorado School of Mines (CSM)**
10:55 – 11:25 a.m.	Q&A
11:25 – 12:05 p.m.	Discussion, evaluation, and written comments
12:05 – 1:05 p.m.	**Lunch (on your own)**
1:05 – 1:50 p.m.	***11 - Project # FE0001293*** – Integrated Water Gas Shift Membrane Reactors Utilizing Novel, Non-Precious Metal Mixed Matrix Membranes – *John P. Ferraris*, **University of Texas at Dallas (UTD)**
1:50 – 2:20 p.m.	Q&A
2:20 – 3:00 p.m.	Discussion, evaluation, and written comments
3:00 – 3:15 p.m.	**BREAK – Foyer D**
3:15 – 4:00 p.m.	***12 - Project # NT42456*** – Production and Storage of Hydrogen from Coal Using C1 Chemistry – *Gerald P. Huffman*, **University of Kentucky - Consortium for Fossil Fuel Liquefaction Science (CFFLS)** *Christopher Roberts and Mario Eden,* **Auburn University**
4:00 – 4:30 p.m.	Q&A
4:30 – 5:10 p.m.	Discussion, evaluation, and written comments
5:10 – 5:25 p.m.	**BREAK – Foyer D**
5:25 – 6:10 p.m.	***13 - Project # FE0001248*** – Yeager Airport Hydrogen Vehicle Test Project – *William A. Davis*, **West Virginia University Research Corporation (WVU)**
6:10 – 6:40 p.m.	Q&A
6:40 – 7:20 p.m.	Discussion, evaluation, and written comments

Thursday, October 21, 2010 – Salon D

7:00 – 8:00 a.m.	**Registration – Foyer D**
8:00 – 8:45 a.m.	***14 - Project # NT0005988*** – Coal Fuels Alliance: Design and Construction of Early Lead Mini Fischer-Tropsch Refinery – *Rodney Andrews*, **University of Kentucky - Center for Applied Energy Research (CAER)**
8:45 – 9:15 a.m.	Q&A
9:15 – 9:55 a.m.	Discussion, evaluation, and written comments

Thursday, October 21, 2010 – Salon D

9:55 – 10:10 a.m.	**BREAK – Foyer D**
10:10 – 10:55 a.m.	***15 - Project # NT42449*** – Production of High-Hydrogen Content Coal-Derived Liquids – *Stephen P. Bergin and Burtron H. Davis*, **Integrated Concepts and Research Corporation (ICRC)**
10:55 – 11:25 a.m.	Q&A
11:25 – 12:05 p.m.	Discussion, evaluation, and written comments
12:05 – 1:05 p.m.	**Lunch (on your own)**
1:05 – 1:50 p.m.	***16 - Project # NT42761*** – Enhanced Hydrogen Economics Via Co-Production of Fuels and Carbon Products – *Elliot B. Kennel*, **West Virginia University (WVU)**
1:50 – 2:20 p.m.	Q&A
2:20 – 3:00 p.m.	Discussion, evaluation, and written comments
3:00 – 3:15 p.m.	**BREAK – Foyer D**
3:15 – 4:00 p.m.	***17 - Project # FE0000435*** – Methanol Economy – *G. K. Surya Prakash and Robert Aniszfeld*, **University of Southern California (USC)**
4:00 – 4:30 p.m.	Q&A
4:30 – 5:10 p.m.	Discussion, evaluation, and written comments
5:10 – 5:25 p.m.	**BREAK – Foyer D**
5:25 – 6:25 p.m.	***18 - Project # NT42457 / FE0000699*** – Continuation of Crosscutting Technology Development at CAST – *Rick Honaker*, **University of Kentucky Research Foundation (UKY)** *Roe-Hoan Yoon and Christopher Hull*, **Virginia Polytechnic Institute & State University (VPI)**
6:25 – 6:55 p.m.	Q&A
6:55 – 7:35 p.m.	Discussion, evaluation, and written comments

Friday, October 22, 2010 – Salon D

7:00 – 8:00 a.m.	**Registration – Foyer D**
8:00 – 8:45 a.m.	***19 - Project # NT42804*** – Long-Term Environmental and Economic Impacts of Coal Liquefaction in China – *Jerald J. Fletcher*, **West Virginia University (WVU)**
8:45 – 9:15 a.m.	Q&A
9:15 – 9:55 a.m.	Discussion, evaluation, and written comments
9:55 – 10:10 a.m.	**BREAK – Foyer D**
10:10 – 12:10 p.m.	**Meeting Wrap-up Session**

APPENDIX C: PEER REVIEW PANEL MEMBERS

After reviewing the scientific areas and issues addressed by the 19 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, in cooperation with the NETL project manager, identified the following areas of expertise as the required skill sets of the FY 2011 Advanced Fuels Peer Review Panel:

- Component, system, and building design
- Component or reactor design; bench and field testing
- Coal/Biomass-to-liquid processes (e.g., Fischer-Tropsch synthesis)
- Integrated gasification combined cycle
- Carbon sequestration and emissions reduction
- Catalysts, cracking, and de-hydrogenation
- Cost estimating and economic analysis
- Synthesis gas or natural gas cleaning
- Transportation fuel
- Hydrogen production, storage, and vehicles
- System analysis and processes
- Environmental analysis
- Membranes and supports
- Biomass (e.g., grass, wood, and algae)
- Data collection, modeling, and simulation

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 six individuals who had served on prior ASME Peer Review Panels were qualified to serve on the Advanced Fuels Peer Review Panel.

Appropriate résumés were then submitted to the Advanced Fuels Peer Review Executive Committee for review. The following seven members were selected for the FY 2011 Advanced Fuels Peer Review (* indicates a prior Panel member):

- Daniel J. Kubek*, Gas Processing Solutions, LLC – *Chair*
- Brian Gleeson*, Ph.D., University of Pittsburgh
- Robert N. Miller, Ph.D., Air Products
- William R. Owens*, Ph.D., Consultant
- Ravi Prasad*, Ph.D., Helios-NRG, LLC
- James C. Sorensen*, Sorensenergy, LLC
- Michael R. von Spakovsky*, Ph.D., Virginia Polytechnic Institute and State University

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.

FY 2011 Advanced Fuels Peer Review Panel Members

Daniel J. Kubek, Panel Chair

Mr. Kubek is the sole principal of Gas Processing Solutions LLC, which provides technology consultation for synthesis gas and natural gas purification and separation. During his professional career, he spent 18 years (1988–2006) with Universal Oil Products LLC (UOP) and 18 years with their parent company Union Carbide Corporation (1970–1988), retiring in May 2006. His career of technical expertise is based in separations engineering, having worked in the fields of absorption, adsorption, distillation, extraction, and membrane permeation. He has worked in engineering design, research and development, plant technical service, and applications engineering.

During the last few years of his professional career, Mr. Kubek was a senior technology manager in UOP's Gas Processing Technical Center within the Engineering Department. He was directly involved in the technology development, systems integration, and engineering design of UOP gas processing technologies into world-scale plants. He was the process manager responsible for all process design packages for multiple gasification projects and served as development manager for UOP's gas processing business.

In 2005, Mr. Kubek was awarded UOP's Don Carlson Award for Career Technical Innovation. From 1996 to 2006 he served as UOP's representative to the Gasification Technologies Council's Board of Directors. He is the holder of eight patents and has co-authored 17 technical publications. Mr. Kubek received a B.S. degree in chemical engineering from Rutgers University and earned a M.S. in chemical engineering from Purdue University.

Brian Gleeson, Ph.D.

Dr. Gleeson is the Henry S. Tack Professor in the Department of Mechanical Engineering and Materials Science at the University of Pittsburgh and an associate senior scientist at Ames Laboratory in the Materials and Engineering Physics Program. His primary research focus is on the thermodynamics and kinetics of gas/solid and solid/solid reactions. Particular emphasis is on the high-temperature degradation of metallic alloys and coatings. Related to this emphasis, his current research interests include active and passive high-temperature oxidation of alloys and coatings, deposition and characterization of metallic coatings, diffusion and thermodynamic treatments of both gas/solid and solid/solid interactions, and structure/property relationships of materials.

Prior to Dr. Gleeson’s position at the University of Pittsburgh and his role as associate senior scientist at Ames Laboratory, he was a professor at Iowa State University in the Department of Materials Science and Engineering. He also served numerous roles at Ames Laboratory and was a lecturer in the Department of Materials Science and Engineering at the University of New South Wales.

In 2005, Dr. Gleeson received the Research and Development 100 Award from *R&D Magazine* for *Novel High-Temperature Coatings with Pt-Modified Ni and* Ni_3Al *Alloy Compositions.* Dr. Gleeson has been a contributing author of over 100 publications, is the editor of the international journal *Oxidation of Metals*, and is an international advisory board member of the international journal *Materials and Corrosion*. Dr. Gleeson has a B.S. and M.S. in materials science and engineering from the University of Western Ontario in Canada, and a Ph.D. in materials science and engineering from the University of California at Los Angeles. He also completed a post-doctoral fellowship at the University of New South Wales in Australia.

Robert N. Miller, Ph.D.

Dr. Miller has a broad interdisciplinary technical background with 32 years of industrial experience and 8 years in academia, primarily in the field of coal and energy science and technology. He currently has leadership responsibility at Air Products for developing and securing government/industry partnerships to advance strategic technology initiatives. Since 1987, he has successfully led the development of Air Products' government-funded research and technology proposals in the fields of gas separation membranes, hydrogen energy, alternative liquid fuels, and many environmental and energy efficiency projects and processes. His principal skills include marketing, presentation and writing proficiency, technical and business proposal preparation, contract negotiation and consultation for procurement processes, and program issues in U.S. Government contracting. In addition, Dr. Miller is currently responsible for managing Air Products Research Alliance with Pennsylvania State University. Dr. Miller also represents Air Products on the Vision 2020 Chemical Industry Steering Committee and the Alternative Fuels Renewable Energy Council and is a member of the Technical Advisory Board of the Pittsburgh Coal Conference.

Dr. Miller has a keen interest in clean alternative energy and hydrogen. Since 1992, Dr. Miller stewarded numerous hydrogen research and development initiatives to support growth of the company's global leadership position in hydrogen. As a member of a cross-functional team formed to investigate advanced concepts for hydrogen, he pioneered hydrogen energy research programs in separation, production, storage, delivery, and infrastructure that today form the backbone of Air Products' emerging hydrogen energy business. For example, he conceptualized and developed the DOE Las Vegas hydrogen energy station project, the nation's first integrated hydrogen co-production station demonstration, as well as the DOE/Penn State hydrogen refueling station project which demonstrated lowest-cost on-site production/refueling. Currently, Dr. Miller is developing technology opportunities related to climate change and sustainability.

Dr. Miller's participation in hydrogen and clean energy activities cuts across many national and international meetings and forums, where he has lectured on all aspects of hydrogen energy technology. He has been an invited lecturer on hydrogen energy technology at various private and public forums nationwide, and has been active in numerous government-sponsored hydrogen workshops, including the Hydrogen Roadmap workshop in 2003, which defined the hydrogen vision for the nation. Dr. Miller serves periodically as a Peer Reviewer for the DOE Basic Energy Sciences and small business innovation research programs, the DOE Hydrogen Program, the DOE Biomass Program, and the DOE University Coal Research Programs. He currently is an elected member of the Technical Advisory Board of the International Pittsburgh Coal Conference where he has served as session chair and organizer of the hydrogen-to-coal and carbon management topics for the past five years. In 2008, as a member of the Technical Oversight Committee he chaired a symposium on "Hydrogen Storage via Glass Microspheres," held at the 2008 American Ceramic Society Conference "Material Innovations in an Emerging Hydrogen Economy". In 2008, he was on the technical oversight committee for the Advanced Materials for Hydrogen Conference and participated as session chair. He also served on the Governor's Energy Advisory Board in Pennsylvania from 2003 to 2004 which advised the Environmental Secretary on clean energy technology pathways, including hydrogen and fuel cell technologies.

Before Air Products, Dr. Miller worked for Exxon Research and Engineering Co. where he utilized his expertise in coal science to develop fundamental property correlations that could predict multidimensional coal utilization performance in support of Exxon’s coal acquisition objectives. Dr. Miller's work at Exxon inspired the creation of the DOE’s National Premium Coal Bank in 1983, for which Dr. Miller served as both peer reviewer and panelist.

William R. Owens, Ph.D.

Dr. Owens is an energy consultant with an emphasis on fossil and renewable energies. 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. Dr. Owens 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. Instrumental in the success of international programs, Dr. Owens has a strong appreciation for the understanding of the relevance of international activities. Dr. Owens' experience includes systems with bituminous coal, anthracite coal, and sub-bituminous western coals. He has worked with alternate fuel systems, including natural gas, hydrogen, gasifier fuel-gas, oil, and oil-shale systems.

Dr. Owens was a senior director in a Clean Coal Technology proposal. He was responsible for the project coordination, project economics, financial plan which included the negotiations with venture capitalists, and the commercialization plan. Dr. Owens has provided DOE with detailed support in outreach programs, deregulation of the electric utility industry, and international programs. He is the author of more than 50 technical publications and reports in the research, engineering, and application of advanced fossil energy power generation systems. He has a B.S. from Pennsylvania State University, a M.S. from Drexel University, and a Ph.D. from the University of Maryland. All of his degrees are in mechanical engineering.

Ravi Prasad, Ph.D.

Dr. Prasad of Helios-NRG, LLC and formerly a corporate fellow of Praxair Inc., has 60 U.S. patents and broad industrial experience in developing and commercializing new technologies, launching technology programs ($2–$50 million), supporting business development, building cross-functional teams, and setting up joint development alliances. He is a founding member of an alliance involving Praxair, British Petroleum, Amoco, Phillips Petroleum, Statoil, and Sasol to develop ceramic membrane synthesis gas (syngas) technology for gas-to-liquid processes.

Dr. Prasad also established and led programs for ceramic membrane oxygen technology; co-developed proposals to secure major DOE programs worth $35 million in syngas and $20 million in oxygen; identified novel, solid-state oxygen generation technology; and conceived and implemented a coherent corporate strategy in nanotechnology. He has championed many initiatives in India, including small on-site hydrogen plants, small gasifiers, and aerospace business opportunities; and developed implementation plans resulting in a new research and development center in Shanghai.

Dr. Prasad is the director and a board member of the National Hydrogen Association, a member of the steering committee for Chemical Industry V2020, and has been a recipient for Chairman's & Corp Fellows awards for technology leadership. He has authored or co-authored 30 publications, is co-author of a book on membrane gas separation, and has presented at over 20 conferences and invited lectures. Dr. Prasad has a B.S. in mechanical engineering from the Indian Institute of Technology in Kanpur, India, and an M.S. and Ph.D. in mechanical engineering and chemical engineering from the State University of New York, Buffalo, New York.

James C. Sorensen

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, a M.S. in chemical engineering from Washington State University, and a M.B.A. from the Harvard Business School.

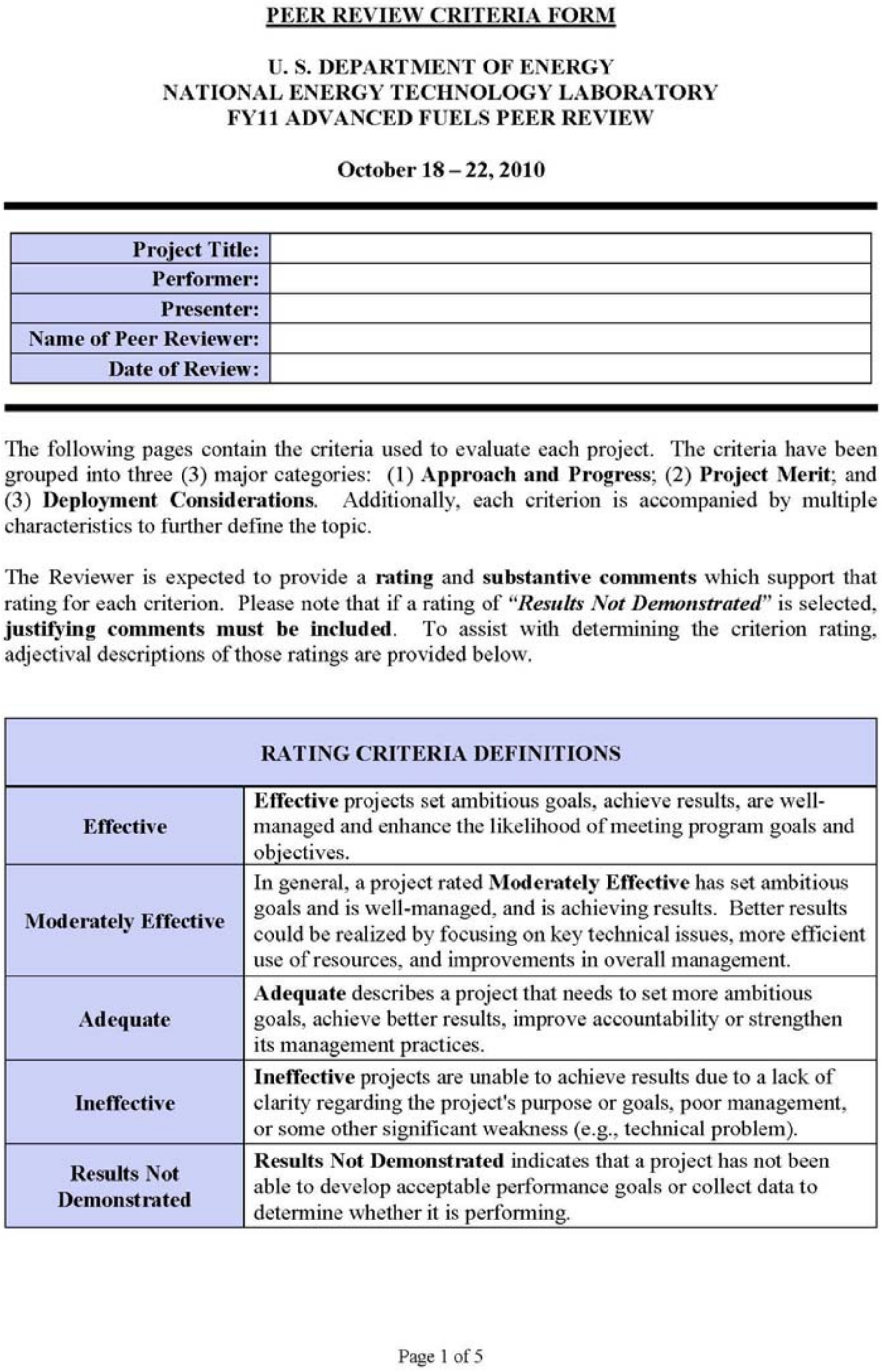
Michael R. von Spakovsky, Ph.D.

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 the 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 lead 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.

His 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 is membership in the American Institute of Aeronautics and Astronautics, fellow of the ASME, member of the Executive Committee for the 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 a M.S. and Ph.D. in mechanical engineering from the Georgia Institute of Technology.

APPENDIX D: PEER REVIEW CRITERIA FORM



PEER REVIEW CRITERIA FORM

U. S. DEPARTMENT OF ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY
FY11 ADVANCED FUELS PEER REVIEW

October 18 – 22, 2010

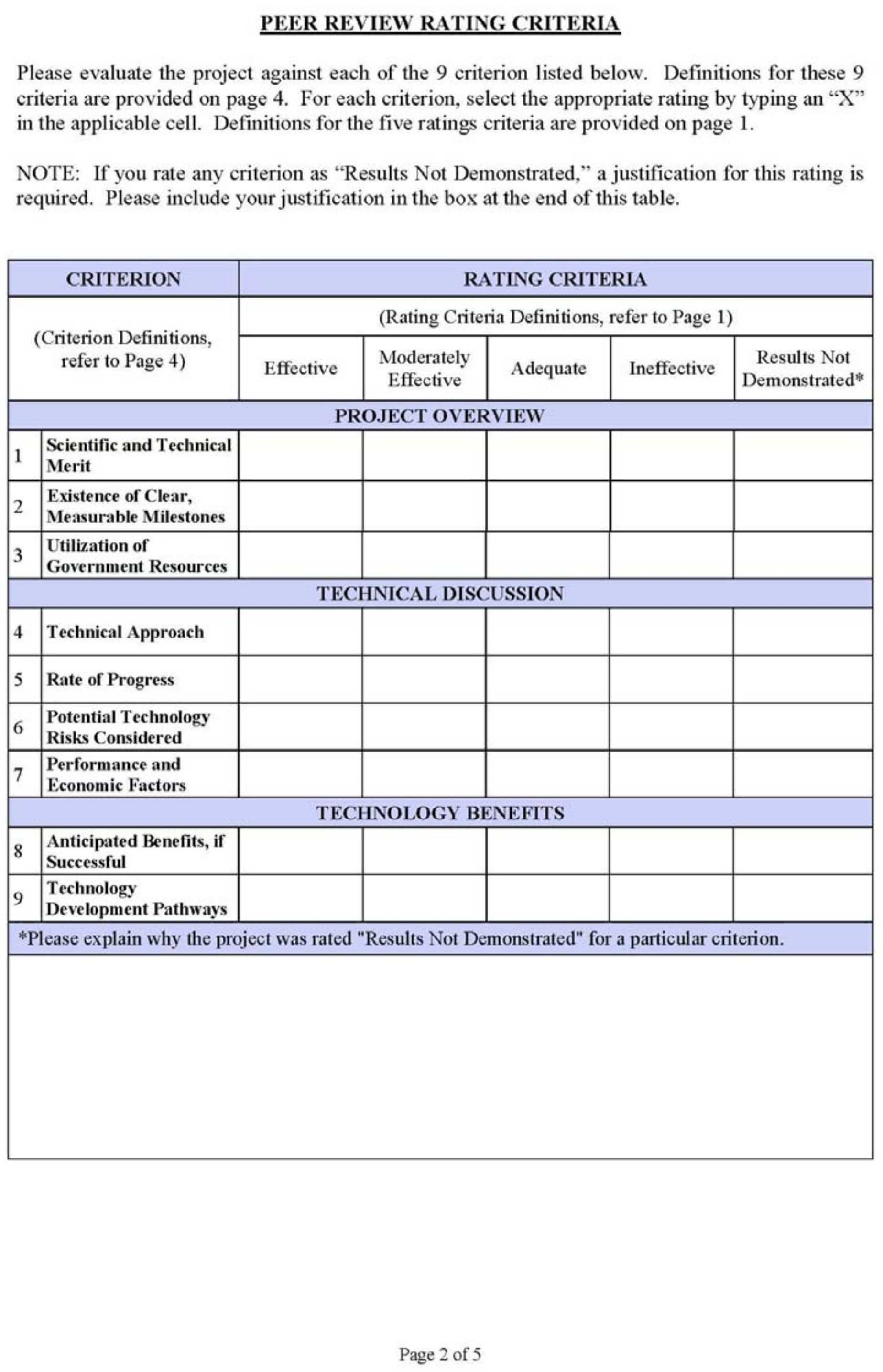
Project Title:	
Performer:	
Presenter:	
Name of Peer Reviewer:	
Date of Review:	

The following pages contain the criteria used to evaluate each project. The criteria have been grouped into three (3) major categories: (1) **Approach and Progress**; (2) **Project Merit**; and (3) **Deployment Considerations**. 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 rating, adjectival descriptions of those ratings are provided below.

RATING CRITERIA 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.

Page 1 of 5

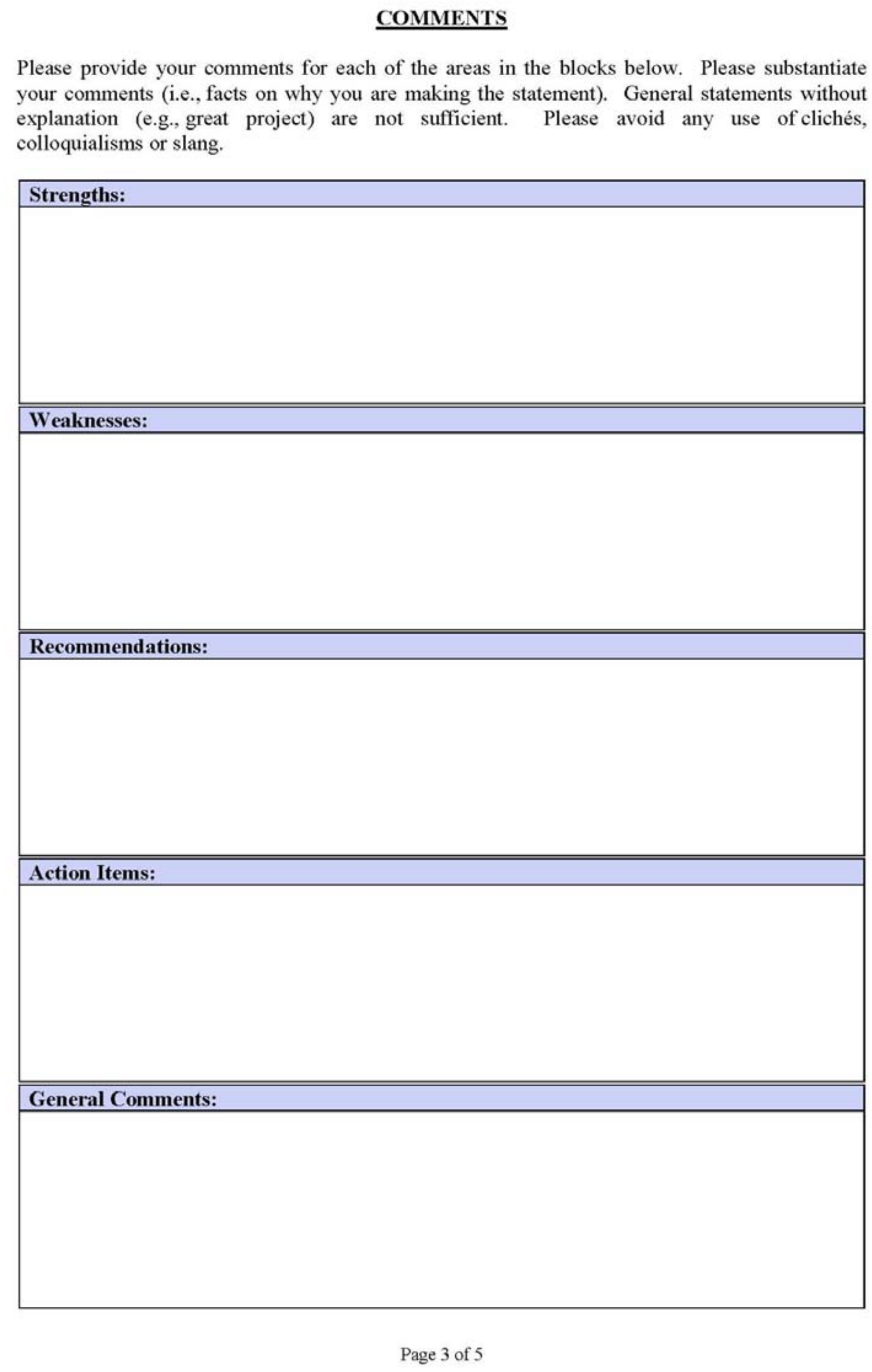


PEER REVIEW RATING CRITERIA

Please evaluate the project against each of the 9 criterion listed below. Definitions for these 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 criteria 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.

CRITERION		RATING CRITERIA				
(Criterion Definitions, refer to Page 4)		(Rating Criteria 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:

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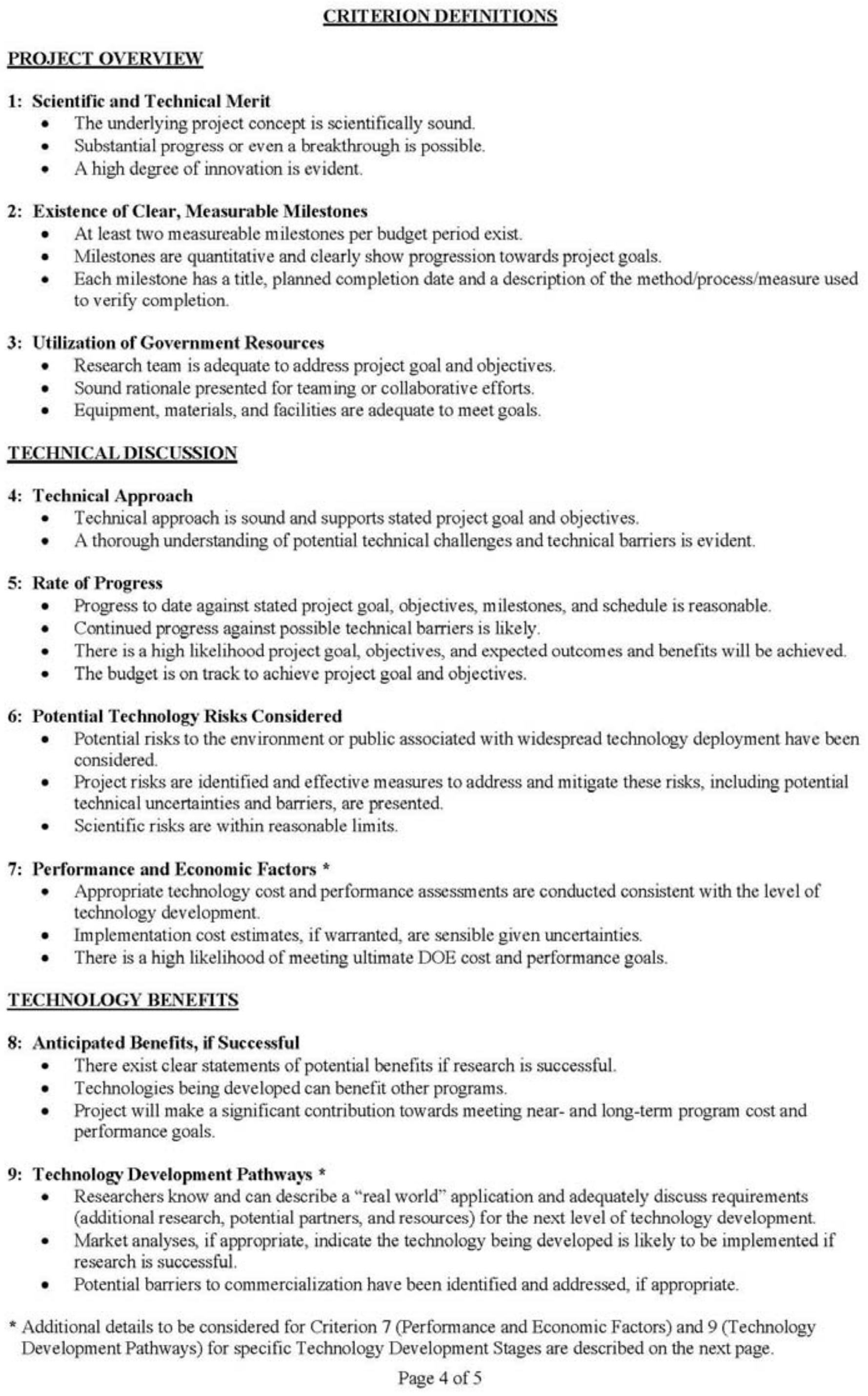

CRITERION DEFINITIONS

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 measureable 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.

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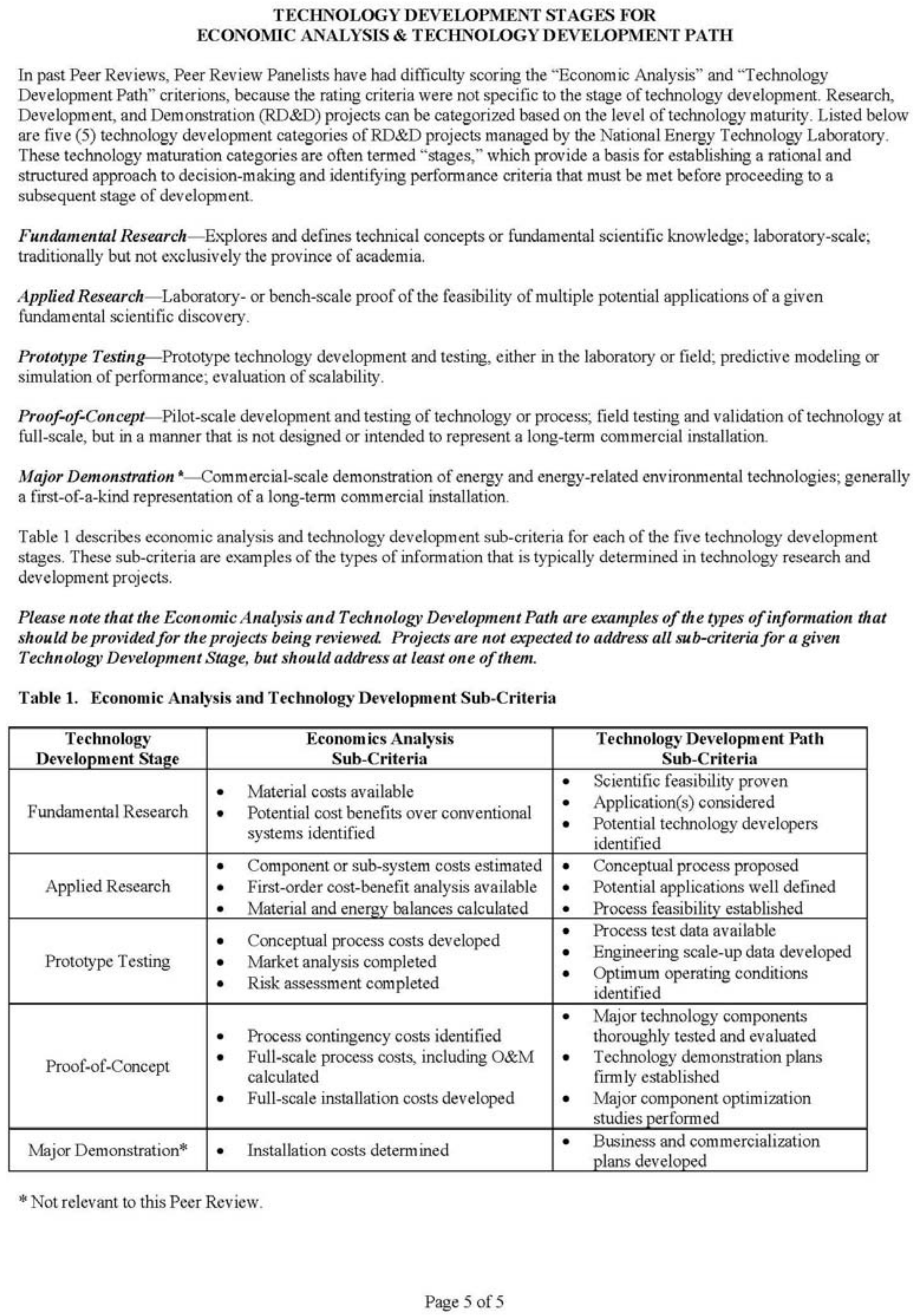

TECHNOLOGY DEVELOPMENT STAGES FOR ECONOMIC ANALYSIS & TECHNOLOGY DEVELOPMENT PATH

In past Peer Reviews, Peer Review Panelists have had difficulty scoring the "Economic Analysis" and "Technology Development Path" criterions, because the rating criteria were not specific to the stage of technology development. 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	• Material costs available • Potential cost benefits over conventional systems identified	• Scientific feasibility proven • Application(s) considered • Potential technology developers identified
Applied Research	• Component or sub-system costs estimated • First-order cost-benefit analysis available • Material and energy balances calculated	• Conceptual process proposed • Potential applications well defined • Process feasibility established
Prototype Testing	• Conceptual process costs developed • Market analysis completed • Risk assessment completed	• Process test data available • Engineering scale-up data developed • Optimum operating conditions identified
Proof-of-Concept	• Process contingency costs identified • Full-scale process costs, including O&M calculated • Full-scale installation costs developed	• Major technology components thoroughly tested and evaluated • Technology demonstration plans firmly established • Major component optimization studies performed
Major Demonstration*	• Installation costs determined	• Business and commercialization plans developed

* Not relevant to this Peer Review.

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APPENDIX E: ADVANCED FUELS PROJECT SUMMARIES

Presentation ID Number	Project Number	Title
01	DE-FE0004001.410.01.22	Analysis of Coal to Hydrogen Systems
02	FC26-05NT42469	Scale-Up of Hydrogen Transport Membranes for IGCC and FutureGen Plants
03	DE-FE0004908	Advanced Hydrogen Transport Membranes for Coal Gasification
04	FC26-07NT43058	Composite Pd and Alloy Porous Stainless Steel Membranes for Hydrogen Production and Process Intensification
05	DE-FE0004967	Advanced Palladium Membrane Scale-Up for Hydrogen Separation
06	FY10.MSE.1610884.663	Coal & Biomass Derived Fuels
07	FWP-49601	Development of Dense Ceramic Membranes for Hydrogen Separation
08	DE-FE0000507	Demonstration of Pressurizing Coal/Biomass Mixtures Using Posimetric Solids Pump Technology
09	FC26-05NT42465, DE-FC0003466	National Center for Hydrogen Technology
10	DE-FE0001009	Nanoporous, Metal Carbide, Surface Diffusion Membranes for High Temperature Hydrogen Separations
11	DE-FE0001293	Integrated Water Gas Shift Membrane Reactor Utilizing Novel, Non-Precious Metal Mixed Matrix Membranes
12	FC26-05NT42456	Production and Storage of Hydrogen from Coal Using C1 Chemistry
13	DE-FE0001248	Yeager Airport Hydrogen Vehicle Test Project
14	FC26-08NT0005988	Design and Construction of Early Lead Mini Fischer-Tropsch Refinery
15	FC26-06NT42449	Production of High-Hydrogen Content Coal-Derived Liquids
16	FC26-06NT42761	Enhanced Hydrogen Economics Via Co-Production of Fuels and Carbon Products
17	DE-FE0000435	Methanol Economy
18	DE-FC26-05NT42457, DE-FE0000699	Continuation of Crosscutting Technology Development of CAST
19	FC26-06NT42804	Long-Term Environmental and Economic Impacts of Coal Liquefaction in China

01: FE0004001.410.01.22

Project Number DE-FE0004001.410.01.22	**Project Title** Analysis of Coal to Hydrogen Systems			
Contacts DOE/NETL Project Mgr.	**Name** Larry Rath	**Organization** NETL-OSAP-Systems Division	**Email** Larry.Rath@netl.doe.gov	
Principal Investigator	Larry Rath	NETL-OSAP-Systems Division	Larry.Rath@netl.doe.gov	
Partners	Research and Development Solutions LLC Electronic Systems Professional Alliance Booz Allen Hamilton			
Stage of Development				
__Fundamental R&D	_X_Applied R&D	__Prototype Testing	__Proof of Concept	__Demonstration

Technical Background

NETL has published and continues to update and expand its comprehensive Cost and Performance Baseline for Fossil Energy Power Plants. This project expands the expertise gained through these previous studies as well as the cost and performance assessments for central hydrogen production in conjunction with the Hydrogen Analysis Project (H2A) and DOE's Hydrogen, Fuel Cells, and Infrastructure Technologies Program.

This project intends to develop credible performance and cost estimates of near-mature fossil-based technologies that should be available for near-term commercial deployment with an online date of 2015. These technologies have relatively uncertain installed costs but do not include added costs or performance uncertainty associated with a first-of-a-kind facility design. This uncertainty was reflected primarily in the level and type of contingency applied to specific process island costs as well as the financial risk structure for calculating the cost of hydrogen production.

To build on these previous DOE baseline studies, this project assesses the cost and performance of the following: (1) state-of-the-art hydrogen production from coal and natural gas with carbon capture and storage (CCS), and (2) a coal-to-hydrogen plant with CCS that incorporates advanced technologies under development in the DOE research and development (R&D) portfolio.

The advanced technologies within DOE's R&D program being evaluated by this project include the following:

- Eltron membrane for hydrogen separation
- Worcester Polytechnic Institute (WPI) membrane for hydrogen separation
- Research Triangle Institute (RTI) warm-gas cleanup (WGCU)
- Ohio State University (OSU) calcium looping

All major process material and energy flows were modeled by Research and Development Solutions LLC/Parsons and Electronic Systems Professional Alliance/Booz Allen Hamilton using Aspen Plus software. Process units and major equipment sizes were estimated based on major material and/or energy flow. Costs were scaled from those costs presented in the Cost and Performance

Baseline for Fossil Energy Plant reports. In those reports, equipment estimates were prepared by a commercial engineering firm (WorleyParsons) based on recent design/build projects. Operating and maintenance costs were estimated based on operating labor assumptions and included maintenance labor and material costs. Consumables were estimated for major process chemicals, catalysts, and utilities based on annual usage. Fuel costs were estimated based on annual facility throughput and availability.

For this study, a spare gasifier was utilized to allow 90% availability and it was assumed that availability is equivalent to capacity factor. Historically, NETL has reported costs on a total plant cost (TPC) basis. For this study, a representative basket of owner's costs have been developed and costs are reported on a TPC basis as well as on a total overnight cost (TOC) basis that includes both TPC and owner's costs. Financing costs, including escalation during construction, were added to the TOC to provide the total as-spent cost. Sensitivity analyses were conducted around major cost drivers including capacity factor.

Relationship to Program

This project will support important membrane separation systems advances within the Hydrogen from Coal Research focus of the NETL Advanced Fuels Program through the following tasks:

- Provide guidance to Office of Fossil Energy (FE) R&D by defining cost and performance benchmarks for state-of-the-art fossil-based hydrogen production.
- Allow for the development of meaningful FE R&D program goals and provide a credible baseline for comparison of cost and performance improvements resulting from funded research activities.
- Show cost and performance impact of advanced hydrogen separation technologies.
- Identify and assess the need for enabling technologies for hydrogen membrane separation (such as WGCU).

Primary Project Goal

The primary goals of this project include the following:

- Complete a comprehensive, credible publicly distributable systems study that estimates performance and cost of advanced fossil-based hydrogen production with CCS.
- Evaluate potential process improvements and cost reductions resulting from successful R&D of advanced technologies for coal-to-hydrogen plants with CCS, assessing the cumulative impact of multiple technologies as appropriate.

Objectives

The main project objective is to provide systems studies that assess the performance and cost impact of advanced technologies funded under DOE's R&D program. To accomplish this objective, the project involves the creation of a credible baseline of state-of-the-art technologies in order to quantify the cost and performance benefits of advanced technologies. Each advanced technology is to be assessed in a consistent manner, while also taking full advantage of the performance aspect of new unit operations and developing creative approaches to characterizing and modeling novel and conceptual technologies. The project includes the analysis of the following cases:

- Baseline natural gas to hydrogen with pressure swing adsorption (PSA) and CCS

- Baseline coal to hydrogen with PSA and CCS
- Coal to hydrogen with Eltron Membrane and CCS
- Coal to hydrogen with RTI WGCU, Eltron membrane, and CCS
- Coal to hydrogen with WPI membrane and CCS
- Coal to hydrogen with RTI WGCU, WPI membrane, and CCS
- Coal to hydrogen with OSU calcium looping and CCS

02: FC26-05NT42469

Project Number	**Project Title**			
FC26-05NT42469	Scale-Up of Hydrogen Transport Membranes for IGCC and FutureGen Plants			
Contacts	**Name**	**Organization**	**Email**	
DOE/NETL Project Mgr.	Arun C. Bose	NETL – Gasification Division	Arun.Bose@netl.doe.gov	
Principal Investigator	Carl Evenson	Eltron Research Inc.	cevenson@eltronresearch.com	
Partners	Eastman Chemical Company			
Stage of Development				
__Fundamental R&D	__Applied R&D	_X_Prototype Testing	__Proof of Concept	__Demonstration

Technical Background

The project technology is based on the use of a dense metallic composite membrane system for the separation of hydrogen and carbon dioxide from a coal-based synthesis gas stream, although it does have wider applicability to other hydrogen-containing streams. These membranes have been shown to meet or exceed the DOE 2010 targets for flux, selectivity, and cost (see table below).

The membrane has been operated at 1,000 pounds-force per square inch gauge (psig) and differential pressure up to 500 psig on simulated synthesis gas (syngas) compositions. Membrane life has been shown for about 8,000 hours. Some early work on impurity testing has shown tolerance to sulfur up to 20 parts per million (ppm). The membrane has also been integrated into a water-gas-shift (WGS) reactor, facilitating high conversion of carbon monoxide. Process design and economics studies have shown cost and thermal efficiency benefits. Membranes have been tested with all syngas components, including carbon monoxide, carbon dioxide (CO_2), hydrogen sulfide, water, and hydrogen (H_2). Membranes have also been exposed to “live” or raw syngas from a coal gasifier and tested. These exposure tests were not flux tests; those will occur later this year.

Performance Criteria	2010 target	2015 Target	Current Eltron Membrane
Flux, scfh/ft^2	200	300	450
Operating Temperature, °C	300–600	250–500	250–440
Sulfur Tolerance (ppmv)	2	20	20 (prelim.)
System Cost (\$/ft^2)	500	<250	<200
ΔP operating Capability (psi)	400	800–1,000	1,000
Carbon Monoxide Tolerance	Yes	Yes	Yes
Hydrogen Purity (%)	99.5	99.99	>99.99
Stability/Durability (years)	3	>5	0.9
Permeate Pressure (psi)	N/A	N/A	400

A 12 pounds-per-day (lb/day) unit is currently being constructed for testing on an actual coal gasifier slipstream at Eastman Chemical Company in FY11 Q1/Q2.The membrane module for that unit will contain two membrane tubes, each 5 feet long. Membrane tubes up to 5 feet in length have been manufactured and coated. Sealing methods have been successfully demonstrated under water-gas shift feed in high pressure laboratory reactors. Tubes up to 2 feet in length—the longest that can be tested in existing equipment—have also been tested. Many of these tubes were prepared by cutting sections from the 5 foot lengths mentioned above to verify successful catalyst deposition.

Relationship to Program

This project will support important membrane separation systems advances within the Hydrogen from Coal Research focus of the NETL Advanced Fuels Program. Several benefits will be conferred to a FutureGen-style plant when the technology is commercialized:

- High-purity hydrogen (>99.999%) can be delivered from coal-based syngas at lower cost than conventional technology.
- Retention of CO_2 at high pressure will lower the capture cost and improve the higher heating value efficiency of a plant capturing CO_2 for sequestration, primarily through significantly reduced compression requirements.
- Technology may enable process simplification and intensification when incorporated into membrane reactors (concept demonstrated under separate small business innovation research contract).
- Technology can be applied for recovery of hydrogen from other systems such as natural gas partial oxidation, diesel or naphtha reforming, refinery streams, chemical processes, and fuel processing for fuel cells.

Primary Project Goal

The primary goal of this project is to develop a high throughput, low cost H_2 separation system suitable for application with coal-based synthesis gas, including improved tolerance for contaminants (e.g., sulfur and mercury) and enabling cost-effective capture of CO_2 for sequestration.

Objectives

Program objectives are grouped into five major areas.

MATERIALS DEVELOPMENT

- Develop and test membrane alloy systems that give the best flux without risk of membrane embrittlement.
- Develop catalyst compositions that do not limit flux and provide the requisite tolerance to impurities.
- Understand the importance of the interface between the membrane and catalyst.

PERFORMANCE SCREENING

- Establish the range of operating conditions for the system giving the best performance using WGS composition syngas.
- Evaluate the effect of impurities on performance.
- Perform life tests of membranes longer than 600 hours.

PROCESS DESIGN

- Integrate the system into integrated gasification combined cycle flow sheets, testing different configurations with and without coproduction of power and H_2.
- Evaluate the impact of different impurity management techniques.
- Compare economics, including capital expenditures and operating expenditures, with those of alternative technologies.

MECHANICAL DESIGN

- Address manufacturing issues for scaling up the system, taking into account maintenance costs, initial capital costs, and system robustness.
- Address issues such as welding, sealing, catalyst deposition techniques, and alloy manufacture for tubular system.

SYSTEM SCALE-UP

- Design, build, and operate 12 lb/day system on coal-based syngas slipstream, developing operating procedures and gathering initial engineering data for further scale-up.
- Design, build, and operate a 250 lb/day unit integrated with warm-gas cleaning.

03: DE-FE0004908

Project Number	**Project Title**			
DE-FE0004908	Advanced Hydrogen Transport Membranes for Coal Gasification			
Contacts	**Name**	**Organization**	**Email**	
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Stage of Development				
__Fundamental R&D	__Applied R&D	_X_Prototype Testing	__Proof of Concept	__Demonstration

Technical Background

Praxair has been working on developing hydrogen transport membrane (HTM) technology for many years and has completed some of this work through successful DOE programs. The first Praxair DOE-funded project developed an integrated HTM water-gas shift reactor and led to substantial progress in substrate development, enabling the production of leak-free membranes with high flux. Another project modeled integrated HTM processes around hydrogen production from coal and established performance and cost targets for the membrane. In the most recent project, Praxair and Colorado School of Mines (CSM) modeled, produced, and tested different palladium (Pd) alloy membranes and will demonstrate a multi-tube hydrogen purifier. The current Praxair project will continue the partnership between Praxair and CSM and is expected to lead to further improvements in membrane performance.

Praxair has advanced many facets of HTM technology, including the development of palladium-gold (Au) membranes supported on porous zirconia that have surpassed several hundred hours of life without performance degradation. These membranes have also achieved 20 thermal cycles without degradation, exceeding the primary objective of 10 thermal cycles. After the initial 10 thermal cycles were successfully completed, an air purge was done to try to increase flux and an additional 10 thermal cycles were completed before the tube was removed intact.

More importantly, Praxair has achieved milestones in scaling up HTM technology beyond the laboratory. Praxair has designed and built a multi-tube hydrogen purifier and has advanced substrate manufacturing to the point where successful substrates are consistently made by extrusion. This reactor is about 15 inches long with a 4-inch diameter and is expected to purify about 1 kg/hr of hydrogen. Praxair has designed other large-scale membrane reactors; lessons learned from those reactors will also be applied to design the Phase II and Phase III reactors.

Praxair also has experience testing palladium membranes integrated with a water-gas shift reactor. Testing of this membrane demonstrates its ability to increase the hydrogen yield in the case of a combined conventional water-gas shift reactor and pressure swing adsorption (PSA) unit. Water-gas shift removes sufficient hydrogen to increase CO conversion. Furthermore, hydrogen that permeates the membrane is purified, eliminating the need for PSA or other purification to produce hydrogen at sufficient purity for polymer electrolyte membrane (PEM) fuel cells. Other modeling work showed that operating a membrane reactor at higher temperature provides an opportunity to make the reactor smaller and potentially provides a significant capital cost savings compared to a shift reactor/PSA combination.

Praxair also developed a model to predict reactor performance with and without methanation. The required membrane area depends on conditions but is estimated to be about 10 ft^2 to produce about 2,000 scfh of hydrogen. The maximum amount of hydrogen that can be produced in a membrane reactor decreased significantly—from about 2,600 scfh to about 2,400 scfh—due to methanation. Therefore, it is critical to eliminate methanation to fully benefit from the use of a membrane in the reaction. It is vital to ensure that the catalyst does not lead to methanation in a membrane reactor, where the gas composition can be different than a typical water gas shift reactor, so as not to reduce the effectiveness of the integrated reactor.

The Colorado School of Mines has also achieved technology and scale-up advances by increasing their electroless plating process from 2” tubes to 12” tubes without sacrificing membrane quality. Palladium alloys, including palladium-silver (Ag), have been produced at laboratory scale using a single plating bath. It is expected that this technology can be expanded to include other alloys. A highly advanced support is required to optimize the performance of an electroless plated membrane; this support should include small surface pores that can easily be bridged by the metal film, while simultaneously providing minimal resistance to gas flow. Praxair’s asymmetric porous zirconia supports are ideally suited for these requirements because they have few pores greater than 0.2 microns in diameter and high gas permeance.

CSM has also developed electroless plating baths that do not require complexing agents such as ethylenediaminetetraacetic acid (EDTA), which can cause carbon contamination and lead to pinhole formation when exposed to gas streams containing carbon dioxide (CO_2). The current plating process begins with an activation step in which the support surface is coated with palladium acetate. The support is then heated in air to decompose the organic ligand and reduced in a hydrazine solution to produce Pd^0. These metallic palladium nanocrystallites act as a catalyst for the electroless plating reaction, promoting it on the surface rather than in the plating bath. The plating bath applies a small amount of palladium in each cycle and can be repeated as necessary to produce films of the desired thickness.

The addition of other metallic elements to the film can improve material properties. For example, alloys with Au have demonstrated high sulfur tolerance while alloys with Ag have high permeability and resistance to low-temperature hydrogen embrittlement. Two methods for adding metallic elements include sequential plating, in which layers of palladium are alternated with layers of the alloying element and annealed, and coplating, in which the alloying element and palladium are in the same bath and applied to the support simultaneously. CSM has produced binary and ternary alloys with Au, Ag, copper (Cu), ruthenium (Ru), and platinum (Pt).

The electroless plating process can produce alloy membranes that combine the high flux of a thin metal film with the excellent mechanical strength of the Praxair support. The performance of a Pd-Au-Ru membrane was tested in pure hydrogen and in a gas mixture containing 3% carbon monoxide (CO), 14% CO_2, 56% hydrogen gas (H_2), and 27% H_2O, achieving a maximum of over 800 scfh/ft^2 at 400°C and 200 psi. Increasing the temperature would increase flux, but 400°C is about the expected temperature for the exit of a high-temperature shift reactor in a gasification system. The membrane also showed no decrease in flux due to the other components of the gas mixture, including 3% CO.

Adding to the expertise of Praxair and CSM, T3 Scientific has developed MembraGuard, a proprietary ultrathin film coating designed to protect the underlying palladium alloy membrane from trace reactive gases such as sulfur compounds, halides, CO, or mercury found in coal-derived synthesis gas (syngas). MembraGuard is robust, has high hydrogen permeability, and is thermally compatible with the underlying membrane. Sulfur resistance was demonstrated up to 100 ppm between 400°C to 500°C with superior performance compared to untreated membranes. T3 Scientific tested 25μm-thick Pd membranes with and without the coating at 500°C using a mixed H_2/hydrogen sulfide (H_2S)/nitrogen stream. The test showed a drastic reduction in H_2 permeation for the untreated membrane that began almost immediately upon contact with H_2S; the membrane with MembraGuard was unchanged. MembraGuard was thermally stable for over 150 hours at 400°C with no degradation in performance. As a result, MembraGuard will be applied to additional membranes and tested in syngas.

Relationship to Program

This project will support important membrane separation systems advances within the Hydrogen from Coal Research focus of the NETL Advanced Fuels Program. It seeks to advance all aspects of current HTM technology toward a commercial scale and enable the economical large-scale production of larger membranes. Furthermore, the project intends to use those large membranes in commercial-scale hydrogen and power production systems to produce hydrogen and reduce the cost of CO_2 capture in integrated gasification and combined cycle when sequestration is required.

Although this project is focused on producing hydrogen from coal gasification syngas for power generation, the eventual impact of implementing HTM technology is that the cost of hydrogen production from a wide variety of sources, including coal, natural gas, and oil, will decrease using processes designed to capitalize on the unique capabilities of HTM. Hydrogen is currently used to reduce emissions from gasoline and diesel fuel, so reducing its cost and increasing its availability will reduce the cost of refining today's transportation fuels. In the future, low-cost hydrogen could become an important transportation fuel because it does not pollute, does not produce greenhouse gases, and enables PEM fuel cells.

Primary Project Goal

The goal of this project is to design, construct, and operate a functional pre-engineering/pilot-scale membrane reactor that will lead to the commercialization of hydrogen transport membranes for hydrogen production, separation, and purification, with an emphasis on producing hydrogen using syngas derived from coal (or coal-biomass) gasification.

Objectives

The primary project objective is to develop (by the end of Phase III) a full engineering design of a membrane separation unit that is capable of producing at least 4 tons of hydrogen per day from coal-gasification-derived syngas.

The specific objective of Phase I is to demonstrate the performance of a hydrogen separation membrane producing a minimum of 2 lbs of hydrogen per day from gasifier-derived syngas based on the HTM technology developed by Praxair and the Colorado School of Mines. The Praxair-CSM Pd-Au membranes surpass the 2015 DOE flux goal (tests without sulfur contamination). In addition, the Pd-Au membrane has superior sulfur resistance when compared to Pd or most Pd alloy membranes. Ruthenium incorporated into Pd-Au alloys improves the tensile strength of the membranes without reducing flux, which enables thinner membranes. The palladium alloy layers are deposited onto ceramic substrates with engineered pore structures. The substrates are produced by extrusion, a proven commercial manufacturing method, and the 5–10 micron layer of palladium alloy is deposited by electroless plating. These accomplishments led Praxair to design and build a multi-tube hydrogen purifier capable of purifying 1 kg/hr (400 scfh) of H_2 to meet PEM fuel specifications. The multi-tube purifier represents an important step toward implementing HTM on a commercial scale.

During Phase I of the proposed program, engineering work will also be performed to optimize the process for using HTM reactors in coal gasification systems for co-producing hydrogen and electric power. The project team will determine the impact of incorporating water-gas shift inside the membrane module or using a steam sweep stream to reduce the permeate side hydrogen partial pressure for hydrogen co-production.

The major objective of the Phase II project is to demonstrate the performance of a multi-tube design on gasifier-derived syngas, with the goal of achieving at least 95% hydrogen recovery. To accomplish this, it is necessary to develop and demonstrate a contaminant management strategy that may include sorbent guard beds to capture chlorides and other contaminants, membrane alloys such as Pd-Au with high contaminant resistance, process conditions such as high temperature that mitigate the impact of contaminants, and MembraGuard technology to shield the materials that are susceptible to degradation.

In Phase II, the proposed project focuses on the design, fabrication, installation, and demonstration of a pilot-scale reactor to produce at least 100 lbs of hydrogen per day when integrated with an operating coal (or coal-biomass) gasifier. The results of the Phase II effort will provide the basis for Phase III, the full engineering design of a membrane separation unit capable of producing at least four tons/day of hydrogen from coal gasification derived syngas.

For a full engineering design to be practicable, it is critical to be able to produce commercial quantities of substrates and membranes at a reasonable cost. Praxair’s extrusion substrate manufacturing approach coupled with advanced Pd-alloy plating techniques that minimize processing steps and time has the potential to provide the commercial membranes needed. A process to simultaneously coat all alloy components would further reduce manufacturing time and cost and will be pursued as part of the proposed program.

04: FC26-07NT43058

Project Number FC26-07NT43058	**Project Title** Composite Pd and Alloy Porous Stainless Steel Membranes for Hydrogen Production and Process Intensification			
Contacts DOE/NETL Project Mgr.	**Name** Jason Hissam	**Organization** NETL- Fuels Division	**Email** Jason.Hissam@netl.doe.gov	
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Partners	Adsorption Research Inc.			
Stage of Development				
__Fundamental R&D	_X_Applied R&D	__Prototype Testing	__Proof of Concept	__Demonstration

Technical Background

The main purpose of this project is to develop an integrated, cost-effective, hydrogen production and separation process using a unique hydrogen separation membrane for water-gas shift reactors. The unique approach will help achieve the objective specified in the solicitation: “the development of advanced technologies that offer the potential to consolidate two or more processes/units, such as gas separation processes in one module that would be integrated downstream of a coal gasification system designed to produce a pure stream of hydrogen.”

The separation of hydrogen from reformate requires the utilization of gas separation processes that will provide high fluxes, high selectivity of separation, and the ability to operate at temperatures around 350°C–400°C. Dense palladium (Pd) and Pd-alloy membranes supported on porous metal substrates are especially well suited for high-temperature hydrogen separations and productions. Composite Pd and Pd-alloy porous metal membranes have high hydrogen permeability relative to other hydrogen permeable inorganic materials (e.g., silica, tantalum, and nickel) and excellent chemical resistance to oxidation and corrosion. Although Pd tubes can be fabricated to withstand higher pressures and to provide a reasonable hydrogen flux, the practical applications for stand-alone Pd membranes is limited, primarily due to the practical limitations associated with making thin Pd tubes and sheets. Composite dense Pd-alloy membranes, on the other hand, alleviate both problems of low flux and poor mechanical strength.

The introduction of Pd-alloy membrane reactors in a water-gas shift (WGS) context will be particularly dependent on the membrane cost. In addition to lowering the cost of Pd, the use of dense composite membranes has the added advantages of good mechanical strength for high-pressure operations, higher hydrogen fluxes, lower membrane areas, thinner membrane layers, and lower material cost. Each of the benefits can further contribute to reducing operating, capital costs, and energy consumption. The criteria for the successful implementation of composite Pd and Pd-alloy membrane modules and membrane reactors for WGS reactors include the following:

- Hydrogen separation membranes exhibiting high hydrogen selectivity and high permeability for reasonable process economics and superior mechanical, chemical, and thermal stability to sustain long-term operation at elevated temperatures and pressures

- The porous support of the composite hydrogen separation membranes exhibiting good mechanical strength for high-pressure operation and uniform pore size for easy deposition of a thin, uniform, defect-free Pd alloy layer for separations
- Simple membrane module construction and easy integration to the other process equipment.

Commercially available hydrogen separation modules do not satisfy all the above criteria, but a composite Pd-alloy membrane on porous stainless steel (PSS) or other porous metal supports satisfies all the above criteria with the added advantages of resistance to cracking, simplicity of module construction, and integration with other process equipment.

A unique, patented technology to synthesize robust composite thin Pd and Pd-alloy membranes has been developed in the principal investigator's laboratory at Worcester Polytechnic Institute. The synthesis uses an electroless plating process to produce membranes that are stable between 350°C–450°C for over 6,000 hours. The benefits of this manufacturing process, in comparison to alternatives, include the following:

- It is made with a patented, novel intermetallic diffusion barrier to prevent loss of permeance at high temperatures.
- It is plated on a porous metal support for mechanical strength at high pressures, low Pd alloy layer thickness (~ 5 µm), and chemical resistance to the feed gases.
- It is made of Pd-alloys that avoid hydrogen embrittlement and crack formation during cycling.
- It is scalable and modular to accommodate small-to-large diameter and length tubular dimensions by connecting sections with commercial welding techniques.
- It can be integrated into a water-gas shift reactor to effect one-step hydrogen production from coal gas at small-to-large scales.

In addition, the proposal includes technology development that will enable the implementation of an integrated catalytic membrane WGS reactor/hydrogen purifier to produce pure hydrogen from the coal gas stream. This reactor will implement novel ultra-thin Pd-alloy membranes on a porous metal support for process intensification, which consists of an advanced gas cleanup and WGS membrane reactor. The shift reactor will contain the commercially available WGS catalyst such as the KATALCO 71-series high-temperature shift (HTS) catalyst produced by Johnson Matthey; simultaneous reaction and hydrogen separation will occur in the reactor, yielding expectations of at least 90% recovery of the total hydrogen produced in the system.

Furthermore, the proposed separator/membrane shift converter makes the process more efficient and economical by eliminating the high- and low-temperature shift reactors and multistage preferential oxidation reactors, as well as the hydrogen separator (e.g., pressure swing adsorption [PSA]). In this process, a shift catalyst will be packed in the annular space between the porous stainless steel tubes that will be externally coated with a very thin layer (~5–10 µm) of a Pd-alloy membrane. This supported membrane will selectively separate hydrogen from the synthesis gas. In addition, developing an advanced gas cleaning process to eliminate sulfur compounds will involve developing very efficient PSA cycles, which will employ adsorbents in an innovative form, and will achieve high energy efficiency along with very high performance (recovery and purity).

Relationship to Program

This project will support important membrane separation systems advances in the Hydrogen from Coal Research focus of the NETL Advanced Fuels Program. The proposed separator/membrane shift converter makes the process more efficient and economical by eliminating the high- and low-temperature shift reactors and multistage preferential oxidation reactors, as well as the hydrogen separator (e.g., PSA). In this process, a shift catalyst will be packed in the annular space between the porous stainless steel tubes that will be externally coated with a very thin layer (~5–10 µm) of a Pd-alloy membrane. This supported membrane will selectively separate hydrogen from the synthesis gas. In addition, developing an advanced gas cleaning process to eliminate sulfur compounds will involve developing very efficient PSA cycles, which will employ adsorbents in an innovative form, and will achieve high energy efficiency along with very high performance (recovery and purity).

A major objective and thematic axis of the proposed research plan is the development of a systematic and comprehensive framework for process intensification tailored to the particular hydrogen production system and energy technology under consideration. Process intensification represents a new paradigm in the design of chemical processes and energy production systems necessitated by growing competitive pressures in the broader chemicals and energy sectors to meet market demands on a global scale and in a cost-effective manner, as well as requirements for corporate responsibility towards environmental protection, safety, and energy efficiency.

Primary Project Goal

The primary goal of the project is to develop advanced process intensification technologies that reduce the number of unit operations required for hydrogen production from coal gases produced from an advanced integrated gasification combined cycle (IGCC) plant. The proposed process intensification will reduce the production of pure hydrogen from the synthesis gas to two unit operations consisting of an advanced synthesis gas clean-up and composite Pd or Pd-alloy membrane WGS shifter, which could be integrated downstream in the hydrogen-producing IGCC gasification system. The high-pressure carbon dioxide (CO_2) from the membrane shifter would be appropriate for recycling, sequestration, and/or conversion to industrially useful products and the creation of a natural CO_2 sink.

Objectives

The objectives of the project include the following:

1. Research and development of advanced gas clean-up technologies for sulfur removal
2. The synthesis of composite Pd and Pd-alloy porous stainless steel membranes for WGS shift reactors with long-term thermal, chemical, and mechanical stability with special emphasis on the stability of hydrogen flux and selectivity
3. Demonstration of the effectiveness and long-term stability of the WGS membrane shift reactor for the production of fuel-cell quality hydrogen
4. The development of a systematic framework toward process intensification to achieve higher efficiencies and enhanced performance at a lower cost

5. A rigorous analysis and characterization of the behavior of the resulting overall process system, as well as the design of reliable digital process control and supervision systems
6. A detailed economic analysis for the assessment of the economic viability of the proposed intensification strategy through a comprehensive calculation of the cost of energy output and its determinants (e.g., capital cost, operation cost, and fuel cost), followed by comparative studies with other existing pertinent energy technologies

05: DE-FE0004967

Project Number DE-FE0004967	**Project Title** Advanced Palladium Membrane Scale-up for Hydrogen Separation			
Contacts	**Name**	**Organization**	**Email**	
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Principal Investigator	Sean Emerson	United Technologies Research Center	emersosc@utrc.utc.com	
Partners	Power+Energy, Inc. (P+E) Energy & Environmental Research Center at the University of North Dakota (EERC)			
Stage of Development				
__Fundamental R&D	__Applied R&D	_X_Prototype Testing	__Proof of Concept	__Demonstration

Technical Background

This project is a continuation of the United Technologies Research Center (UTRC) team's approach to increase the technology readiness level of palladium (Pd)-based metallic membranes for hydrogen (H_2) separation from coal-biomass gasifier exhaust or similar H_2-containing gas streams, in particular those developed under DOE contracts DE-FC26-05NT42453 and DE-FC26-07NT43055.

The current project is aimed at demonstrating the separation of H_2 from coal-derived synthesis gas (syngas) at the pre-engineering/pilot scale using a proprietary, surface-modified, palladium-copper (Pd-Cu) tubular membrane separator. It will include testing of laboratory-scale separators capable of producing 2 lbs of H_2 per day and of pilot-scale separators capable of producing 100 lbs of H_2 per day. UTRC's subcontractor, Power+Energy, Inc. (P+E) will manufacture the separators, and the Energy & Environmental Research Center at the University of North Dakota (EERC) will test the separators downstream of a coal gasifier.

The main objective of Phase I of the project is to construct, test, and demonstrate a Pd-Cu dense metallic tubular membrane separator capable of producing 2 lbs of H_2 per day at a minimum 95% recovery when operating downstream of an actual coal gasifier. The project will also acquire engineering data to reliably scale up Pd-Cu membrane separators to a size of 4 tons per day (tpd) of H_2 and assess the combined effects of coal gas constituents and trace contaminants on membrane performance and durability. The data will be evaluated against the DOE's 2015 targets for H_2 membrane separation and used in an engineering analysis of the separation and production method using NETL guidelines.

Under previous contracts, significant work has been done through atomistic modeling and laboratory experimentation to develop an understanding of the performance of Pd-Cu systems. Notably, previous research has evaluated the impact of membrane poisons such as carbon monoxide and hydrogen sulfide, and has included carrying out durability testing on laboratory-scale modules under DOE test protocol conditions identical to the ones specified for the current project.

Pd-Cu DURABILITY IN THE PRESENCE OF CARBON MONOXIDE (CO) AND HYDROGEN SULFIDE (H_2S)

A 527-hour test under DOE protocol conditions of a Pd-Cu membrane was conducted through project DE-FC26-07NT43055. The testing was performed under pure H_2 as well as DOE test conditions 1, 2a, and 2b in the presence of CO and H_2S. Under the specific test conditions, the pure H_2 flux of this separator was 45±2 $ft^3ft^{-2}h^{-1}$ with a H_2 recovery of >80% at 450°C and 200 pounds per square inch absolute (psia). Upon exposure to the DOE test 1 conditions, this flux decreased to 14±2 $ft^3ft^{-2}h^{-1}$ with a similar recovery. When 20 ppmv H_2S was introduced during test 2a conditions, the flux was further reduced to 11±1 $ft^3ft^{-2}h^{-1}$ with a corresponding decrease in recovery to (61±7)%; however, membrane performance remained stable during the 100+ hours at each condition. Finally, when the H_2 concentration was decreased and the sulfur level increased to 40 ppmv, the flux was reduced to 6±1 $ft^3ft^{-2}h^{-1}$ with a H_2 recovery of (50±6)%. The decrease in H_2 flux due to composition effects was completely reversible based on measurements taken with pure H_2 between each of the steps and on the fact that the membrane did not leak. This further supports the conclusion that Pd-Cu is sulfur resistant and not susceptible to sulfur corrosion.

EFFECT OF CONTAMINANTS ON Pd-Cu MEMBRANE HYDROGEN PERMEABILITY

One of the goals of the current project is to quantify the effect of gas composition and temperature on separator hydrogen permeability. Experience at UTRC has shown that the presence of other gaseous species results in lower hydrogen permeabilities. By quantifying these effects in a permeability model, membrane performance can be better predicted over a wide range of gas compositions and pressures. Work performed under DOE contract DE-FC26-07NT43055 established that the hydrogen permeability of a Pd-Cu separator can be represented by Equation 1, where the impact of non-hydrogen gas species is represented by competitive, reversible adsorption.

$$Q_{eff} = \frac{Q_{H_2}}{1 + K_{CO}P_{CO} + K_{CO_2}P_{CO_2} + K_{H_2O}P_{H_2O} + K_{N_2}P_{N_2} + K_{H_2S}P_{H_2S}}$$

In this equation, Q_{H_2} is the pure hydrogen permeability of the membrane in units of $mol.s^{-1}.m^{-1}.Pa^{-0.5}$. Q_{eff} is the effective permeability of the membrane in the presence of other gases, and the species partial pressures are in Pa. For the conventional Pd-Cu system, the impact of carbon dioxide (CO_2), water (H_2O), and nitrogen (N_2) was minimal with nearly equivalent adsorption coefficients. Hydrogen sulfide had the strongest impact and CO had an effect on hydrogen permeability that was an order of magnitude lower.

TECHNICAL PATH FORWARD WITH SURFACE MODIFIED Pd-Cu

The prime path for this contract is based on a high flux, surface-modified dense metallic Pd-Cu tubular membrane micro-channel separator. Pd-Cu membranes are already in commercial use by P+E and have been shown to be sulfur tolerant. This micro-channel design minimizes the challenges of sealing the membrane separators in a robust manner, and most effectively mitigates the thermal and chemical stresses on the separator, while achieving a high membrane packing density and reducing the H_2 separation footprint. The proprietary surface treatment has been shown to increase the flux by a factor of 5^{-6}.

At the end of DE-FC26-07NT43055, a surface-modified Pd-Cu single-tube separator was tested with a variety of gas mixtures to elucidate the impact of different gas species on the enhanced Pd-Cu. Unlike previous tests, these experiments were performed under low hydrogen recovery conditions (<10%) to better simulate “differential” conditions and simplify direct calculation of the permeability. The separator was tested under DOE protocol test conditions 1 (1%CO, no H_2S) and 2A (1% CO, 20 ppmv S) for five hours each without any change in performance due to the introduction of sulfur. This suggests that enhanced Pd-Cu membranes retain the sulfur resistance of the standard Pd-Cu, but with increased permeability.

The project team performed parameter estimation to determine the coefficients that would describe the effect of different gas species on the hydrogen permeability. For the data that was available, there was a statistically significant impact due to the presence of carbon monoxide; other gas species, such as nitrogen, carbon dioxide, and water, appeared to have a negligible effect on hydrogen permeability. The resulting fitted permeability model is shown in Equation 2, where the permeability (Q) is given in units of mol.s^{-1}.m^{-1}.Pa$^{-0.5}$, the temperature is in Kelvin, and the partial pressure of carbon monoxide is in Pa.

$$Q = \frac{Q_{H_2}}{1 + K_{CO}P_{CO}} = \frac{e^{(-18.275+2.1014\left(1-\frac{673.15}{T(K)}\right))}}{(1 + e^{(-14.216-5.5942(\frac{673.15}{T(K)}-1))P_{CO}(Pa))}}$$

The preliminary data obtained on the advanced Pd-Cu membrane will be verified and expanded during the current project in order to support the design and testing of larger units under real gasifier conditions.

Relationship to Program

This project will support important membrane separation systems advances in the Hydrogen from Coal Research focus of the NETL Advanced Fuels Program. If the project is successful, it will contribute the following benefits:

1. A palladium-based hydrogen separation from coal-derived syngas will have been demonstrated at a pre-engineering scale, which is critical for the development of a viable H_2 economy based on coal/biomass processing with CO_2 capture.
2. The palladium-based membrane separators resulting from this project are based on existing, commercially manufactured separators, which will make it easier to scale up to a larger-scale demonstration.
3. Reliable, long-term durability and corrosion data on both the palladium-based membrane and separator materials of construction shall be obtained, which will be necessary to validate the DOE’s 2015 goal of 5-year separator life.

Primary Project Goal

The primary goal of this project is to construct, test, and demonstrate a Pd-Cu metallic tubular membrane micro-channel separator capable of producing 2 lbs/day of H_2 at ≥95% recovery when operating downstream of an actual coal gasifier.

Objectives

The Phase I project objectives are as follows:

- Construct, test, and demonstrate a Pd-Cu metallic tubular membrane micro-channel separator capable of producing 2 lbs/day of H_2 at ≥95% recovery when operating downstream of an actual coal gasifier.

- Quantify the impact of simulated gas composition and temperature on separator performance.
- Compare the performance and durability of a surface-modified, higher H_2 flux Pd-Cu membrane with the baseline Pd-Cu tubular membrane.
- Evaluate various materials of construction for the separator structural parts to ensure durability under harsh gasifier conditions.
- Perform an engineering analysis using NETL guidelines of the separator design based on gasifier test performance for the co-production of electric power and clean fuels.
- Select a gasification facility partner for Phase III.

06: FY10.MSE.1610884.663

Project Number FY10.MSE.1610884.663	**Project Title** Coal & Biomass Derived Fuels		
Contacts DOE/NETL Project Mgr.	**Name** Charles Taylor	**Organization** NETL – ORD – Chemistry & Surface Science Division	**Email** Charles.Taylor@netl.doe.gov
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Partners	Dominic Alfonso, NETL Todd Gardner, NETL Bret Howard, NETL Dirk Link, NETL Chris Matranga, NETL Dan Sorescu, NETL Marvin Albao, Oak Ridge Institute for Science and Education Mike Ciocco, URS Corporation Adefemi Egbebe, URS Corporation Sonia Hammache, URS Corporation Brian Kail, URS Corporation Janice, Panza, URS Corporation Paul Zanhuis, URS Corporation		

Stage of Development				
X_Fundamental R&D	__Applied R&D	__Prototype Testing	__Proof of Concept	__Demonstration

Technical Background

NETL has taken a multi-pronged research approach to address the technical hurdles associated with the conversion of coal/biomass-to-liquids (CBTL) transportation fuels. The research to date includes a wide range of topics such as molecular modeling of catalytic reactions, the extraction and conversion of algae oils, development of catalysts, assessment of the effects that various coals and biomass have on reaction rate and product distribution, and the effects of containments on the gasification and Fischer-Tropsch (FT) process. Each of the five tasks of this project is discussed in more detail below.

TASK 1

Relative to other experimental projects in the area of clean fuels production, computational chemistry methods, and in particular first-principles calculation methods, are uniquely positioned to assist in solving the problems associated with CBTL. The main reasons for this suitability are related to the possibility that these methods can extract fundamental information at the atomic scale about the reactivity of various chemical species involved in the FT process and about the role played by different surface sites with low metal coordination (e.g., surface steps or kinks).

It is well known from previous experimental and theoretical studies, including those of NETL, that active species can be produced with smaller energy requirements at low metal-metal coordination numbers. For this reason, identification of such sites is essential for further optimization of the FT processes and for further development of the corresponding catalysts. Besides these activated sites, the use of different promoter-modified metal catalysts can also provide unique pathways for discovering new synthetic routes. In particular, the effect played by different promoter species upon adsorption and activation reactions is important to quantify to provide a deeper-level understanding of the role played by these promoters. This understanding can then be used for further optimization of the catalysts. This research complements the current experimental research tasks at NETL related to FT synthesis and co-gasification of coal and biomass.

TASK 2

Product gas separation and purification are a critical part of the thermochemical conversion of coal and biomass feeds to fuels and energy. The goal of this task is to investigate materials and approaches for the efficient separation of hydrogen (or carbon dioxide) from synthesis gas (syngas) produced from the thermochemical conversion of coal and biomass feeds.

This project task also aims to assess the viability of the technology for integration with the water-gas shift (WGS) reaction. Gasification will be an important process in the production of hydrogen, syngas for subsequent liquid fuels production, electricity, and heat. Efficient gas separation is an important component of all gasification schemes currently under consideration; it is especially critical when considering carbon dioxide (CO_2) separation for control, storage, and/or reuse. These separations generally occur under severe or unfavorable conditions, including at high temperature and pressure, and in the presence of catalytic poisoning, corrosive gases, or low concentration of the target gas. Materials currently used or under investigation for these applications suffer from various performance limitations such as low selectivity, short lifetimes and susceptibility to catalytic poisoning, and corrosive degradation by gas stream contaminants including hydrogen sulfide (H_2S), ammonia (NH_3), halides, particulates, and other contaminants. For the full potential of gasification with CO_2 control to be realized, efficient methods must be developed to overcome these separation limitations. Separation techniques investigated within this task are primarily hydrogen-selective metal membranes, but could also include materials and technologies such as sorbents, inorganic hollow fibers, and novel catalytic and protective inorganic coatings applied to traditional separation materials. This project team will work closely with fundamental computational and experimental groups within NETL in an effort to develop an understanding and new approaches to separation technologies. Although the separation technologies developed within this project will be tested using ideal gas streams, promising samples will be evaluated per the recently developed NETL hydrogen membrane test protocol and will meet DOE targets of flux, costs, chemical robustness, and mechanical integrity.

TASK 3

Coal and biomass-derived syngas contains contaminants that may negatively impact FT synthesis catalysts. Efficient technologies developed for cleaning coal syngas, which are also suitable for biomass cleaning, reduce most contaminants to acceptable levels. However, the remaining impurities may still negatively affect FT synthesis catalysts over time.

One of the most-investigated poisons present in syngas is sulfur. Though its impact on FT synthesis catalysts has been thoroughly investigated, the deactivation mechanisms of sulfur on FT catalysts are not fully comprehended and present many contradictions. Research demonstrated that sulfur poisoning of cobalt-based catalysts can cause a shift in the selectivity to lighter hydrocarbons;

however, other research reported that sulfur poisoning caused the selectivity to move toward higher hydrocarbons at low sulfur addition and to lighter hydrocarbons at high sulfur addition.

TASK 4

Conventional WGS catalysts are known to be susceptible to poisoning by a wide variety of trace impurities present in syngas, including halides, alkalis, alkaline earth, sulfur (H_2S and carbonyl sulfide [COS]) and nitrogen compounds (NH_3 and hydrogen cyanide [HCN]). In order to optimize hydrogen (H_2) and fuel production technologies, it is necessary to develop more robust catalytic materials that are able to tolerate both variances in syngas composition due to the seasonal variances in biomass, and elevated trace impurity levels. In addition, the study of catalytic behaviors in the presence of unique coal and biomass-derived syngas impurities is necessary to process this syngas optimally into H_2, fuel, and power.

TASK 5

The growth of microalgae and the subsequent production of liquid fuels from algae lipids offer a unique combination of CO_2 utilization and liquid fuel production. The algae absorb CO_2 during growth and produce biological oils (typically mixtures of free acids, esters, and glycerides) in the process. Potential yields of over 10,000 gallons of bio-oil per acre per year have been projected. These oils can be chemically transformed into transportation fuels, typically through transesterification to produce biodiesel (a methyl ester-based fuel). However, these oxygenated fuels have certain undesirable properties for some applications. A promising route from algae to liquid fuel is to produce a petroleum-like mixture of hydrocarbons, which provides a fuel that is transparent to the end user, as the functionality of alkanes is the same whether it came from crude oil or from algae lipids. Further, these renewable hydrocarbon fuels will have low sulfur and aromatic content, leading to cleaner-burning transportation fuels. However, it is currently unknown how the CO_2 and other constituents of flue gas, such as nitrogen oxides (NO_x) and sulfur oxides (SO_x), will affect the algae growth and lipid production process.

Relationship to Program

This project will support important co-production with coal and biomass advances within the Coal and Biomass Liquids Research focus of the NETL Advanced Fuels Program. A discussion of how each project task relates to the program is provided below.

TASK 1

The proposed theoretical work complements the experimental investigations at NETL on iron carbide catalysts. In concerted efforts with this group at NETL, the project team will be able to provide a comprehensive picture of the atomistic mechanism involved in the adsorption and dissociation processes of carbon monoxide (CO) in the active FT phase of iron (Fe) catalysts. If successful, this project will place NETL at the forefront of scientific research because no other group to date has been able to provide this information on the atomic scale.

TASK 2

The work conducted under this task will lead to a better understanding of the interactions of gas separations materials, such as the interactions between metal alloys and gasification stream components. These interactions can cause degradation of membrane performance via catalytic poisoning, corrosion, embrittlement, etc. Understanding these effects will enable the design of higher performance, lower cost, and longer life membranes, thereby improving efficiency of membranes applied to gasification systems.

TASK 3

The work conducted under this task will lead to a better understanding of the interaction of contaminants on FT catalytic surfaces. Ultimately, this effort will lead to more robust catalysts with better conversions, longer operating lifetimes, and higher hydrocarbon yields.

TASK 4

This research task will lead to the development of more robust catalytic materials with greater selectivity and lifetimes. This task will allow for the optimal conversion of domestic fuels (coal and biomass) to produce synthesis gas that will be converted into hydrogen and liquid fuels.

TASK 5

The successful development of algae-to-fuels technologies will enable the synthesis of liquid transportation fuels while also offering carbon management opportunities by using CO_2 emissions from fossil-derived power generation to fuel the photosynthetic reactions of microalgae.

Primary Project Goal

The primary goal of this project is to investigate, evaluate, and develop technologies to advance the efficient conversion and upgrading of energy, while also promoting end-use flexibility and complete carbon capture. The project efforts will utilize fundamental and applied scales of research to focus on the development of reaction chemistry and gas separations technologies associated with energy conversion processes.

TASK 1

The main goal of this project task is to characterize the adsorption and reaction properties of the elementary gas-phase species in the presence of alkali promoters on different types of iron surfaces using first-principles density functional theory calculations. The main goal of this task is to identify the role played by these promoters, specifically how the electronic and energetic properties of the adsorbed chemical species are modified as a function of different coverage of alkali promoters.

TASK 2

The main goal of this project task is to investigate and develop materials and approaches for the efficient separation of hydrogen (or carbon dioxide) from syngas produced from the thermochemical conversion of coal and biomass feeds, as well as the feasibility of integrating these technologies with the WGS reaction. Primary components of this work include the impurity resistance of metal-based membrane technologies and the development of alternative separation materials.

TASK 3

The main goal of this project task is to investigate the effect of contaminants present in coal-biomass syngas on FT catalysts in a fluidized bed reactor and continuously-stirred tank reactor units. The project team will study the effect of single contaminants on conversion, reaction rate, and selectivity; the synergy of the contaminants when added concurrently; and the regeneration of the spent catalysts under reduction conditions. The spent catalysts will also be characterized using techniques such as H_2-chemisorption to measure the concentration of active sites on the catalyst; BET (Brunauer-Emmett-Teller) equations will be used to determine the surface area and assess changes in the structure and chemistry of the catalysts.

TASK 4

The main goal of this task is to evaluate and develop catalyst technology to optimally process coal and biomass-derived syngas into hydrogen and liquid fuels. The introduction of biomass into the gasification process will introduce a new spectrum of contaminants, such as the vapors of alkali metals (e.g., sodium and potassium compounds) and ammonia which could either render the WGS catalysts inactive or degrade their selectivity.

TASK 5

The goal of this project task is to examine the effectiveness of selected algae species for use in carbon management and fuel production strategies when coupled with simulated effluent gas from coal or natural gas-fired power plants. This will be accomplished by introducing NO_x and SO_x contamination into the typical CO_2 feed during algal growth, and evaluating the net effect of these contaminants on photosynthetic rate, biomass production, lipid production, and lipid composition. After removing the lipids from these species, or after identifying a suitable surrogate material, the project team will assess several promising catalysts and reaction conditions that produce hydrocarbon fuels from surrogate bio-oil samples as well as possible algal lipid extracts.

Objectives

The gasification of fossil fuels, possibly combined with biomass, will be an important process in the production of hydrogen, syngas for subsequent liquid fuels production, electricity, and heat. A variety of gasification schemes are under consideration and gas separations are an important component of all of these schemes. Efficient gas separations are especially critical when considering CO_2 separation for control, storage, and reuse.

TASK 1

The specific objectives of Task 1 include the following:

- 1.1A: Identify the stability properties of alkali promoters on the Fe surface.
- 1.1B: Determine the diffusion properties of alkali promoters on the Fe surface.
- 1.2A: Determine the adsorption and activation properties of CO in the presence of alkali promoter species.
- 1.2B: Develop a first-principles-based kinetic modeling for CO methanation on Fe surfaces.

TASK 2

This task consists of two primary components: (1) contaminant-resistant metal membrane development and (2) alternative separation materials development. The specific objectives of the Task 2 subtasks include the following:

- 2.1: Develop contaminant-resistant metal membranes that are highly catalytic for hydrogen dissociation, permeable to hydrogen, and resistant to poisoning and degradation by gasification stream components.

- 2.1A: Investigate multi-component Pd-based alloys designed to develop a catalytic, protective inorganic surface layer.
- 2.1B: Investigate multi-component Pd-based alloys with inorganic additives or components that can be made to migrate to advantageous locations within the membrane.
- 2.1C: Investigate non-Pd-based metal alloys (crystalline and/or amorphous) for their potential as corrosion-resistant membrane materials and as compatible supports for Pd-based corrosion resistant alloys.
- 2.2: Develop separation materials that are alternatives to the dense metal based systems being investigated.
- 2.2A: Assess the potential of inorganic hollow fibers for H_2 separation from syngas.
- 2.2B: Investigate coating technologies that can protect the surfaces of superpermeable metal membranes to prevent catalytic poisoning and degradation and improve catalytic activity.

TASK 3

Coal and biomass-derived syngas contains contaminants that may affect FT synthesis catalysts in a disastrous manner. Efficient technologies developed for cleaning coal syngas are very suitable for biomass cleaning as well. Most of the contaminants are reduced to an acceptable level by these processes. However, the remaining impurities may still negatively affect FT synthesis catalysts over time.

TASK 4

This task will be divided into two primary components: (1) Evaluation of containments on conventional WGS catalysts, and (2) synthesis and testing of nanoparticle WGS catalysts. The specific objectives of these tasks include the following:

- 4.1: Evaluate the effects of coal and biomass-derived contaminants on FT and WGS fuel production catalyst technology.
- 4.2: Develop methods for growing model Fe, Fe-oxide, and Fe-carbide, copper, and other catalysts particles on single-crystal substrates.

TASK 5

The research will be divided into three tasks with the following objectives:

- 5.1: Determine the effective changes in algae growth rate and lipid production rate in the absence and presence of contaminants in the gas feed.
- 5.2: Determine quantity and composition changes in lipids produced under various growth conditions.
- 5.3: Develop catalyst systems and processes for converting the algal lipids to alkane-based fuels that are chemically transparent from petroleum-derived alkane-based fuels.

07: FWP-49601

Project Number FWP-49601	**Project Title** Development of Dense Ceramic Membranes for Hydrogen Separation			
Contacts DOE/NETL Project Mgr.	**Name** Richard Dunst	**Organization** NETL – Gasification Division	**Email** Richard.Dunst@netl.doe.gov	
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Partners	National Energy Technology Laboratory, University Energy Systems Inc. CRL Energy Ltd. University of Houston Department of Mechanical Engineering			
Stage of Development				
__Fundamental R&D	X Applied R&D	__Prototype Testing	__Proof of Concept	__Demonstration

Technical Background

Hydrogen is considered the fuel of choice for the electric power and transportation sectors. Like electricity, hydrogen is an energy carrier; therefore, it must be produced from fossil fuels and other resources using various technologies. During its production, hydrogen is separated from gas streams containing other species. The Office of Fossil Energy (FE) at DOE sponsors a wide range of research, development, and demonstration programs to maximize the use of vast domestic fossil resources and ensure a fuel-diverse energy sector while responding to global environmental concerns.

Ceramic membranes are of interest to DOE because they provide a simple, cost-effective method for separating hydrogen from mixed streams, allowing more efficient management of hydrogen supplies and thereby improving the economics of converting domestic coal reserves to electric power, hydrogen, and liquid fuels. Membrane separation units that can selectively permeate hydrogen gas (H_2) and retain carbon dioxide (CO_2) and carbon monoxide (CO) are also promising for pre-combustion CO_2-capture in integrated gasification combined cycle (IGCC) plants. After CO_2 removal, the H_2-rich synthesis gas (syngas) can be used as a fuel in a combustion turbine to produce electric power. Supported by NETL, Argonne National Laboratory is developing dense hydrogen transport membranes (HTMs) for separating hydrogen from mixed gases, particularly product streams generated during coal gasification, thus producing CO_2 at elevated pressure and reducing CO_2 compressor load. Hydrogen separation with HTMs is nongalvanic (i.e., it does not use electrodes or an external power supply to drive the separation), and hydrogen separated from the feed stream is highly pure, so post-separation purification steps are unnecessary.

Initially, HTM materials development followed a three-pronged approach. In one approach, the project team investigated single-phase mixed (ionic/electronic) conducting ceramics (perovskites doped on A- and B- sites). Single-phase membranes gave low hydrogen flux due to their low electronic conductivity. In the project team's second approach, they developed ceramic-metal composite (cermet) membranes containing mixed-conducting ceramics mixed with a metal. In cermets, the metal enhanced the hydrogen flux by increasing the electronic conductivity. In their third approach, they dispersed a metal with high hydrogen permeability (e.g., palladium [Pd], palladium silver [Pd-Ag], palladium copper [Pd-Cu], etc.), in a thermodynamically and mechanically stable ceramic matrix (e.g., aluminum oxide [Al_2O_3] or zirconium oxide [ZrO_2]). Cermets made by the third approach presently exhibit the highest hydrogen flux. The project team is now revisiting earlier investigations of Group IV and V non-precious-metal membranes for H_2/CO_2 separation that are compatible with warm gas cleanup and water gas shift reaction temperatures (≈350°C). These new membranes should be cheaper than the Pd-based membranes.

This project aims to identify materials with suitable hydrogen permeability and develop methods for fabricating thin, dense membranes from such materials. Chemical, mechanical, and thermal stability of the membranes are studied. Because HTMs will contact gas streams containing H_2, water (H_2O), hydrogen sulfide (H_2S), CO, methane (CH_4), CO_2, etc., in concentrations that are typical of syngas from coal-based gasifiers, the stability of the HTMs are also studied. Extensive tests have been conducted with HTMs made by mixing ≈50 vol% Pd with yttrium oxide (Y_2O_3)-stabilized ZrO_2. Using several feed gas mixtures, the project team measured the nongalvanic hydrogen permeation rate, or flux, for the cermet membranes in the temperature range 400°C–600°C. The flux followed Sievert's law and varied linearly with the inverse of membrane thickness. With 90% H_2/bal (balance) helium (He) at ambient pressure as feed gas, an ≈20 μm thick membrane on a porous substrate gave a measured flux of ≈26 cm^3[standard temperature and pressure]/min-cm^2 (≈52 standard cubic feet per hour [scfh]/ft^2) at 400°C and ≈32 cm^3[STP]/min-cm^2 (≈64 scfh/ft^2) at 500°C; the pressure of the H_2(sweep) was 0.065 atm at 400°C and 0.077 atm at 500°C.

Because product streams from coal gasification are corrosive, good chemical stability is critical for HTMs; therefore, the project team tested the effect of contaminants on the chemical stability of cermet membranes. H_2S, which is particularly corrosive, impedes hydrogen permeation through membranes with Pd or Pd alloys by forming palladium sulfide (Pd_4S). To test the chemical stability of HTMs, the project team determined the Pd/Pd_4S phase boundary and monitored a membrane's flux in tests at ≈400°C–600°C with feed gas containing 51% H_2, 31% CO_2, 1% CO, balance He & steam at ambient pressure.

Long-term (≈4 months) tests showed that the flux was stable in the above gas stream at ≤500°C. Microstructure evaluations showed that Pd_4S did not form in 10–20 ppm H_2S/10% H_2 at 500°C or in 1–5 ppm H_2S/10% H_2 at 400°C. It should be noted that the sulfur tolerance drops with decreasing temperature for constant H_2 concentration in the H_2S/H_2 gas stream, and it goes up with increasing H_2 concentration at constant temperature, e.g., at 400°C the sulfur tolerance increases from 1–5 ppm to ≈20 ppm when H_2 concentration increased from 10% to 73%.

HTMs must also have good mechanical integrity at high temperature and high pressure. The project team recently constructed a reactor in which the hydrogen flux of membranes can be measured at temperatures and pressures specified in NETL's Test Protocol for Testing of Hydrogen Separation Membranes. In this reactor, they have tested a ≈150-μm-thick cermet membrane on porous support and a Pd-Au alloy membrane prepared by Pall Corp., as per test protocol.

The project team interacted with the NETL in-house researchers during construction of the membrane test reactor and during the Pd/Pd_4S phase equilibrium studies. The project team has an agreement with CRL Energy Ltd. to test the performance of membranes in a coal gasifier slip stream. The mechanical properties of HTMs were evaluated through their collaboration with the University of Houston. Recently, Argonne has teamed with Universal Energy Systems, Inc. to fabricate defect-free thin films of HTM on porous metallic tubes using a modified sputtering process.

The HTM work has produced 4 patents, 29 publications in peer-reviewed international journals, and 20 conference proceedings. A cermet membrane developed during this project received an R&D 100 Award (selected by an independent judging panel and the editors of *Research & Development* magazine as one of the 100 most technologically significant products introduced into the market place). The present status of membrane development at Argonne and the challenges involved in bringing this technology to fruition will be presented in this project peer review meeting.

This project addresses the technology focus area of "Advanced Membrane Separation Systems" in DOE-FE's and NETL's *Hydrogen from Coal Program Research, Development, and Demonstration Plan*. NETL's Hydrogen and Clean Fuels Program supports DOE's goals in the *Hydrogen Posture Plan*, and DOE's FutureGen Project to produce electricity and clean fuels from coal with near-zero emissions. This project also addresses NETL's research needs for its Carbon Sequestration Program. Membrane separation units that selectively permeate H_2 and retain CO_2 and CO are promising for IGCC plants. Coupling warm gas cleanup with an HTM could increase the process efficiency of an IGCC plant by eliminating Selexol regeneration steam requirements and auxiliary power, and also by producing CO_2 at elevated pressures.

In its report on the hydrogen economy, the National Research Council concluded that coal must be a significant component of the R&D effort to make large amounts of hydrogen if energy security is the primary driver. Argonne's HTM project is one of the enabling technologies for producing abundant, economically attractive hydrogen and other clean fuels for the dual purposes of increasing energy security and reducing carbon dioxide emissions. The technical targets for hydrogen membranes list a flux of 300 scfh/ft^2/100 psi Δp (Δp is the difference in hydrogen partial pressure, pH_2, across the HTM) in the range 250°C–500°C by 2015. So far, the project team has measured a flux of ≈64 scfh/ft^2 at 500°C and ≈52 scfh/ft^2 at 400°C with an HTM with thickness of ≈20 μm and with feed gas (90% H_2/bal He) and the sweep gas (nitrogen [N_2]) both at ambient pressure. High-pressure measurements with a 0.86-mm-thick HTM at 490°C (pH_2 [feed]=283 psia; pH_2 [sweep]=2 psia) showed a flux of ≈2.2 scfh/ft^2, which scales to ≈95 scfh/ft^2 for a 20-μm-thick HTM of similar properties. Assuming Sievert's law behavior, calculations show that an Argonne HTM with similar properties and thickness of ≈2 μm should give a flux of ≈300 scfh/ft^2/(ÄpH_2=100 psi) (pH_2 [feed]=150 psia; pH_2 [sweep]=50 psia). Work at Argonne continues on fabricating and testing thinner membranes.

DOE's technical target requires the HTM to be resistant to contaminants (CO and H_2S). Tests have already shown that the flux of the project team's HTMs is stable in gas streams with >10% CO. Sulfur tolerance was established as a function of temperature and H_2 concentration by evaluating the microstructures of HTMs after their exposure to known H_2S concentrations and, thereby, determining the

Pd/Pd_4S phase boundary. The dense membrane's selectivity for hydrogen is theoretically infinite; hence, the membranes developed in this project meet the hydrogen purity target (99.99%), provided the thin membranes are defect free and the connections between membrane and gas inlet and outlet are free of leaks. To meet the cost target (<$100/ft^2 in 2015) by significantly reducing the amount of Pd in the membrane, thin film membranes on porous support structures are being developed. In addition, the project team is revisiting earlier work that they did with membranes made from Group IV and V non-precious metals that are cheaper and have potential to be compatible with warm gas cleanup and water gas shift reaction conditions for H_2/CO_2 separation.

HISTORY/CONTEXT LEADING TO THE HYDROGEN TRANSPORT MEMBRANES PROJECT:

During fiscal years (FY) 1992–1997, the project team performed R&D (funded by DOE-FE) on dense ceramic membranes for natural gas-to-liquid fuel conversion. In that work, the project team developed dense ceramic membranes that were mixed conductors, i.e., exhibited both electronic and oxygen-ionic conductivities. The membranes selectively transported oxygen from air on one side of the membrane to the membrane's other side, where the oxygen reacted with methane to form syngas. The dense membrane transported only pure oxygen in the form of oxygen ions. No nitrogen was transported through the membrane. Because the mixed-conducting material transported electrons with the oxygen ions, the membranes operated without any electrodes (i.e., non-galvanically), thereby making the process energy efficient and reducing the cost of converting methane to syngas by ≈35% compared to steam reforming or partial oxidation processes.

The project team's research demonstrated the concept of utilizing dense, mixed-conducting, oxygen transport membranes (OTMs) for syngas production. The OTM R&D at Argonne resulted in five patents and numerous publications. The OTM work also received an R&D 100 Award in 1995 and a Federal Laboratory Consortium Award for Excellence in Technology Transfer in 1996. In FY1998, the OTM project was moved to industries for scale-up and large-scale demonstrations. In addition to syngas production, the OTMs are being scaled up for IGCC and oxy-fuel combustion by Air Products & Chemicals and Praxair. Around December 1997, through the Federal Energy Technology Center (presently NETL), DOE-FE continued the project at Argonne while shifting emphasis to the development of dense ceramic membranes for separating pure hydrogen from mixed gas streams. Argonne's experience, expertise, and accomplishments in the development of OTMs were strong reasons for DOE-FE to continue the HTM project. In many ways, the expertise required to develop OTMs is closely related to that needed to develop membranes for separating hydrogen, which is the aim of the present HTM project. As directed by NETL, Argonne's effort originally focused on developing membranes that would operate at 800°C–900°C, and the project team had a cooperative research and development agreement with Eltron, Praxair, and ITN Energy, Inc. During this fiscal year the emphasis of HTM shifted to membranes that can function at lower temperatures (≈350°C), i.e., compatible with warm gas cleanup and water gas shift reaction temperatures; therefore, the team has started addressing the technical challenges involved in developing non-precious metallic membranes. Argonne did preliminary work with niobium membranes and measured hydrogen flux at 400°C and reported the results a few years ago. At that time, Argonne was instructed to focus on cermet-type membranes that can function at higher operating temperatures.

Relationship to Program

This project will support important advances in membrane separation systems within the Hydrogen from Coal Research focus of the NETL Advanced Fuels Program. Cost-effective ceramic membranes will benefit hydrogen-based power production and transportation applications. Using ceramic membranes to separate hydrogen from a shifted syngas stream will also benefit CO_2 storage efforts by producing highly concentrated CO_2 streams at elevated pressure. Previous studies showed that ceramic membranes can potentially increase hydrogen production by 32% and increase carbon capture by 13% over conventional pressure swing adsorption technology. A July 27, 2010 NETL news release emphasized the benefits of hydrogen separation membranes in stating that “analysis of advanced IGCC power systems indicates hydrogen membrane separation technologies could increase overall power plant efficiency and decrease electricity costs for the consumer. Hydrogen produced from the separation could be utilized as an additional turbine fuel or be further used to co-produce other fuels and chemicals.” Membrane separations might also help mitigate greenhouse gas (GHG) emissions by isolating CO_2 produced during gasification and facilitating its permanent geological sequestration or storage. HTMs might also be used in dehydrogenation reactions for producing olefins, hydrogen production from natural gas, and separation of H_2 in petrochemical processing.

Primary Project Goal

The primary goal of this project is to develop dense HTMs that separate hydrogen and produce CO_2 at high pressure from coal-gasifier-produced product streams at commercially significant fluxes under industrially relevant operating conditions.

Objectives

The project objective is to develop membranes that have high selectivity for hydrogen, give industrially significant flux, withstand high pressure and temperature, have low cost, and are mechanically strong and chemically stable in the presence of steam and impurities present in coal gasifier gas streams. Hydrogen separation membranes can be classified into five broad categories: porous (micro- and nano-porous), polymeric, metallic, dense mixed-conducting, and dense cermet membranes. Pore-closing/plugging and poor selectivity for hydrogen are major problems with porous membranes. Polymeric membranes are generally limited to lower temperatures that are not suitable for the coal-to-hydrogen program. Pd metallic membranes give high hydrogen flux but they suffer from hydrogen embrittlement, CO and H_2S poisoning, and catastrophic failure due to phase changes. Pd-alloys seem to have better tolerance to sulfur and CO, and several ongoing projects in this area are funded by NETL. The project team is developing cermet membranes because they offer the following advantages: theoretically infinite selectivity for hydrogen; capability to operate in high-temperature and high-pressure gas streams (suitable for FutureGen plants); no pores to plug/close; they supply CO_2 stream at coal gasifier pressures (important for CO_2 sequestration); and they tolerate steam, CO, CO_2, CH_4, and H_2S. Recently the project team began investigating again the technical challenges with using Group IV and V (non-precious) metallic membranes for H_2/CO_2 separation that is compatible with warm gas cleanup and water gas shift reaction temperatures (≈350°C).

Membrane development at Argonne focused initially on $BaCe_{0.8}Y_{0.2}O_{3-\delta}$ (BCY), a mixed proton/electron conductor whose high total electrical conductivity suggested that it may yield a high hydrogen flux without using electrodes or external electrical circuitry. Despite its high total electrical conductivity, however, BCY's low electronic conductivity does not allow a high nongalvanic hydrogen flux. To increase the electronic conductivity, and thereby increase the hydrogen flux, the project team developed various cermet membranes with 40%vol–50%vol of a metal (or alloy) dispersed in a ceramic matrix. In the cermet membranes, the metal enhances the hydrogen permeability of the ceramic phase by increasing the electronic conductivity of the composite. If the metal (or alloy) has high hydrogen permeability, it is called a hydrogen transport metal and can provide another transport path for hydrogen. An ≈20-μm-thick cermet membrane, containing a hydrogen transport metal (Pd) in a thermodynamically and mechanically stable yttria-stabilized zirconia ceramic matrix, presently exhibits the highest hydrogen flux (≈64 scfh/ft^2) at 500°C under ambient pressure conditions, and functions well as a hydrogen separation membrane.

Because HTMs will come into contact with gas streams containing H_2S, CO, CO_2, CH_4, and steam in "real-world" applications, the project team is studying their stability in simulated syngas mixtures that are typical of a gasifier stream. Preliminary data on stability in mixed-streams have been collected. In order to meet/exceed the DOE flux target, the project team is modifying the microstructure and surface exchange activity of HTMs and fabricating thinner membranes on porous support structures. The project team is measuring the flux in cermets at 400°C–600°C and up to ≈300 psig to evaluate the membrane performance. In order to evaluate the durability, the project team has measured the fracture toughness of their cermet membranes in the temperature range 25°C–1,200°C. Measured mechanical properties will be used in a life-time analysis model to predict mean time to failure (Weibull analysis). Combining water gas shift and hydrogen separation steps in a single membrane reactor would allow process intensification and increase efficiency; therefore, the team will investigate the water-gas shift activity of HTMs. Using an HTM to remove hydrogen from the shift reaction will increase the hydrogen yield by forcing the reaction to go forward toward completion (i.e., exceeding the thermodynamic equilibrium limit). The project team is also developing non-precious-metallic membranes (niobium [Nb], vanadium [V], tantalum [Ta], zirconium [Zr], and alloys thereof) that have potential to meet DOE flux targets at 350°C. The operating temperature of these new membranes is comparable to warm gas cleanup and water gas shift reaction conditions, and the DOE NETL Pathway Study finds the development of such a membrane would not only improve process performance and reduce the cost of electricity, but it would also help to reduce the incremental cost of carbon capture.

In coordination with NETL and its support team, the project team will evaluate the opportunities and economics of process integration. The project team will team with industrial partners to plan for scaling-up the HTM technology and demonstrating its viability in a prototype demonstration unit.

08: DE-FE0000507

Project Number DE-FE0000507	**Project Title** Demonstration of Pressurizing Coal/Biomass Mixtures Using Posimetric Solids Pump Technology			
Contacts DOE/NETL Project Mgr.	**Name** John Stipanovich	**Organization** NETL – Fuels Division	**Email** John.Stipanovich@netl.doe.gov	
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Partners	Christopher Wright, Idaho National Laboratory			
Stage of Development				
__Fundamental R&D	__Applied R&D	_X_Prototype Testing	__Proof of Concept	__Demonstration

Technical Background

NETL is exploring affordable technologies and processes to convert domestic coal and biomass resources to high-quality liquid hydrocarbon fuels. This interest is primarily motivated by the need to increase energy security and reduce greenhouse gas emissions in the United States. Gasification technologies are flexible and efficient conversion pathways to utilize coal and biomass resources. A critical technical barrier to adoption of coal/biomass gasification is the ability to deliver solids to a pressurized reactor using a dry conveyance method. The Posimetric pump technology has been demonstrated for coal feedstocks at pressures up to 1,000 pounds-force per square inch gauge (psig), but it has not been demonstrated yet for coal/biomass mixtures.

In this project, General Electric (GE) Global Research will characterize the critical material properties of coal/biomass mixtures that relate to Posimetric pump operation, translate those properties to estimates of pump performance, define biomass pretreatment specifications for successful pump operation on coal/biomass mixtures, and conduct pilot-scale pump demonstration trials with suitably pretreated coal/biomass mixtures. GE Global Research will collaborate with Idaho National Laboratory (INL) and GE Energy to execute this plan, relying on INL's biomass feedstock pretreatment expertise and GE Energy's expertise in Posimetric pump technology. The outcome of this project will be a pressurized demonstration of the pump for coal/biomass mixtures and an economic assessment of the pump technology and biomass pretreatment methods. Successful demonstration of the Posimetric pump for high-pressure delivery of coal/biomass mixtures addresses one of the key technical risks of dry-feeding technology for pressurized gasification.

The scope of this project includes the three major types of coal: bituminous, sub-bituminous, and lignite; and three biomass types: pine, switchgrass, and corn stover. These feedstocks encompass a wide range of material properties and biomass sources (e.g., woody, herbaceous, agricultural byproduct, energy grass). Coal/biomass mixtures will be produced using these feedstocks in the range of 0%—50% biomass by weight, with special emphasis on 30% and 50% biomass content. Limited characterization of 100% coal will be performed to establish a benchmark against which the performance of coal/biomass mixtures can be compared.

Relationship to Program

This project will support important advances in coproduction with coal and biomass within the Coal and Biomass to Liquids Research focus of the NETL Advanced Fuels Program. The successful development of technology for feeding pressurized coal/biomass mixtures would be a significant advancement toward large-scale production of low-net-carbon fuels using pressurized entrained-flow gasification. Pressurized entrained-flow gasification is preferred over atmospheric gasification for fuel production due to its high efficiency, low tar formation, and lower capital cost at large scale. Compared to other commercial dry-feeding technologies, the Posimetric pump offers potentially reduced operating costs and improved gasification efficiency. Posimetric pressurization of coal/biomass mixtures allows for synergistic use of the high energy density of coal and the carbon neutrality of biomass to produce fungible, low-net-carbon hydrocarbon fuels from domestic feedstocks at a commercially relevant scale.

Primary Project Goal

The primary project goal is to demonstrate that the GE Posimetric pump can operate at pressures up to 650 psi on coal/biomass mixtures containing at most 50% biomass by weight.

Objectives

The following technical objectives will be achieved during this project:

- *Identify primary biomass characteristics to enable dry-feeding coal/biomass mixtures with the Posimetric pump.* To achieve this aim, the project team will assess the effect of biomass particle size, size distribution, and moisture content on coal/biomass mixture performance in bench-scale characterization experiments. Biomass properties will be systematically varied to develop understanding of their effects on coal/biomass mixture bulk density, permeability, friction, compression behavior, and flowability. These essential performance criteria will be used to estimate the performance of the Posimetric pump at high pressure. Using this understanding of how biomass properties affect estimated Posimetric pump performance, the project team will optimize the biomass properties to achieve successful estimated pump operation at high pressure. Such results will allow the project team to predict how the optimized coal/biomass mixtures would perform in demonstration-scale pump trials later in the project.

- *Define the most favorable feedstock pretreatment scheme to produce coal/biomass mixtures that are appropriate for use in the Posimetric pump.* In order to optimize biomass properties for coal/biomass mixture Posimetric pump operation, raw biomass must be ground and dried using the most economically and technically attractive methods. Grinding methods that rely on different fracture mechanisms (e.g., cutting and shattering) may produce biomass with unique properties. For example, a shredding-type mechanism may produce more elongated particles than a shattering-type mechanism. Different types of biomass may be better suited for processing in specific types of grinding methods. Further, the cost of grinding is directly linked to the capacity of the equipment, which can be affected significantly by the moisture content of the biomass. The project team will assess how biomass particle size and size distribution are affected by the grinding method employed, and determine the most desirable process configuration to grind and dry biomass.

- *Demonstrate pressurized operation of the Posimetric pump for coal/biomass mixtures at a reasonable scale.* Upon successful characterization and optimization of biomass properties for use in coal/biomass mixtures, coal/biomass mixture trials will be conducted in a demonstration-scale Posimetric pump. Through these trials, the project team will demonstrate the ability of the Posimetric pump to deliver coal/biomass mixtures at pressures up to 650psi, and will measure performance parameters such as pump mass throughput, drive torque, operable pressure range, and gas leakage rate.

- *Perform a preliminary technical and economic evaluation of Posimetric pressurization of coal/biomass mixtures, including feedstock pretreatment.* To determine the economic impact of using the Posimetric pump for high-pressure delivery of coal/biomass mixtures, the project team will perform a preliminary economic evaluation, which can ultimately be used in a broader economic analysis of the CBTL (coal/biomass to liquids) process. INL will prepare an economic analysis of the biomass pretreatment process, and GE will analyze the experimental Posimetric pump results for coal/biomass mixtures. GE will synthesize these separate analyses to create a cohesive estimate of the economic impact of dry-feeding coal/biomass mixtures using the Posimetric pump.

09: FC26-05NT42465; DE-FC0003466

Project Number	**Project Title**			
FC26-05NT42465, DE-FC0003466	National Center for Hydrogen Technology			
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Partners	Aboriginal Cogeneration Corporation Advanced Biomass Gasification Technologies, Inc. Air Products and Chemicals, Inc. Basin Electric Power Cooperative ConocoPhillips Company ePower Synergies, Inc. Electric Power Research Institute G F Truss, Inc. General Hydrogen Corporation GreatPoint Energy Great River Energy IdaTech LLC Intellection Holding Pty Ltd. North American Coal Corporation North Dakota Industrial Commission Porvair Filtration Group Ltd. Prairie Public Broadcasting, Inc. Pratt & Whitney Rocketdyne, Inc. Resurfice Corporation Rio Tinto SGL Group – The Carbon Company Siemens Power Generation, Inc. TXU Power University of Wyoming Verendrye Electric Cooperative, Inc. Xcel Energy, Inc. Xethanol Corporation			
Stage of Development				
__Fundamental R&D	_X_ Applied R&D	_X_ Prototype Testing	__Proof of Concept	__Demonstration

Technical Background

Formed in 2004 and founded upon the Energy & Environmental Research Center's (EERC's) more than 60 years of experience in hydrogen systems, the National Center for Hydrogen Technology (NCHT) project develops and pursues commercialization of technologies that produce and utilize hydrogen for fuels and chemicals; as a coproduct with power; and other uses. Since the NCHT's inception, the EERC has received more than $60 million in funding for hydrogen-related projects ($20 million for the NCHT project, which includes congressionally directed project funds) involving more than 85 partners (27 with the NCHT).

The NCHT project's 22 activities span a broad range of technologies that align well with Advanced Fuels Program goals and, specifically, those described in the *Hydrogen from Coal Program Research, Development, and Demonstration (RD&D) Plan*. Technical activities include: development of hydrogen production technologies by gasification and gas cleanup with domestic coals, especially cheap, abundant coals; extension of novel, proprietary EERC bonding technologies to join high-temperature, hydrogen-compatible materials that enable more efficient hydrogen and power production; and development of tools to increase efficiency and reliability of gasification systems through improved fuel selection and preparation, among others. Of particular note are NCHT's efforts to provide a flexible gasifier facility capable of larger-scale, more realistic testing of advanced technologies (e.g., low-cost hydrogen separation membranes), which directly address DOE "high cost" and "lack of demonstration" technical barriers. This technical breadth and close working relationship with DOE and numerous partners endow the EERC with the capacity to quickly respond to evolving DOE needs, especially in areas such as warm-gas cleanup and hydrogen purification.

RISK MANAGEMENT APPROACH

To a great extent, the NCHT project pursues technologies that permit it to leverage and extend the EERC’s experience and unique facilities focused upon fossil fuel and hydrogen technology development. While the project exploits the expertise of its many partners, its core capabilities are provided by the EERC’s more than 345 scientists, engineers, and staff applying a 60-year history of research in hydrogen and gasification. The EERC has one of the largest, single-site collections of pilot-scale gasifiers in the world—a site comprising 250,000 square feet of laboratories, demonstration facilities, fabrication shops, and offices. Risk is reduced because much of the project comprises activities that are (1) well-defined with limited inherent uncertainty (e.g., testing, data collection and optimization), (2) systematically planned with active partner involvement, and (3) performed using EERC-designed gasification equipment for which the EERC has thousands of hours of operating experience. Risk is further reduced by the ability of the EERC to quickly marshal its resources to resolve problems that the project might encounter.

CURRENT-YEAR ACTIVITIES

Activity 1.10 (A1.10). Historically, combustion has been the preferred route to obtaining energy from coal because of its simplicity and low cost; consequently, knowledge and commercialization of combustion technologies far exceed that of other routes, such as gasification. However, combustion loses its advantage to gasification when carbon capture or hydrogen and fuels production requirements are imposed. While interest in carbon capture and hydrogen and fuels production is increasing—expected to subsequently increase attention on gasification technologies—knowledge and commercialization of gasification technologies are limited in general. One such crucial deficiency is the understanding of and ability to predict ash behavior in gasification systems. Slag flow, slag attack on refractory, ash deposition on heat-transfer surfaces, corrosion and erosion of system materials, and gas cleanup profoundly affect the performance and reliability—and thus economics—of gasification systems. The ability to relate coal characteristics to equipment and process requirements would provide a substantial advantage when selecting coals as feeds to existing gasification systems or when designing and operating gasifiers with specific coals. This activity seeks to collect and experimentally generate coal characterization and performance information for various gasifiers, and then incorporate these into models to produce a tool capable of predicting ash behavior based on coal characteristics, gasification system configuration, and operating parameters. The resulting models will be validated using case studies of full-scale systems.

Activity 1.12 (A1.12). A1.12 includes tests of two technologies using the transport reactor development unit (TRDU), which is a pilot-scale gasifier capable of firing up to 500 pounds per hour of fuel and producing 400 standard cubic feet per minute of synthesis gas (syngas). The first technology thermally pretreats coal to reduce moisture and impurities (e.g., mercury) content to improve efficiency and to reduce the complexity and expense of incorporating emission control equipment into gasification systems. Removing moisture prior to transporting and feeding coal to a gasifier reduces weight and increases the energy content of coal, thereby improving the efficiency of the transportation system and gasifier. Removing hazardous impurities (e.g., mercury), whose emissions are regulated before introduction into the gasification system reduces the challenge of removing impurities at elevated temperatures or the inefficiency of cooling and reheating the product stream to remove the impurities. This activity will perform a seven-day gasification test, feeding both treated and untreated coals, to evaluate the performance of the gasifier under a variety of operating conditions. The results should provide better estimates of the value of the technology as well as guidance for further development. The second technology applies hydrogen separation membranes to separate syngas into a carbon dioxide stream for sequestration and a hydrogen stream that is adequately pure for fuel, chemical, and power applications. Membranes have an economic advantage over other separation technologies because of the fact that they produce carbon dioxide streams at system pressures that could be more than 1,000 psi for gasifiers as compared to less than 10 psi for pressure swing absorbers. This significantly reduces the compression needed for sequestration, which is nominally 2,000 psi. With no moving parts and, potentially, no steam or other additional energy inputs, hydrogen separation membranes promise to be reliable and inexpensive. Thus, based upon ideal laboratory data, the costs of using membrane technologies are estimated to be substantially less than those of conventional separation technologies. However, membranes can suffer from chemical processes (e.g., hydrogen embrittlement, contaminant poisoning), seal difficulties, and fabrication issues that reduce their practicality and utility and increase their costs. Unfortunately, membranes are still in a relatively early stage of development, so little testing has been performed under conditions and at scales comparable to those that they would experience when commercialized. This lack of experience creates uncertainty regarding whether membranes are capable of functioning commercially in their current state of development, and if not, what is required to enable them to function commercially and at what ultimate cost. A1.12 seeks to reduce this uncertainty by observing hydrogen separation membrane responses to exposure to a coal-based syngas slipstream from the TRDU for up to 200 hours at about a 2 lb/day hydrogen production rate under conditions comparable to those expected commercially. The results of testing will be incorporated into process and economic models to estimate cost of power production and carbon dioxide capture and sequestration. Testing will also expose membrane deficiencies that will need to be resolved prior to commercialization to guide future development efforts. Among others, these deficiencies include most of the barriers to hydrogen separation called out in the *Hydrogen from Coal Program RD&D Plan*.

Activity 1.13 (A1.13). As noted above, gasification technologies have economic advantages over conventional combustion technologies when carbon sequestration is required. Gasification possesses similar advantages in electric power generation applications, an example of which is integrated gasification combined cycle (IGCC) technology. It gasifies coal and then separates the syngas into a carbon dioxide stream (which is directed to sequestration) and a hydrogen stream (which becomes fuel for the gas turbine). While commercialization has been limited, one such plant in Spain discovered potentially harmful deposition of iron and nickel carbonyl compounds in equipment. To avoid this, the plant manufacturer is developing proprietary coatings that can be applied to equipment surfaces to retard or halt carbonyl deposition. The EERC will simultaneously expose coupons that were treated by the manufacturer and untreated coupons to a syngas atmosphere, which is very similar to that of the plant in Spain by using its small pilot-scale coal-fed gasifier and, if necessary, a nickel and iron carbonyl generator. The EERC will also perform various analytical tests to evaluate the efficacy of the treatment.

Activity 3.5 (A3.5). Conventional small, on-site hydrogen production units produce hydrogen at low pressure. The NCHT is developing a novel, proprietary technology, simplified high-pressure hydrogen production, as well as an associated high-pressure, pressure swing absorber hydrogen purifier to provide hydrogen at elevated pressure without costly hydrogen compression and capable of accepting coal-derived hydrogen carriers as feedstock. A3.5 will upgrade the hydrogen purification sub-system and optimize the system to deliver 700 bar hydrogen at 1 kilogram per minute.

Relationship to Program

This project will support important advances in membrane separation systems within the Hydrogen from Coal Research focus of the NETL Advanced Fuels Program.

A1.10. Coal properties have profound effects on gasification system performance and availability, affecting not only the gasifier but also downstream gas cleanup, hydrogen purification, and carbon dioxide capture. The tool being developed by A1.10 has the potential to guide equipment design for feed coals of interest as well as to guide coal selection, blending, equipment operation, and maintenance based on coal characteristics. The result of this is increased efficiency and reduced capital, operating, and maintenance costs because of improved designs (e.g., less “overdesign” and more focused design improvements), as well as more predictable and optimized operations, and more predictable maintenance scheduling.

A1.12. A1.12 activities will employ the TRDU to assess the performance of thermally treated coal and hydrogen separation membranes. The TRDU, which is capable of processing 500 pounds per hour of coal and producing 400 standard cubic feet per minute of syngas, offers the opportunity to test and demonstrate novel technologies at larger scale and over longer term—closer to commercial scale—than lab and many pilot units. If successful, thermal *pretreatment of coal* to reduce moisture and contaminants (e.g., mercury) could reduce costs associated with warm-gas cleanup emission control equipment. It also permits the opportunity to geographically relocate cleanup to a more suitable location—suitable, for example, with respect to disposition of contaminants or equipment space. *Hydrogen separation membranes* have promised cheaper and more compact syngas purification with higher-pressure carbon dioxide streams (enabling cheaper carbon dioxide capture) than conventional separation technologies. Testing of such membranes generally has been under carefully controlled conditions that lack many of the constituents found in commercial syngas streams. The results have been incomplete estimates of gas cleanup requirements and of performance (e.g., durability, sensitivity to contaminants, flux variation), which have limited the accuracy of cost estimates, the identification of mediation requirements, and the evaluation of the practical value of the technology. A1.12 will provide a realistic demonstration of membrane capability by exposing membranes to conditions resembling commercial processes: coal-based syngas volumes, for current tests of 2 pounds per day of hydrogen (but capability for future testing of 100 pounds per day) at more efficient elevated temperatures and pressures for extended durations (up to 200 hours). In addition to improving the quality of cost estimates and identifying required technology enablers, this testing will aid in determining the extent to which different membranes have addressed the “hydrogen separation” barrier defined by DOE, such as seal technology, resilience to thermal cycling, selectivity, membrane structural integrity and performance, and poisoning of catalytic surfaces, among others. Beyond coal-based syngas, the lessons learned and development resulting from the testing potentially can aid other applications such as natural-gas-based hydrogen and separation of hydrogen from mixtures in refinery and chemical processes.

A1.13. The objective of A1.13 is to test metal coatings that are expected to be able to retard or stop the deposition of iron and nickel carbonyl compounds on treated metal surfaces. If the treatments are successful, the solution will avoid potentially more expensive and disruptive alternative solutions, and the solution will be applicable to other syngas equipment and gasification applications.

A3.5. Safety and security concerns associated with storing and transporting hydrogen have increased interest in on-site hydrogen production. While coal gasification scales up very easily, small-scale units of this sort present challenges. A3.5 can enable coal’s participation in on-site hydrogen production by developing a more efficient, cheaper processing unit for hydrogen carriers that are produced by large, efficient centralized coal facilities.

NCHT project success supports expanded use of domestic coal to coproduce hydrogen with power, fuels, and chemicals, as well as provides economic, environmental, and security benefits.

Primary Project Goal

The NCHT draws upon resources from across the EERC, including the EERC’s internationally recognized coal gasification and emission control expertise, to pursue DOE goals of coproducing hydrogen with power using high-efficiency gasification at near-zero emissions and reducing the cost of hydrogen production by 25% over current coal-to-hydrogen technology.

Objectives

MILESTONES

For the current year, the NCHT project’s four technical activities have five milestones.

M1.10.1, A1.10, will deliver software based on EERC test runs that predict ash behavior in gasification systems based on the incoming fuel properties. The milestone will be satisfied when the initial validation work is reported.

M1.12.1, A1.12, will evaluate and compare the performance of a partner’s thermally treated coal with untreated coal and will assess performance of hydrogen separation membranes using the EERC’s 500-pound-per-hour coal transport reactor demonstration unit. The milestone will be satisfied when the draft test plan is provided to the partners.

M1.13.1, A1.13, will expose then analyze and evaluate the effect of a syngas stream produced by a small, pilot-scale coal-fed gasifier upon candidate materials for incorporation into future advanced (IGCC) power plants. A1.13's first milestone will be satisfied after completion of modifications to the test specimen holder and heater and upon commencement of the first test.

M1.13.2, the second A1.13 milestone, will be satisfied upon completion of exposure of test specimens.

M3.5.1, A3.5, will upgrade the gas cleanup system and optimize the performance of the EERC's simplified high-pressure hydrogen production process. The milestone will be satisfied when parametric test results are available.

WORK PLAN

With the resources and risk management approach d as a guide to work plan development, the following are work plans for the current activities. The A1.10 work plan performs several tasks concurrently: (1) identifying key coal property, system configuration, and operating parameters; (2) collecting data from the technical literature and previous EERC and current NCHT research and generating experimental data describing ash behavior in gasification systems; (3) developing mathematical models of coal ash behavior; (4) designing the user interface; and (5) generating computer code. As key coal, system, and operating parameters are identified and data are received, they will guide development of and be incorporated into the ash behavior models. As the models develop, they will merge with the user interface from the tool. Case studies of full-scale gasification systems will be collected to serve as a means to validate the model and tool. The A1.12 work plan involves modifying the TRDU to be capable of installing and exposing hydrogen separation membranes to a slipstream of syngas at the desired conditions, receiving treated and untreated coals and test membranes, and then running seven-day tests of the coals and tests of up to 200 hours of the membranes. The A1.13 work plan involves modification of the bench-scale gasifier by adding side-by-side coupon holders, an electric heater and, if necessary, a metal carbonyl generator. After exposing coupons for up to 200 hours in coal-derived syngas, analytical tests will be performed to determine the extent of metal carbonyl deposition on the treated and untreated specimens. The A3.5 work plan involves enlarging the reformer and adding high-pressure hydrogen separation equipment. When completed, experimental runs will be performed to optimize the unit in terms of catalyst and operating parameters. Following this, a short-term small-scale verification and demonstration test will be performed. All of the above activities will conclude with preparation of final reports.

POTENTIAL REAL-WORLD APPLICATIONS

In addition to coproduction of hydrogen from coal with power, real-world applications of the results of NCHT activities include: advanced gasifiers for synthetic natural gas, alcohols, diesel, and chemical production from coal, biomass, and other fuels; use in refinery and fertilizer production processes; and other carbon dioxide separation applications. Additional applications also exist for the materials development and distributed hydrogen production activities within the program.

10: DE-FE0001009

Project Number	**Project Title**			
DE-FE0001009	Nanoporous, Metal Carbide, Surface Diffusion Membranes for High Temperature Hydrogen Separations			
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Partners	Dr. Ashok Damle, Pall Corporation, Ashok_Damle@pall.com			
Stage of Development				
X Fundamental R&D	__Applied R&D	__Prototype Testing	__Proof of Concept	__Demonstration

Technical Background

Colorado School of Mines is developing transition metal carbides as inexpensive substitutes to platinum group metals (PGMs) for use in high-temperature hydrogen (H_2) membranes. This project stems from recent theoretical studies that use density functional theory to show that hydrogen binding energy for molybdenum carbide (Mo_2C) is similar to platinum and alloys of platinum group metals. It also responds to the DOE call for the development of high-temperature H_2 membranes that contain no PGMs.

To the best of the project team's knowledge, the concept of using transition metal carbides for H_2 separation membranes has not been previously explored. Carbide materials are very thermally stable (melting points exceeding 2,000°C) and are chemically stable over a wide range of conditions (e.g., they are used to catalyze the water-gas shift reaction, hydrodesulfurization, hydrocarbon reforming, etc.).

One of the strategies of this project is to create nanoporous, transition metal carbide films to serve as surface diffusion membranes. The key development in metal carbide catalysis came from Boudart and coworkers, who developed a method to convert dense molybdenum trioxide (MoO_3) into high surface area Mo_2C by temperature-programmed reaction (TPR) using mixtures of hydrogen and methane (CH_4). The mechanism for the MoO_3 to Mo_2C transformation involves the substitution of carbon for oxygen in the MoO_3 lattice, with little displacement of the Mo atoms during the reaction. Because the molar volume of Mo_2C is smaller than the molar volume of MoO_3, micropores form as the oxide transforms to the carbide. The MoO_3 is also converted into Mo_2C without having metallic molybdenum (Mo) as a reaction intermediate. In addition, metal sintering is avoided, unsupported catalysts can be prepared with very high surface areas ($\geq$100 m^2/g), and corresponding pore sizes are below 3 nm. Tungsten carbides can also be synthesized using analogous conditions—pore size can be engineered by modification of the TPR conditions for the production of Mo_2C. Both molybdenum and tungsten carbides chemisorb hydrogen, which is the basis for chemically stable, low-cost, hydrogen separation membranes. To enable the surface diffusion mechanism, dense oxide films will be deposited on porous supports, followed by TPR to create the nanoporous structure required.

As a corollary to the project's experiments with porous molybdenum carbide as a surface diffusion membrane, this project is also examining the use of this material as a catalyst layer on dense metal membranes. Palladium (Pd) and Pd alloys dominate this field due to the fact that they are able to both catalyze the hydrogen dissociation reaction and rapidly permeate the dissociated hydrogen. Several crystalline, body-centered cubic (BCC)-structured elements—vanadium (V), niobium (Nb), tantalum (Ta), and zirconium (Zr)—have much higher permeability for the dissociated H_2 species than Pd, but have limited catalytic activity for the hydrogen dissociation reaction. This issue is typically addressed by coating the super-permeable BCC metal with a thin catalyst layer that is active for hydrogen dissociation, such as Pd. However, the resulting membranes often have a narrow range of operating temperatures—if the range is too low, the temperature will promote embrittlement of the BCC metal membrane layer, but if the range is too high, the temperature will cause alloying of the catalyst layer with the permeable layer and result in loss of permeability. A low-cost hydrogen dissociation layer that can operate at higher temperatures than a metallic catalyst is therefore being pursued by this project as both a novel discovery and potentially a great spur to the development of BCC-phase dense metal membranes. Preliminary results demonstrate that nanostructured Mo_2C films can serve as the catalyst layer for H_2 dissociation, enabling vanadium or other BCC metal foils to serve as a high temperature membrane for H_2 separation.

To investigate both the surface diffusion and catalyst layer on dense metal membrane concepts in parallel, this project has conducted and is continuing to conduct the activities that follow.

FACILITIES DEVELOPMENT

A significant fraction of the first nine months of this project were dedicated to building or upgrading the project team's facilities to execute the studies described below. The following capabilities have been fully installed and are all now operational:

- Modification of a PECVD reactor to accepts both planar supports and the tubular AccuSep supports provided by the project team's industrial collaborators at Pall.
- Construction of a TPR apparatus for the conversion of dense oxides into nanoporous metal carbides. It includes a residual gas analyzer (RGA) as an online process monitor.
- Purchase, installation, and commissioning of the Micrometrics pore size analyzer. This instrument includes both physisorption and chemisorption capabilities.
- Upgrade of a mixed gas permeation apparatus for performance testing of the H_2 membranes produced in this work. This system enables the use of the DOE NETL Test Protocol for H_2 Separation Membranes (DOE/NETL-2008/1335)
- Acquisition and installation of a Mo_2C target for magnetron sputtering of nanostructured films.

SYNTHESIS OF NANOPOROUS, MOLYBDENUM CARBIDE FILMS

This project is developing a two-stage process that involves the synthesis of dense oxide films by plasma-enhanced chemical vapor deposition (PECVD) followed by carburization using TPR. The deposition rate needs to be high, as it is expected that the required thickness will be in the range of 0.5–5 µm. Optimum thickness will reflect a competition between maximizing flux and completely sealing the macropores present in the underlying support to ensure selectivity. The porous supports that are being investigated include the following:

- Pall AccuSep® tubular supports that consist of zirconia on stainless steel supports
- Planar stainless steel discs
- Planar alumina and silica supports
- Silicon wafers: used as controls and for characterization

PECVD was chosen for its ability to produce uniform coatings on non-planar substrates at both high rate and at ambient temperature. This project is also exploring the use of pulsed power modulation to improve the conformality of film deposition on these meso-structured supports. Synthesis of MoO_3 films has been accomplished using mixtures of MoF_6 (molybdenum fluoride), H_2, and O_2. The first co-reagent scavenges F (fluorine) while the latter forms the oxide. The parameters that were optimized with respect to rate and quality include the following:

- MoF_6 flow rate
- O_2:MoF_6 and H_2:MoF_6 ratios
- Radio frequency (RF) power and operating pressure

The dependence of these variables was found to be nominally identical to the Colorado School of Mines' previous work with PECVD synthesis of WO_3 (tungsten oxide) from analogous gas mixtures: tungsten fluoride (WF_6)/H_2/O_2. Conditions were identified that produced films at a high rate (>50 nm/min) with high refractive indices (~2.2). Chemical and structural analysis confirmed that the films were fully oxidized and free of fluorine impurities. While trace amounts of F were present on the surface of the as-deposited films, they can be removed with a light sputter clean; there is no evidence of F in the bulk.

The spectra from the Mo 3d5 region from an as-deposited film after the TPR carburization procedure displays the doublet due to spin-orbit coupling in d orbitals. The primary peak is located at a binding energy (BE) of 233.0 eV, in good agreement with the expected position for Mo in its fully oxidized +6 state. The intensity of the doublet is in agreement with the theoretically expected 3:2 ratio, further confirming the absence of sub-stoichiometric compounds. After carburization, the Mo doublet is shifted to a BE of 228.4 eV, while retaining the 3:2 ratio indicating that it in single oxidation state. The peak position is consistent relative to metallic Mo that appears at BE = 227.8 eV.

The spectra displaying the C1s region indicates that the as-deposited MoO_3 films have adventitious carbon located at a BE of 285 eV due to surface contamination, which can be readily removed with sputter cleaning. After carburization, the electronic state of carbon in the Mo_2C is distinctly shifted, appearing at 283.4 eV.

PRODUCTION OF PINHOLE-FREE FILMS ON POROUS SUPPORTS

An essential first step to the production of surface diffusion membranes is the elimination of pinholes. The as-received stainless steel supports being evaluated by the project have huge, micron-size pores. Dip coating with the polymer eliminates much of the surface roughness. Taking this one step further, a 30-minute MoO_3 deposition makes the oxide appear to be very smooth and deposited conformally on the templated, polymer surface; after deposition, the polymer layer is removed via oxidation. This project has recently produced leak-free oxide-coated supports that are now being carburized.

OPTIMIZATION OF TPR CARBURIZATION PROCESS

The TPR conditions used for carburization were optimized using MoO_3 powders while the project team was developing their thin film deposition capabilities. The approach was to adapt recipes that are well-described in the catalysis literature. The primary variables used in the TPR process include the following:

- Choice of hydrocarbon—e.g., CH_4, ethane (C_2H_6)—and % dilution in H_2 (20–80%)
- Ramp rate (0.5–5°C/min)
- Soak temperature (600°C –900°C) and duration (1–4 hrs)

A thorough investigation of these parameters above was conducted; metrics for analysis included X-ray diffraction (XRD), surface area, pores size, and carbon monoxide (CO) uptake. Results show that temperature and reaction time were the most important keys for achieving the hexagonal, β-Mo_2C phase. Conditions that employed temperatures ≥700°C and reaction times ≥3 hours always yielded pure â-Mo_2C. Parameters such as ramp rate and the percentage of CH_4 had a negligible impact on crystal structure, but they are expected to impact the pore size distribution.

To further quantify the nanostructure, studies using the Micrometrics instrument are currently under way. Initial results show BET surface areas >20 m^2/g, and the project team expects that this can be further optimized. More importantly, when standard TPR conditions are applied to MoO_3 thin films, a complete transformation to the carbide phase is observed. The carbide film remained well-adhered to the substrate, and the project will explore the H_2 separation performance of these materials in the next quarter.

FABRICATION AND PERFORMANCE OF CARBIDE/VANADIUM COMPOSITE MEMBRANES

For dense metal membrane composites, the optimal thickness for the catalyst layer is expected to be thin (5–50 nm), as its role is limited to H_2 dissociation due to the underlying BCC metal providing selectivity. This project’s initial synthesis efforts have focused on magnetron sputtering. The typical sputter rate using the refractory target is, as expected, low (~1 nm/min), but it is sufficient for the fabrication of the thin catalyst layers—a separate carburization step is not necessary and the technique offers the ability to clean the BCC metal *in situ*. The as-received V foils have a significant oxide layer, which is expected to impede transport. This oxide is removed using an argon (Ar) sputter treatment before deposition of the carbide layer.

As with the surface diffusion membrane concept, it is expected that the structure and morphology of the carbide layer will be critical to its performance as a H_2 dissociation catalyst. To that end, the project team conducted a preliminary evaluation of sputter parameters, through which it was found that substrate temperature has a profound impact on microstructure. Dramatic transformations were observed as temperature was increased from ambient to 600°C. Films sputtered at room temperature display the cubic α phase and a nanocrystalline morphology. At 200°C, the crystallinity improves dramatically, as the nanocrystals appear to coalesce. A further increase in temperature to 400°C yields a smooth, disordered film. However, at 600°C, the films begin to adopt the hexagonal â crystal structure, which is accompanied by a rougher, nanostructured surface.

The project has recently commenced performance evaluation of the V/carbide composite membranes. In these experiments, a Mo_2C target was used to apply catalytic layers by sputtering on both sides of dense vanadium foils. The membranes were then sealed into 0.5" vacuum coupling radiation (VCR) fittings with Ag-coated nickel (Ni) washers and mounted in a furnace. Membranes were heated under flowing inert gas, and then single-gas permeation experiments were conducted with H_2 and nitrogen (N_2) at varying temperatures, with the feed pressure as high as 100 psig and the permeate pressure kept at ambient conditions (12 psia). Testing showed that none of the membranes under consideration had any detectable N_2 permeance during the testing period. Hydrogen permeance in the Mo_2C-sputtered membranes showed a square root dependence on pressure gradient, suggesting that the rate-limiting step in H_2 transport was diffusion through the bulk, not dissociation or adsorption/desorption. The maximum hydrogen flux measured was at 700°C and 100 psig feed pressure, and was 0.088 $mol/m^2/s$ = 23.7 $scfh/ft^2$. By comparison, a palladium membrane of equivalent thickness would be expected to have a hydrogen flux of approximately 0.41 $mol/m^2/s$ = 110 $scfh/ft^2$ under the same conditions. Because palladium presently costs 600 times more than vanadium, this reduced flux may not be critical. As a control experiment, a vanadium membrane with no Mo_2C layer was also tested and found to have zero hydrogen permeability, strongly suggesting that the catalytic activity of the Mo_2C for hydrogen dissociation is key to hydrogen transport. While these initial experiments seem quite promising, this project will have to further investigate both the mechanism and the stability of the metal carbide/V composite membranes in the next quarter. Parameters of interest include dependence on V thickness, carbide thickness, and carbide morphology.

Relationship to Program

This project supports important membranes separations systems advances in the Hydrogen and Coal Research focus of the NETL Advanced Fuels Program. The benefits of this project stemming from the replacement of Pd (or other precious metals) in membranes for hydrogen separations include the potential for reduction in cost of materials, the energy and CO_2 footprint to produce them, and the dependency on foreign sources. This project is also educating future scientists in the areas of energy, clean coal utilization, and membrane separations. For example, during the first year, two postdoctoral researchers, four graduate students, five undergraduate students, and three high school students have worked directly on this project. Many of these have been co-authors on papers presented at national meetings.

Primary Project Goal

The primary goal of this project is to demonstrate the viability of transition metal carbide-based membranes as cost-effective alternatives to platinum group metals for meeting DOE NETL 2015 hydrogen separation performance targets.

Objectives

This project aims to achieve the following objectives:

- Fabricate nanoporous, transition metal carbide-based surface diffusion membranes.
- Fabricate composite membranes using BCC metals and transition metal carbide catalysts.
- Test and optimize the performance of the membranes described above.
- Develop strategies for the selective repair of large pores (>3nm).

- Explore the performance of analogous metal sulfides in these applications.
- Meet DOE NETL 2015 targets for hydrogen flux and selectivity.

11: DE-FE0001293

Project Number DE-FE0001293	**Project Title** Integrated Water Gas Shift Membrane Reactor Utilizing Novel, Non-Precious Metal Mixed Matrix Membranes			
Contacts DOE/NETL Project Mgr.	**Name** Jason Hissam	**Organization** NETL – Fuels Division	**Email** Jason.Hissam@netl.doe.gov	
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Partners	Dr. Benjamin Mattes, Santa Fe Science & Technology Inc.			
Stage of Development				
_X_ Fundamental R&D	__Applied R&D	__Prototype Testing	__Proof of Concept	__Demonstration

Technical Background

The University of Texas at Dallas is developing non-precious metal mixed-matrix membranes (MMMs) for integration into a water-gas shift membrane reactor for hydrogen (H_2) separations under NETL test protocol conditions. This project responds to the DOE 2015 challenge to develop high-flux hydrogen separation membranes that are robust and stable.

MMMs comprise select porous additives and thermally and chemically stable polymers. Carbon molecular sieve and pure zeolite membranes offer very attractive permselectivity properties relative to polymeric materials, but processing challenges and high costs hinder their industrial development. High-performance polymers are low-cost and easy to process, but pure polymers have seemingly reached a limit in the tradeoff between permeability and selectivity. MMMs are formed by combining nanoporous materials with polymers, enabling the membranes to benefit from the properties of both materials and holding great promise for hydrogen / carbon dioxide (CO_2) separations.

MMMs have included nanoporous materials such as carbon molecular sieves, zeolites, metal oxides and, more recently, carbon nanotubes and fullerenes and metal-organic frameworks. This project has identified the zeolitic imidazolate frameworks (ZIFs)—a new class of metal organic frameworks that includes materials isostructural with several zeolite phases—as a promising family of additives for MMMs. ZIFs exhibit high thermal (up to 500°C) and chemical stability (steam, organic solvents, and H_2S). ZIFs also comprise inorganic/organic hybrid molecular sieves that exhibit some of the highest surface areas ever reported and selective adsorption of target gases generated during coal processing. Pure ZIF membranes have shown promise for gas separations, but are subject to the same limitations as pure zeolite membranes. Nevertheless, ZIF preparations are generally high-yielding and scalable, and some ZIFs are commercially available. The hybrid nature of ZIFs facilitates their interaction with high-performance polymers, thus promoting good interfacial contact. Some ZIFs are also hydrophobic—in the case of ZIF-8, the hydrophobic pore could help to facilitate the diffusion of H_2 while minimizing the diffusion of water (H_2O), thus preventing the loss of H_2O from the reactor. Several ZIFs have been shown to be stable at NETL test protocol conditions.

The high performance polymers of interest in developing MMMs include commercially available polyimides such as Matrimid® and VTEC®, polybenzimidazole (PBI), and those synthesized in The University of Texas at Dallas laboratory, including 6FDA derivatives and PIM-1. These polymers are stable above 250°C and can be cross-linked to further enhance their separation properties.

A challenge with MMMs is creating good contact between the polymer and the additive. An effective interface enables good dispersions of molecular sieve materials at high loadings. The key parameters in controlling the interfacial properties include the particle size, shape, composition, and pore architecture of the additive, as well as the functionality of the polymer. A nanoporous particle will be effectively wetted by a polymer if its surface possesses organic functionality (i.e., like dissolves like), as is the case for the ZIF metal-organic frameworks. The project team has already succeeded in producing defect-free flat MMMs of ZIF-8 in Matrimid, with unprecedented loadings as high as 50% (weight per weight [w/w]).

This project's strategy for fabricating MMMs is first dispersing the ZIF nanocrystals in an organic solvent by stirring and sonication. ZIF dispersion can be improved by using a resonant acoustic mixer, which rapidly breaks up the aggregates without destroying the ZIF crystals. This step may be followed by a particle pre-coating step from a dilute polymer solution. The polymer matrix solution is then added to the ZIF solution with stirring and sonication. The suspension is concentrated, and then deposited as a flat membrane using an automatic film applicator housed in a laminar flow hood. Alternatively, the ZIF/polymer suspension can be either dip- or spray-coated onto tubular porous alumina supports or hollow fibers. The membranes are then carefully annealed in a vacuum oven to remove casting solvent.

The project team synthesized and characterized nanocrystals of the chemically and thermally stable ZIF-7, ZIF-8, and ZIF-69 using X-ray diffraction, scanning electron microscopy, thermogravimetric analysis, and nitrogen adsorption. Procedures are currently being developed for the synthesis of ZIF-20 and ZIF-95 nanocrystals (micrometer-sized crystals of these materials were obtained). Based on this work, the project team has determined that ZIF-8 and ZIF-95 are stable in the presence of steam and/or H_2S, and is continuing testing of the other ZIF materials.

The project team also tested PBI, VTEC, and Matrimid as flat membranes at 200°C and 5 atmosphere (atm) for gas permeation. Permeabilities were determined to be consistent with those reported in the literature; permeabilities for helium (He), nitrogen (N_2), and CO_2 in VTEC increased from 3.6, 0.02, and 0.74 at 35°C to 53.81, 2.51, and 9.47 Barrers, respectively. The calculated $He/CO_2 = 5.7$ selectivity of this membrane was comparable to that reported for $H_2/CO_2 = 7.5$, tested at 300°C. No evidence of plasticization occurred in the membrane. Cross-linkable and cross-linked 6FDA-DABA-DAM, 6FDA-durene, and PIM-1 polymers were synthesized with high molecular weights (>100 kiloDaltons [kDa]). The project team is currently measuring ZIF MMMs for H_2/CO_2 separations. H_2 selectivity by ZIFs is achieved through the sieving effect of the small pore apertures. For example, the pore aperture of ZIF-8 (0.30 nm) favors the transport of H_2 over CO_2 thereby increasing the H_2/CO_2 selectivity of the MMM from 2.0 for pure Matrimid to 7.0 for a 50% (w/w) ZIF-8/Matrimid MMM (feed: 50/50 mixture of H_2 and CO_2).This results from an increase in the diffusivity selectivity for H_2.

Mixed-matrix membranes from Matrimid, VTEC, and 6FDA-durene polymers containing ZIF loadings up to 60% (w/w) were successfully prepared and tested for gas permeation at 35°C. ZIF-8 (50% w/w)/6FDA-durene demonstrated permeability/selectivity properties above the Robeson bound for H_2/CO_2 separation (400% increase in permeability [P] and 70% increase in selectivity [α] compared to the pure polymer).

Relationship to Program

This project supports important membranes separations systems advances in the Hydrogen and Coal Research focus of the NETL Advanced Fuels Program. The benefits of this project stemming from the replacement of palladium (Pd) or other precious metals in membranes for hydrogen separations include the potential for reduction in cost of materials, the energy and CO_2 footprint to produce them, and the dependency on foreign sources.

This project is educating future scientists in the areas of energy, clean coal utilization, and membrane separations. For example, during the first year, two postdoctoral researchers, four graduate students, five undergraduate students, and three high school students have worked directly on this project. Many of these have been co-authors on papers presented at national meetings.

Primary Project Goal

The primary goal of this project is to develop non-precious metal mixed-matrix membranes comprising chemically and thermally stable polymers and zeolitic imidazolate frameworks and to integrate them into a water-gas shift membrane reactor for hydrogen separations under NETL test protocol conditions.

Objectives

The achievement of the primary project goal requires optimization of the membrane components (e.g., ZIFs, polymers) and their integration into functional modules for water-gas shift membrane reactors. Hence, the project team must first screen ZIFs for use in MMMs (year 1: milestone 1), acquire (or synthesize) and screen alternative polymers (year 1: milestone 2), and fabricate and test MMMs in different configurations (year 1: milestones 3, 4, and 6). Adsorption properties of the ZIF additives at high temperature and pressure are also being measured (year 1: milestone 5 revised).

Year 1 milestones include the following:

1. Screen ZIFs for use in MMMs (x-ray diffraction [XRD], thermal gravimetric analysis [TGA], H_2O, and H_2S exposure).
2. Acquire and synthesize alternative polymers (PBI, VTEC, and cross-linked 6FDA).
3. Fabricate and characterize flat ZIF/Matrimid and ZIF/alternative polymer membranes.
4. Fabricate and characterize ZIF/polysulfone hollow fiber membranes.
5. Install a high-pressure volumetric analyzer (HPVA-100, Micromeritics) and obtain temperature/pressure adsorption isotherms of hydrogen and carbon dioxide from targeted ZIFs up to 15 atm and 300°C, conditions at which water-gas shift reactors operate (revised milestone).
6. Perform permeability studies of flat ZIF/Matrimid and ZIF/alternative polymer membranes (high temperature and pressure, pure and binary gas mixtures).

In year 2, the project team will be transitioning to a new membrane geometry (year 2: milestone 1), fabricating hollow fiber MMMs using high-temperature polyimides (year 2: milestone 2), measuring permeability properties of ZIF/polymer MMMs in the integrated water-gas shift membrane reactor using pre-water-gas shift synthesis gas composition (year 2: milestones 3 and 5), and conducting long-term stability studies of the MMMs at high temperature and pressure, and in the presence of water and hydrogen sulfide (year 2: milestone 4).

Year 2 milestones include the following:

1. Fabricate and characterize tubular ZIF/polymer membranes.
2. Fabricate and characterize ZIF/polybenzimidazole hollow fiber membranes.
3. Permeability studies of flat or tubular ZIF/polymer as well as ZIF/polysulfone and ZIF/polybenzimidazole hollow fiber membranes in the integrated water-gas shift membrane reactor using pre-WGS synthesis gas.
4. Long-term stability studies of MMMs at high temperature and pressure, and in the presence of water and synthesis gas contaminants (e.g., hydrogen sulfide [H_2S]).
5. Construct the integrated water gas shift membrane reactor (milestone moved from year 1).

In year 3, the project team will extend its studies to other ZIF/polymer systems using post-WGS synthesis gas compositions generated in situ (year 3: milestones 1 and 2). In addition, permeability studies of the most promising ZIF/polymer MMMs will be conducted in the presence of H_2S using the facilities at DOE-NETL Pittsburgh.

Year 3 milestones include the following:

1. Fabricate and characterize ZIF/VTEC polyimide hollow fiber membranes.
2. Perform permeability studies of ZIF/polymer MMMs using post-WGS synthesis gas.
3. Perform permeability studies of ZIF/polymer MMMs using the DOE-NETL Pittsburgh facility (using synthesis gas that includes H_2S).

12: FC26-05NT42456

Project Number FC26-05NT42456	**Project Title** Production and Storage of Hydrogen from Coal Using C1 Chemistry			
Contacts DOE/NETL Project Mgr.	**Name** Donald Krastman	**Organization** NETL – Fuels Division	**Email** Donald.Krastman@netl.doe.gov	
Principal Investigator	Gerald Huffman	University of Kentucky-CFFLS	Huffman@engr.uky.edu	
Partners	Auburn University West Virginia University University of Utah University of Pittsburgh			
Stage of Development				
_X_ Fundamental R&D	__Applied R&D	__Prototype Testing	__Proof of Concept	__Demonstration

Technical Background

The Consortium for Fossil Fuel Science (CFFS) is a research center led by the University of Kentucky that includes participants from the University of Kentucky, West Virginia University, Auburn University, the University of Utah, and the University of Pittsburgh. For many years, the CFFS has been conducting research focused primarily on the conversion of coal and other hydrocarbon resources (e.g., waste plastics, waste tires, and biomass) into clean, high-quality liquid transportation fuels using direct coal liquefaction, Fischer-Tropsch synthesis (FTS), and pyrolysis processes. The CFFS also has extensive experience in the production of hydrogen from gaseous and liquid hydrocarbons. This CFFS project is focused on the development of technology for the production of liquid transportation fuels by FTS from coal-derived synthesis gas (syngas) that is enriched by hydrogen produced by processes that emit little or no carbon dioxide.

Relationship to Program

This project will support important advances in coproduction with coal and biomass within the Co-Production with Coal and Biomass area of the NETL Advanced Fuels Program. As discussed above, the primary goal of the current CFFS research program is to develop novel technology for the production of liquid fuels and hydrogen (H_2) from coal while generating minimal carbon dioxide emissions using novel methods that do not require carbon capture and sequestration. If this goal is met, it should play a major role in making the conversion of coal-to-liquid transportation fuels economically and environmentally viable. Additionally, approximately 60 students have been trained under this research contract. Many of them are choosing to pursue careers in fossil energy research and development, which could eventually be the greatest benefit of the program.

Primary Project Goal

The primary goal of this research project is to develop novel technology for the production of liquid fuels and hydrogen from coal while generating minimal carbon dioxide emissions. The program consists of three major components:

1. Hydrogen production with very low or carbon-neutral carbon dioxide (CO_2) emissions. The goal of this task is to replace the water-gas shift reaction from FTS and eliminate the need for carbon capture and storage (CCS) during the production of liquid fuels from coal.
2. Fischer-Tropsch synthesis with higher activity, selectivity, stability, and carbon monoxide (CO) conversion.
3. Crosscutting research in the areas of systems analysis and catalyst characterization to enhance topics 1 and 2.

Objectives

HYDROGEN PRODUCTION

In previous CFFS research, three H_2-producing processes have been developed that generate little or no carbon dioxide: catalytic dehydrogenation (CDH) of gaseous hydrocarbons, reforming of biocrude in supercritical water; and catalytic electrolysis of water. This project aims to further improve these processes and couple them to FTS in the laboratory. Work on coupling FTS and CDH to produce a viable FTS-CDH reactor system is now in progress.

FISCHER-TROPSCH SYNTHESIS

The primary objective of this project area is to develop catalytic systems and/or unique FT processes such as supercritical fluid FTS (SCF-FTS) that will enhance CO conversion and selectivity. The goal of this task is to develop technology that will yield FT products that are close to the desired final product, maximizing efficiency and minimizing energy use.

CROSS-CUTTING RESEARCH

This project area consists of two activities:

- *Systems Analysis.* Systems analysis provides environmental, logistical, and economic analysis to assess industrial viability. This analysis has been successfully applied to several program projects, including analyses of both gas phase and SCF-FTS processes using performance data obtained by CFFS researchers. Analyses of the catalytic dehydrogenation process, along with updated results for supercritical water reforming, are ongoing. Recently, work has been initiated on analyzing coal/biomass gasification processes.
- *Catalysis Characterization*. The rational design of catalysts is essential to reduce the energy costs associated with each coal and/or biomass conversion pathway to transportation fuels production. Catalysis characterization is also essential to improve the quality and selectivity of the fuel products. The focus of this research program is to employ a broad range of analytical techniques to improve understanding of the structural and electronic characteristics of catalysts to optimize their design. Several novel catalysts have been developed as part of this research program, including precisely size-controlled nanoscale catalysts for liquid fuels applications and CDH, and synthetic doped ferrihydrite nanoflakes for FTS. This activity has significantly enhanced the value of all projects in the contract involving catalyst development.

13: DE-FE0001248

Project Number DE-FE0001248	**Project Title** Yeager Airport Hydrogen Vehicle Test Project			
Contacts DOE/NETL Project Mgr.	**Name** Darryl Shockley	**Organization** NETL – Fuels Division	**Email** Darryl.Shockley@netl.doe.gov	
Principal Investigator	William Davis	WVU Research Corporation	Bill.Davis@mail.wvu.edu	
Partners	Central West Virginia Regional Airport Authority			
Stage of Development				
__Fundamental R&D	__Applied R&D	_X_Prototype Testing	__Proof of Concept	__Demonstration

Technical Background

Energy independence is a critical factor affecting homeland security in the United States and other countries. An adequate and reliable fuel supply is a key component of any strategic plan for economic development and national security. In every nation, decisions regarding the choice of fuel can and do have serious adverse economic and environmental consequences, including budget deficits caused by excess oil imports and ecological degradation caused by pollution. Nevertheless, energy consumption is increasing at a dramatic rate everywhere in the world.

As more countries grow and prosper, the world will see an increased demand and an accelerated depletion of petroleum and foreign oil resources that can be used for transportation. The widespread use of alternative fuels, alternative fuel vehicles, advanced vehicle technologies, and other petroleum reduction technologies in the foreseeable future is not only feasible, but necessary. If Americans are to wean themselves off foreign oil, enjoy cleaner air, celebrate fewer environmentally-related illnesses, and help create jobs in the current U.S. economy, they must first be educated on available and forthcoming petroleum reduction technologies. Once they feel comfortable with advanced vehicle technologies, the acceptance and increased use of these technologies will follow.

In addition, with the expanded implementation of these new technologies will come challenges and uncertainties for those exposed to them. This creates the need to train first responders on how to safely approach and extricate passengers at the scene of an accident involving alternative fuels, alternative fuel vehicles, and advanced vehicle technologies. There also is the need to provide education to government officials, fleet administrators, and others who can spearhead the implementation of these vehicles' use.

Results of an October 2006 public opinion survey, commissioned by the National Alternative Fuels Training Consortium (NAFTC) and conducted by R.L. Repass & Partners, Inc. (Cincinnati, OH), provided evidence that the primary barrier to a consumer buying an alternative fuel vehicle or advanced technology vehicle is a lack of knowledge. Learning about, and becoming comfortable with, alternative fuels, alternative fuel vehicles, and advanced vehicle technologies can be expected to both empower and assist Americans in their acceptance and selection of future transportation purchases.

Since an increased understanding of alternative fuels, alternative fuel vehicles, and advanced vehicle technologies is imperative to their ultimate success and adoption by the American public, there is a critical need to provide this information. NETL has been tasked to determine the effectiveness of hydrogen-powered vehicles. The initial test in West Virginia will be at the Yeager Airport in Charleston, WV. This test will determine the effectiveness of hydrogen vehicles in the hands of everyday users in a complex setting.

The NAFTC's *Hydrogen Vehicle Test Project* is designed to determine the effectiveness of hydrogen-powered vehicles in support of everyday operations at Yeager Airport. The findings will be used to support the further testing of hydrogen stations and vehicles across the state of West Virginia and the United States. The testing and results will also be used to provide information, education and awareness of hydrogen as a vehicle power source to public officials, consumers and others in the test area.. This project's education and outreach efforts will lead to a significantly increased acceptance of the use of hydrogen vehicle technologies by fleet managers and by individual consumers.

Relationship to Program

This project will support advances in hydrogen-powered vehicles as part of the NETL Advanced Fuels Program in the following ways:

- The project will provide data on the usage of hydrogen vehicles in an operational tempo that has not been tested.
- The successful completion of this project will provide data that can be used to develop additional programs using the architecture of the station and vehicles.
- The project will provide information on training requirements for operators, technicians, first responders, and others working on hydrogen projects or operations.

Primary Project Goal

This program will test and evaluate hydrogen vehicles in the state of West Virginia in a mid-tempo business environment at the Yeager Airport hydrogen fueling station. This program will provide demonstrated information to be used in the development of additional programs and education and outreach activities in support of hydrogen vehicles.

Objectives

The objectives of the hydrogen vehicles project are divided into two separate goals, each with its own objectives.

Goal 1. Provide project management for the Hydrogen Vehicle Test Project at Yeager Airport, including the following tasks:

- Purchase of four hydrogen-powered vehicles to be used as test vehicles for the project.
- Reporting, including data collection of vehicles from the operators of vehicles. The NAFTC will monthly collect the data using a format provided by the U.S. DOE NETL.

a. The NAFTC will prepare reports to DOE on the status of vehicles, fuel usage, driver reports and interviews, and other data as determined through coordination with NETL, State of West Virginia personnel, and the NAFTC.
b. The NAFTC will develop and conduct driver training for potential operators of the hydrogen-powered vehicles.

Goal 2. Provide education and outreach for the Hydrogen Refueling Station project at Yeager Airport, including the following tasks:

- The NAFTC will conduct safety training for first responders in Central West Virginia.
- The NAFTC will coordinate a workshop with the Central West Virginia Regional Airport Authority.
- The NAFTC will conduct an education and outreach activity for West Virginia officials after vehicle purchases. This activity will be coordinated with the Central West Virginia Regional Airport Authority, the West Virginia Energy Department, and NETL.
- The NAFTC will coordinate an outreach activity for citizens of the Charleston area and other WV residents to highlight the hydrogen-powered vehicles and their capabilities. This workshop will be coordinated with the Central West Virginia Regional Airport Authority, the West Virginia Energy Department, and NETL.
- The NAFTC will develop a workshop for code officials of other potential hydrogen refueling projects that will allow DOE to duplicate the hydrogen fueling station and vehicle project in other locations throughout West Virginia and the United States.

14: FC26-08NT0005988

Project Number	**Project Title**			
FC26-08NT0005988	Design and Construction of Early Lead Mini Fischer-Tropsch Refinery			
Contacts	**Name**	**Organization**	**Email**	
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Partners	Purdue University Southern Illinois University			
Stage of Development				
__Fundamental R&D	_X_ Applied R&D	__Prototype Testing	__Proof of Concept	__Demonstration

Technical Background

To carry out a program to evaluate the commercial and technical viability of advanced technologies for the production of Fischer-Tropsch transportation fuels manufactured from Illinois basin coal, the Southern Illinois University Coal Research Center, the University of Kentucky (UK) Center for Applied Energy Research (CAER), and the Energy Center at Purdue University entered into a Memorandum of Understanding to form the “Coal Fuel Alliance” to support complementary and joint research focusing on applied and developmental needs for coal/biomass-to-liquids (CBTL) technologies. Accordingly, the overarching objective of this project is to advance the design and construction of this facility at the University of Kentucky CAER. A key expected benefit is the know-how, show-how associated with the facility, which can be used to house test beds for new concepts at a level of expenditure that is affordable. It will provide open-access facilities and information in the public domain to aid the wider scientific and industrial community, and a means to independently review vendor claims and validate fuel performance and quality. Environmental considerations, particularly how to manage and reduce carbon dioxide emissions from CBTL facilities and from use of the fuels, will be a primary objective of the research. More specifically, research at this new CBTL facility will focus on the following technical areas.

COAL & BIOMASS GASIFICATION

This area includes: demonstrated gasifiers suitable for integration with fuel synthesis or hydrogen production; compatibility with emerging coal and biomass feedstocks; vessel design and increased knowledge of bed behavior/agglomeration; and effective process control to maintain gasifier performance and emissions at target levels with varying load, fuel properties, and atmospheric conditions.

GAS CLEANUP/CONDITIONING

Syngas cleaning is an area where there are further opportunities for improvement. It involves cost reduction and the adjustment of the H_2 to CO ratio in the syngas for optimal Fischer-Tropsch performance. Moreover, gas cleaning and conditioning systems to remove contaminants (tar, particulates, alkali, ammonia, chlorine, and sulfur) not suited to downstream catalysts will be important, as will systems for hot gas particulate removal and advanced desulfurization adsorbents.

GAS CONVERSION BY FISCHER-TROPSCH (FT) SYNTHESIS

Although the cobalt catalysts (mostly proprietary) have expected lives of up to five years, there might be cheaper catalyst formulations with similar life expectancies. For iron catalysts, which are cheaper, the thrust for longer life and cheaper production costs would also apply. The robustness (mechanical attrition resistance) of catalysts varies a great deal and especially some iron catalysts could be relatively weak, limiting the separation of catalyst and wax. There is little open access information on these issues, and open R&D will reduce concerns in this area. In the FT synthesis, there is great variation possible to fine tune selectivities (such as olefin/paraffin ratios, degree of branching, chain length, level of oxygenates, and type of oxygenates). The product spectrum is influenced by a large number of parameters like catalyst characteristics (reduction/pretreatment, morphology, promoters, mechanical strength, etc.), process variables (temperature, temperature gradient, pressure, syngas flow rate, syngas composition, gas purity, etc.), and reactor design features. The combination of these process conditions determines the conversion and the selectivity pattern for the chosen system. There are no open R&D facilities where such work can be done at a scale beyond the normal scientific lab scale. Having such a facility or facilities could provide potential project developers with a platform from which to optimize the process for their market needs by integrating the synthesis optimization with the product optimization.

PRODUCT WORK-UP OR REFINING

The discussion here is restricted to the “low-temperature” FT or slurry bed systems, as these are the simplest FT plants that are likely to be built first in the United States. The primary products from the FT reactor are typically separated by a series of thermal steps to separate products in boiling point fractions analogous to a conventional refinery. The lighter gases can, depending on the level of syngas conversion and the value of the energy in the tail gas, be partially cleaned up for recycle (e.g., water removal) or used as a fuel gas in the plant. In some cases (especially when using a Lurgi gasifier), the methane in the gas can be separated out and reformed to produce more syngas. The simplest configuration is likely to be that the light liquids (“naphtha”) can be used either as a petrochemical feedstock or potentially as a gasoline component after significant octane number enhancement through isomerization/alkylation (here research could be applied to improve yields). The next heavier cut would be the “straight run” diesel/fuel oil cut, and lastly there will be heavier waxes, which can be hydro-cracked to bring the boiling point into the diesel range. Variations would be used to produce different grades of jet fuel. Depending on specifications, hydro-isomerization would also be used to improve the cold-temperature properties and lubricity characteristics. In the area of product characteristics, there are likely to be opportunities for analytical method development for simpler and more applicable testing procedures, and collaboration with certification authorities will be desirable. As in a refinery, there are usually “polishing” steps and special fractionation and or hydrotreating steps to ensure that all specifications for a particular product grade will be met. Thus, special grades of fuels and chemicals can be produced in an FT facility, such as special grades of jet and aviation fuels or other “boutique” fuels and chemical components. This is clearly an area for product-specific R&D based on the FT system and by combining the FT system parameters with a multi-purpose continuous product work-up facility, a very powerful tool for companies interested in making particular products can be established. The issue of separating and purifying components and fractions from complex streams in an FT facility is part of the challenge to maximize profits. In this area, creative and novel separation technologies could be developed to add value to a CBTL venture.

ENVIRONMENTAL CONSIDERATIONS

Coal is a complex material and processing it into high-purity clean liquid fuels requires detailed attention to environmental, health, and safety issues. In a generic sense, technologies are available to address the issues regarding the various emissions, effluents, and solids residual materials. The question is to what extent the costs associated with these processing steps will impact the overall viability of a venture. Thus, CBTL facilities can be clean coal facilities and, as with most of the other process units, there are opportunities to enhance the viability by bringing down costs through performance improvement. Specific research topics could include the efficient use and re-use of water; beneficial use of the ash from the gasifiers (this will depend on the type of gasifier selected); further improvements of technologies to capture sulfur from the gasifiers as well as from the power plant; improved mercury capture (depending on gas purification process); control of volatile organic components; and optimization regarding potential CO_2 capture from all CO_2 sources in a CBTL facility.

SYSTEMS ANALYSIS AND INTEGRATION

To support the above activities, it will be essential to have a systems analysis and integration capability. This can be applied for the work plan itself and also to analyze the components in the process facility. These skills will have to be developed and models will have to be verified against the experimental results to enable initial assessments of scale-up opportunities. Developing the software capabilities to control the integrated R&D facility and to apply process engineering optimization to the operation of the facility and to conceptual process configurations will be an ongoing activity. At a more fundamental level, the capability of computational chemistry could be used to assess ways to improve separations and catalysis in various parts of the plant.

SCALE-UP AND DEMONSTRATION

The reactor types used commercially (up to 20,000 barrels per day [bbd] per single reactor) have been fine tuned over a long time and incremental improvements are made continually. Some key factors in reactor design include the hydrodynamics (gas and catalyst dispersion, back mixing, temperature profiles, heat distribution), the withdrawal of the high amount of exothermic heat from the FT reactor, good feed gas distribution (mostly patented technologies), the optimization of recycle streams, the effective recovery of catalyst particles (in fluidized beds in the gas phase and in slurry rectors from the wax), pressure drop (especially for tubular reactors as used by Shell), and catalyst feed and withdrawal systems as might be applicable. Developing and verifying reactor design models become meaningful at reactor diameters above about 2 feet, so that this activity will only be valuable at the larger scale of operation before full commercialization. The products produced in smaller units will nevertheless be typical of FT products. If collaboration with engineering contractors can be established, that could strengthen an RD&D team to focus the R&D on relevant issues that will have an economic impact. Normally design details are protected very well by the technology owners. In a similar way, the expertise for scale-up resides mostly with experienced contractors.

Relationship to Program

This project will support important advances within the Fischer-Tropsch focus of the Co-Production with Coal and Biomass area of the NETL Coal and Biomass to Liquids Research Program.

A key benefit expected is the know-how, show-how associated with the facility, which can be used to house test beds for new concepts at a level of expenditure that is affordable. It will provide open-access facilities and information in the public domain to aid the wider scientific and industrial community, and a means to independently review vendor claims and validate fuel performance and quality.

Environmental considerations, particularly how to manage and reduce carbon dioxide emissions from CBTL facilities and from use of the fuels, will be a primary objective of the research once the facility is constructed. The inclusion of a coal/biomass gasification unit will be used to assess and address the carbon footprint issue associated with coal-to-X facilities.

Primary Project Goal

The primary project goal is to advance the design and construction of a coal/biomass-to-liquids process development unit at the University of Kentucky Center for Applied Energy Research that is capable of producing up to 1 barrel per day of FT liquids and finished products for subsequent testing.

Objectives

The project is divided into three phases, each with its own tasks and objectives.

PHASE 1 : ORIGINAL AWARD - DOE PROJECT DE-FC26-08-NT05988

Task 1.1 Technology Selection
To select and enter into collaborative agreements with the technology vendors for each of the principal processing units envisioned for the coal/biomass-to-liquids process development unit. These include Unitel for natural gas reforming; Rentech and Velocys for Fischer-Tropsch (FT) synthesis; W.R. Grace for fluid catalytic cracking (FCC); and UOP for hydrocracking (HYC), dehydrogenation (DHY), and alkylation (ALK).

Task 1.2 Front End Engineering and Design (FEED) Study
Key technical information for each unit process is being provided to CAER's engineering contractor, Zeton Inc., for use in completing the FEED study. The purpose of the FEED study is to firm up the process design and develop the process and instrumentation designs (P&IDs). Zeton will investigate the optimal skid layout to accommodate the equipment and process units, and suggest an appropriate control system based on its experience. Finally, Zeton will provide a +/-10% cost estimate and a more precise schedule for the detailed design, procurement, and construction phase of the project.

Task 1.3 Architectural and Engineering (A/E) Plans and Specifications for Refinery Building
Within the next several months, CAER anticipates that it will have sufficient information from the FEED study to engage an architectural and engineering company. The A/E firm will provide design and engineering services related to the general site work, building shell, materials of construction, thermal and moisture control, heating, air conditioning and ventilation, fire protection, finishes, equipment, furnishings, special construction, conveying systems, lighting, mechanical, electrical, plumbing, energy efficiency, and special building utility services.

Task 1.4 Construction of Refinery Building
Following receipt of the architectural and engineering plans and specifications, the University of Kentucky's Capital Project Management Division with CAER will bid the project for construction pursuant to Department of Energy approval and Commonwealth of Kentucky procurement statutes.

PHASE 2: FIRST PLUS-UP AND RENEWAL APPLICATION FOR DOE PROJECT DE-FC26-08-NT05988

Task 2.1 Cost Estimation and Feasibility Study for Incorporation of Feed Handling and Preparation, Gasifier and Gas Cleaning/Conditioning and Compression Sections

UK CAER has contracted Zeton Inc. as a teaming partner for completion of a cost estimation and feasibility study. The purpose of this preliminary study is to firm up the requirements for potentially incorporating one or more experimental gasifiers and the necessary feed handling and preparation, and gas cleaning/conditioning and compressions sections. Zeton's deliverables will include:

- Process flow diagrams (PFD) in AutoCAD format showing major equipment items and key instrumentation and process control loops for incorporation of experimental gasifiers and gas cleaning/conditioning system
- A summary of the mass and energy balance for key components and streams in Microsoft Excel format for the desired feed and product stream compositions and flows
- Based on process datasheets, a summary of preliminary sizing information for the major equipment units in Excel format
- A simplified 2-D plan and elevation layout drawing in 11 x 17 formats for the gasifier and gas cleaning/conditioning process modules in AutoCAD format
- A +/-30% cost estimate for the gasifier and gas cleaning/conditioning modules, and a preliminary Gantt chart schedule for a FEED study, procurement, and construction phase of the project

Task 2.2 Fabricate and Install Natural Gas Conditioning and Reformer Section

In this task, the project team will install and commission a natural gas reformer as a failsafe and first means of producing synthesis gas. In addition, they will install and commission certain utilities and ancillary equipment needed for natural gas conditioning and management, including storage vessels, preheaters, metering and mixing, and controls.

Task 2.3 Shakedown and Commissioning of Natural Gas Conditioning and Reformer

In this task, the project team will shakedown and commission the natural gas conditioning and reformer section over a period of months—initially for immediate house gas needs (continuous stirred tank reactor [CSTR] catalyst studies) and eventually for its integration with downstream refinery units, particularly the FT reactor(s) and hydrocracking units.

PHASE 3: SECOND PLUS-UP AND RENEWAL APPLICATION FOR DOE PROJECT DE-FC26-08-NT05988

Task 3.1 Fabricate and Install Syngas Work-up and Conditioning and Compression Section (i.e., CO_2 capture membrane and compression system)

In this task, CAER will install, procure, and commission over a period of months a membrane-based syngas work-up, conditioning, and compression system for adjustment of gas feeds and CO_2 capture and compression. A detailed design will be made to include additional detailed information for the skid-mounted units, such as piping and tubing isometrics, a complete structural design, an ASME stamped vessel design, detailed refractory specifications, detailed electrical conduit and wiring drawings, detailed instrument conduit and wiring drawings, detailed utility drawings, module interface specifications for process flows and safety relief flows, and vendor quotes for all major equipment including equipment-specific drawings. The deliverables will include: executed purchase orders based on vendor quotes;

timely delivery and acceptance of the items ordered; executed contract with a suitable construction contractor or engineering procurement company; and delivered pilot plant skid(s) that comply with specifications.

Task 3.2 Shakedown and Commissioning of Natural Gas Conditioning, Syngas Generation, Syngas Work-up, and Conditioning and Compression Section
In this task, the project team will shakedown and commission the complete natural gas conditioning, syngas generation, syngas work-up, and conditioning and compression section over a period of months—initially for immediate house gas needs (CSTR catalyst studies) and eventually for its integration with downstream refinery units, particularly the FT reactor(s) and hydrocracking units.

Task 3.3 Detailed Design of Long-lead Item: FT Reactor
In this task, CAER will complete a detailed design of an iron-based slurry bubble column FT reactor, which is considered to have the longest lead to commissioning. A detailed design will be made to include additional detailed information for the skid-mounted pilot plant, such as piping and tubing isometrics; a complete structural design; an American Society of Mechanical Engineers (ASME) stamped vessel design; detailed refractory specifications; detailed electrical conduit and wiring drawings; detailed instrument conduit and wiring drawings; detailed utility drawings; module interface specifications for process flows and safety relief flows; and vendor quotes for all major equipment including equipment specific drawings.

15: FC26-06NT42449

Project Number FC26-06NT42449	**Project Title** Production of High-Hydrogen Content Coal-Derived Liquids			
Contacts DOE/NETL Project Mgr.	**Name** Darryl Shockley	**Organization** NETL – Fuels Division	**Email** Darryl.Shockley@netl.doe.gov	
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Partners	EnviRes LLC University of Kentucky Center for Applied Energy Research University of Alaska Fairbanks Emerging Fuels Technology Smith Management Group			
Stage of Development				
__Fundamental R&D	_X_Applied R&D	__Prototype Testing	__Proof of Concept	__Demonstration

Technical Background

Most Fischer-Tropsch (FT) plants with coal feedstocks have used iron catalyst systems for FT synthesis. Iron FT catalyst systems are more tolerant of synthesis gas (syngas) with coal's low hydrogen (H_2)/carbon monoxide (CO) ratios because the iron system can catalyze a significant amount of water-gas shift—and thus increase the effective H_2/CO ratio—at essentially the same time as it catalyzes FT synthesis. Furthermore, iron FT catalyst systems may be more tolerant (or perhaps simply less expensive to replace) than cobalt-based systems to the types and amounts of contaminants that remain in coal-derived syngas, even after cleanup.

Cobalt FT catalyst systems need their incoming syngas to have a H_2/CO ratio of about 2:1 to produce the highest quality products. The H_2/CO ratio of coal-derived syngas must be increased, and the level of cleanup may need to be increased as well for adequate catalyst life. These steps add cost and complexity, but the cobalt catalyst system may (or may not) provide other advantages that more than compensate.

This project, evaluating the potential applicability of cobalt FT catalyst systems to coal-derived syngas, was awarded to ICRC on March 30, 2006, with Syntroleum Corp. as ICRC's partner and provider of both cobalt FT catalyst technology and the project's required 20% cost-share. Syntroleum had financial difficulties, and dropped out of the project in December 2006. NETL managers stated that they wanted the project to continue, if at all possible, along the same general lines as had been planned with Syntroleum, and NETL encouraged ICRC to find a partner (or partners) such as the University of Kentucky (UK) Center for Applied Energy Research (CAER) to replace Syntroleum. The kick-off meeting for the revised ICRC project with EnviRes LLC and CAER as new partners was held in November 2008.

Relationship to Program

This project will support important advances in the co-production with coal and biomass focus of the NETL Advanced Fuels Program. The project is providing real-world data, and then using it to evaluate the overall pros and cons of cobalt versus iron catalyst systems for synthesis of Fischer-Tropsch fuels with coal-derived syngas. It is motivated by the following:

- Iron (Fe) FT catalyst systems have been used by virtually all coal-based FT plants to date.
    - Iron FT catalyst is relatively cheap, and more tolerant of coal's low H_2/CO syngas ratio.
    - Iron can "simultaneously" catalyze water-gas shift and FT synthesis.
- Cobalt (Co) FT catalyst is more expensive than iron, and is generally less tolerant.
    - Cobalt needs syngas H_2/CO ratio boosted to ~2:1, which increases processing cost.
    - Cobalt is sensitive to impurities, so more expensive syngas cleanup may be required.
    - Cobalt's fuel products can be superior, thus requiring potentially less expensive upgrading to obtain high-hydrogen content coal-derived liquid fuels.

Primary Project Goal

The primary goal of this project is to evaluate and compare intrinsic differences between Co and Fe catalysts for Fischer-Tropsch synthesis utilizing coal-derived synthesis gas. Specific parameters to be evaluated include the effect of contaminants contained in coal-derived syngas on catalyst activity and lifetime, the required H_2/CO ratios for efficient conversion, the required level of syngas cleanup to maintain catalyst reactivity, and raw product upgrading requirements to produce high-hydrogen content coal-derived liquids.

Objectives

This project will evaluate both cobalt and iron-based Fischer-Tropsch catalyst systems and provide real-world data in several technical areas. The project team will provide technical analyses and process data on the following core elements required for the integration of FT synthesis technology with coal-derived syngas:

- Sensitivity of cobalt FT catalysts to the types and amounts of impurities in coal derived syngas
- Analysis of impurity removal or syngas cleanup, to include identification of impurities and their expected concentration ranges, and evaluation of removal strategies and the equipment required, including economics of removal
- Technical analysis and economic evaluation of CO water-gas shift and subsequent CO_2 removal, including a study of the types and characteristics of process equipment required
- Evaluation of coke-oven gas cleanup strategy and equipment, and the cost-effectiveness of such equipment, as an additional or alternative (to water-gas shift) source of hydrogen to adjust the ratio of H_2/CO to the required value for the type of FT catalyst system to be used
- Evaluation of the pros and cons of both cobalt and iron FT catalyst systems, including product property differences between raw FT products obtained with cobalt and iron catalysts with clean syngas, and from cobalt catalyst with potential catalyst poisons added, and the equipment required based on commercial catalysts and processes

The project team will assess the plant siting constraints, carbon-capture strategies, and related environmental issues that are certain to accompany the planning, siting, design, construction, and operation of any U.S. domestic commercial coal-to-liquid fuel production project.

The project team will obtain sample quantities of coal-derived FT fuels, for the following:

- Analysis and comparison to other fuels
- Demonstrations involving mobile and stationary engines

Lastly, the project team will assess the feasibility of the use of existing industrial facilities, including an R&D-scale FT plant, as potential near-term domestic sources of coal-derived FT transportation and jet fuel.

16: FC26-06NT42761

Project Number FC26-06NT42761	**Project Title** Enhanced Hydrogen Economics Via Co-Production of Fuels and Carbon Products			
Contacts DOE/NETL Project Mgr.	**Name** John Stipanovich	**Organization** NETL – Fuels Division	**Email** John.Stipanovich@netl.doe.gov	
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Partners	GrafTech inc Koppers Inc Wolfe Engineering Battelle Memorial Institute Columbus			
Stage of Development				
__ Fundamental R&D	_X_ Applied R&D	__Prototype Testing	__Proof of Concept	_Demonstration

Technical Background

This project seeks to convert coal to a suite of products, including binder pitch, coke (both metallurgical grade and anode grade), and crude oil. The concept is to use only low-cost commodity solvents, produced from coke over tars or refinery bottoms, in order to dissolve 90% of the coal (measured on a dry, ash-free basis). This extracted coal is then distilled to produce a material that can be used as binder pitch, a tarry material that is used to make carbon and graphite composites for the metals smelting industry.

The process is licensed to a Canadian company, Quantex Energy Inc., with substantial investment from New Hope Energy, an Australian coal company which plans to build a demonstration plant.

Direct liquefaction historically has sought to produce light crude, requiring an addition of some 5wt%–12wt% hydrogen (17–42 pounds per barrel). This is accomplished at pressures of up to 3,000 pounds per square inch (psig) or 20 millipascal (MPa) and temperatures of about 400°C.

Processes have been developed in the current effort using very little hydrogen (less than 1% by mass), and for certain coals even zero hydrogen is possible. This is possible because commodity products such as pitch and coke have a lower ratio of hydrogen to carbon than many types of carbon. If it is necessary to add a small amount of hydrogen to the solvent for certain coals, this can be done by blending in hydrogenated liquid obtained from a refinery rather than by incorporating a hydrogenation step in the liquefaction process.

In the 1970s, this would not have been a viable process because American refineries mainly operated using sweet light crude. In today's environment, however, American refineries produce millions of barrels per day from heavy crudes, notably from Venezuela and Alberta, Canada.

Liquefaction now requires no gaseous hydrogen. Hydrogen may still be useful for upgrading (i.e., increasing the yield of light products such as gasoline and diesel), as well as hydrodesulfurization and other hydrotreatments. Yet from a capital investment standpoint, there is a great advantage to not using gaseous hydrogen in a new process, even if it will still be used in downstream processes at another facility.

A 2,250-ton reactor, rated at 3,000 psig, is used by Shenhua Group in its direct liquefaction plant in China, and is described as the largest reactor of its kind in history. Such a reactor is not needed in plants incorporating the NETL-sponsored process from West Virginia University (WVU), and thus will be completely omitted in the Quantex Research Corp. plant.

During the course of investigations, the WVU liquefaction process succeeded in producing products such as gasifier fuel, meeting the specifications for the Great Plains gasifier in North Dakota; binder pitch derived from bituminous, sub-bituminous, and lignite coals; anode coke from bituminous coal; metallurgical grade coal from sub-bituminous and lignite coal; and crude oil from bituminous, sub-bituminous, and lignite coals.

Minimization of the greenhouse gas footprint is problematic because there currently is no agreed-upon, standardized methodology for evaluating processes and products. Nevertheless, chemical processes should strive to minimize the need for thermal energy, which might be produced by mining coal.

Relationship to Program

This project will support important advances in the co-production with coal and biomass focus of the NETL Advanced Fuels Program. This project serves to permit the use of abundant domestic coal in an environmentally clean way to produce oil as well as carbon products. Currently, the United States imports about 11 million barrels of petroleum per day, according to the DOE Energy Information Administration, with some 9 million barrels per day coming from outside North America. Although the United States seeks to develop alternative energy supplies to replace petroleum, it may continue to be dependent on imported energy for a long time. Metcoke ovens, another source of coke products and heavy hydrocarbons, likewise represent a significant environmental concern. Hence, the ability to produce clean, indigenous supplies of liquid hydrocarbon fuels and carbon products may continue to be important economically and environmentally for several years to come.

Primary Project Goal

The primary goal of this project is to enhance the environmental considerations and economics of direct liquefaction via processes that supply gasifier fuel, carbon products, and crude oil while minimizing the greenhouse gas footprint.

Objectives

The project has the following objectives:

- BP1: Identification of Products and Co Products; Mass balances; and production of pitches and cokes
- BP2: Production of pitches and cokes; electrode carbon composites.
- BP3: Production of coke in continuous coke production; pilot-scale trials of low-rank coals.

17: DE-FE0000435

Project Number DE-FE0000435	**Project Title** Methanol Economy			
Contacts	**Name**	**Organization**	**Email**	
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Principal Investigator	George Olah	University of Southern California	olah@usc.edu	
Partners				
Stage of Development				
X Fundamental R&D	__Applied R&D	__Prototype Testing	__Proof of Concept	__Demonstration

Technical Background

The era of readily available, inexpensive, and secure sources of fossil fuels seems to be ending. Left unmet, the present challenges surrounding carbon-based fuel availability, higher carbon dioxide (CO_2) levels in the atmosphere, and the impact of global warming may result in regional conflicts, slowing or stagnant growth, or even far worse situations. It is therefore important that the project team address these challenges with transformational ideas and solutions. One such concept conceived by the principal investigator (PI), co-PI, and their coworkers at the Loker Hydrocarbon Research Institute (LHI) at the University of Southern California (USC) is the Methanol Economy, which promotes the use of methanol as a versatile liquid fuel and feedstock.

The PI and co-PI have long research experience in hydrocarbon chemistry. Acid catalyzed conversion of hydrocarbons, such as cracking, isomerization, alkylation, oligo- and poly-condensation, etc., are of fundamental significance. Such fundamental chemistry has been systematically studied in the PI's laboratory at LHI for more than 30 years using methods developed in connection with studies of carbocations and their reactions using superacid media. For the pioneering development of studies on long-lived carbocation chemistry, the PI was awarded the 1994 Nobel Prize in Chemistry. The PI, co-PI, and co-workers have also developed environmentally benign catalyst systems for alkylation of alkenes (high-octane gasoline production) to overcome difficulties connected with use of conventional mineral acids such as hydrofluoric or sulfuric acid. This was commercialized as the Alkad Process. New chemical additives have been explored to improve diesel fuels and make them cleaner burning and less polluting. The use of methane and its oxygenates has been studied in strongly acidic membrane-based direct oxidation fuel cell systems. The direct oxidation methanol fuel cell technology (DMFC) developed at USC in cooperation with the National Aeronautics and Space Administration Jet Propulsion Laboratory (NASA-JPL) has been commercialized by companies such as Toshiba and Smart Fuel Cell for powering hand-held portable devices. New superacid catalyzed carbonylation of alkanes to branched ketones in high conversions and selectivity have also been developed.

The idea behind the Methanol Economy project is to develop fundamental chemistry for the direct conversion of methane to methanol and the utilization of anthropogenic carbon dioxide as a valuable carbon (C) feedstock by chemical and electrochemical means. The direct electrophilic conversion of methane to methanol and higher hydrocarbons and derived products offers a viable alternative to Fischer-Tropsch chemistry. Until recently, the utilization of methane as a chemical building block was limited to free radical reactions (combustion, nitration, chlorination, etc.) and various stoichiometric organometallic insertion reactions. Studies are proposed for the direct electrophilic catalytic conversion of methane to its monosubstituted derivatives, including methyl bromide, and finally its hydrolysis to methanol and/or dimethyl ether. The project team is also pursuing combined high-temperature conversion of methane, carbon dioxide, and water in suitable ratios to syngas and bireforming (for methanol and dimethyl ether synthesis) over a variety of solid oxide catalysts in a pressure flow reactor. In addition to regenerative capture, the reductive electrochemical recycling of anthropogenic carbon dioxide to syngas, formic acid, methanol, and their derivatives will be extensively studied. To achieve the latter cost effectively, the required electrical energy could originate from any of the alternative sources based on solar, wind, nuclear, and unused power during off-peak periods from fossil-fuel burning power plants. The suitability of formic acid as a source for hydrogen or carbon monoxide (CO) as well as an energy carrier for direct oxidation fuel cells will be explored. The proposed studies represent new approaches for efficient transportable fuel and feed stock production and energy storage. The overall intent is to develop renewable and practical energy carriers and feedstocks that can help reduce U.S. dependence on fossil fuels (oil, gas, and coal), and to recycle carbon dioxide into transportable fuels and materials (using unused and underutilized alternative energies) thus lowering, to a certain extent, anthropogenic carbon dioxide (CO_2) concentration in the atmosphere.

Relationship to Program

This project will support important advances in the co-production with coal and biomass focus of the NETL Advanced Fuels Program in the following ways:

- Bromination of methane followed by hydrolysis for the production of methanol could be useful for remote natural gas sites and a useful method to convert natural gas to transportable liquids.
- Bireforming of natural-gas-containing CO_2 streams will also provide a good method to produce methanol through syngas. Such a process may get CO_2 abatement credit.
- Inexpensive materials for CO_2 capture and release under moderate conditions.
- Direct electrochemical reduction of CO_2 to the right ratio of syngas for the production of methanol can use any alternative energy source based on solar, wind, nuclear, geothermal, etc.
- Electrochemical reduction of CO_2 to liquid formic acid can be achieved in high faradaic efficiency under pressure. If carried out under acidic conditions, separation formic acid from water is easy.
- Formic acid can be decomposed exclusively to either hydrogen gas or CO.
- Formic acid is an energy storage medium and can be used in proton exchange-based direct oxidation fuel cells for producing electricity.

Primary Project Goal

The primary goals of this project is to convert natural gas and/or anthropogenic carbon dioxide into methanol and dimethyl ether (DME) and other related materials as versatile fuels (energy carriers) and feedstocks.

Objectives

The project was initially spread over three years beginning September 30, 2009. A fourth year funding has been approved (terms are being negotiated with DOE/NETL) and therefore the project objectives include four years of work. The overall project management and planning is considered Task 1, which is operational throughout the project period.

In Task 2, direct electrophilic bromination of methane (which is still an abundant resource) to methyl bromide in high selectivity and conversion over a variety of catalysts in a quartz flow-reactor will be explored. Efficient hydrolysis of methyl bromide to methanol/DME over a variety of amine-based solid catalysts will be probed (the byproduct hydrogen bromide [HBr] that is produced in bromination of methane as well as hydrolysis can be recycled to bromine by air oxidation, making these processes catalytic in bromine).

In Task 3, bireforming of methane and carbon dioxide and steam to syngas in a pressure flow reactor for conversion to methanol and DME will be studied. Substantial amounts of CO_2, in some places up to 40%, is present in natural gas streams. Therefore, combined conversion of methane, CO_2, and water (bireforming) to the right ratio of syngas to produce methanol and DME is of great significance.

In Task 4, many aspects of capture, chemical, and electrochemical reduction of CO_2 will be investigated, including two-electron reduction of CO_2 to CO and formic acid. CO_2 capture and regeneration materials should be easily available, cost effective, and simple to use under moderate conditions. Direct electrochemical reduction of CO_2 in water to syngas (CO and H_2 in a 1:2 ratio) will be developed. Formic acid (which will be derived by electrochemical reduction) as a potential feedstock for H_2 and CO will be explored.

In Task 5, formic acid will be optimized as a fuel in proton exchange membrane-based direct oxidation fuel cells for potential energy storage.

In Task 6, the efficacy of each process developed will also be analyzed for its potential overall economic success.

The performance period for each task and subtasks are described in the Gantt chart of section 15.

18: DE-FC26-05NT42457; DE-FE0000699

Project Number DE-FC26-05NT42457; DE-FE0000669	**Project Title** Continuation of Crosscutting Technology Development at CAST			
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Partners	West Virginia University, Morgantown, WV University of Kentucky, Lexington, KY University of Utah, Salt Lake City, UT University of Nevada, Reno, NV New Mexico Tech, Socorro, NM Montana Tech, Butte, MT FLSmidth Salt Lake City, Salt Lake City, UT			
Stage of Development				
X Fundamental R&D	X Applied R&D	X Prototype Testing	X Proof of Concept	__Demonstration

Technical Background

In 2008, the U.S. mining industry produced minerals and coal worth $102.4 billion. Some of the raw materials, including coal and uranium, were used to produce 70% of the electricity generated in the United States. According to the 2008 Mineral Commodities Summary, the value-added mineral materials contributed $2.3 trillion to the nation's economy, which accounted for 16% of the GDP. Thus, the domestic mining industry is important to the U.S. economy.

Freshly mined coal (solid fuel) contains mineral matter impurities which produce ash, sulfur dioxide (SO_2), mercury, and other undesirable elements in power plants. Many of these impurities are removed at mine sites to reduce shipping costs, meet customer specifications, and comply with environmental regulations. The efficiency of cleaning coal is high for the coal particles that are large in size (e.g., >0.15 mm). It is difficult, however, to clean finer coal particles. Therefore, many coal producers discard the fine coal to impoundments, creating serious environmental concerns for those living in coal mining communities. According to a recent National Research Council (NRC) report, the U.S. coal industry discards annually 70–90 million tons of fine refuse to slurry impoundments. Assuming that 30–40 million tons of the refuse are recoverable coal, the dollar value of the coal wasted in this manner is estimated to be $1.5–$2 billion per year.

It has been reported that approximately 2.5–3 billion tons of fine coal have been discarded over the years to numerous impoundments in the United States, mostly in Appalachia. These estimates were made more than 20 years ago; therefore, the amount of fine coal discarded to date may be substantially larger, possibly in the range of 4 billion tons. Assuming that roughly one third of this amount is recoverable, the dollar value of the coal that has been discarded in the existing impoundments may exceed $100 billion.

The problems associated with the disposal of fine coal refuse have been created by the lack of appropriate separation technologies. Therefore, the Center for Advanced Separation Technologies (CAST) has been developing advanced technologies that may be used to (1) help companies eliminate the problem at the source, *i.e.*, stop discarding fine coal to impoundments and injecting it into old underground workings, and further ii) to recover the coal from existing impoundments. Citizens groups in Appalachian coal mining districts are lobbying for the elimination of the large impoundments by law. They consider the fine coal impoundments to be the worst form of 'valley-fill mining' and violate the Clean Water Act. The water containing heavy metals and fine coal particles seep into the ground water and enter the drinking water system. They are also afraid of major fatalities in the event a large coal sludge impoundment fails. If they succeed in mandating the elimination of the impoundments by law, the cost of producing coal would rise significantly, and the recoverable coal in existing impoundments, which may be worth over $100 billion as noted above, would be lost. An alternative would be a technological solution to the problem, *i.e.*, developing advanced separation technologies and making them available for companies to use.

In addition to the problems associates with solid fuels, CAST has been developing novel methods of separating gases from each other. In view of the incident in the Gulf of Mexico, the project team can also develop more efficient methods of separating oil from water.

Relationship to Program

CAST is a consortium of seven universities led by Virginia Tech, established to develop advanced separation technologies/processes and knowledge bases that can be used to produce cleaner solid and gaseous fuels from domestic energy resources in an efficient and environmentally acceptable manner. The project expects to produce the following benefits:

- Advanced technologies developed at CAST can be used to produce cleaner-burning solid and gaseous fuels in a manner that can increase environmental quality.
- The advanced fine coal cleaning technologies to be developed at CAST may be used to clean up and/or eliminate troublesome fine coal impoundments and create jobs.
- The new technologies can also help developing countries produce cleaner fuels that can help reduce carbon dioxide (CO_2) emissions.
- The university research at the seven major mining schools will help produce future leaders of the U.S. mining industry.

Primary Project Goal

The primary goal of CAST is to develop technologies that can be used by the U.S. mining industry to create new products, reduce production costs, and meet environmental regulations.

Objectives

Cleaning fine coal is the least efficient and most costly step in processing coal. In addition, the value of fine coal is substantially lower than that of coarse coal. Finer fractions of clean coal produced in the United States have higher ash and moisture contents and, therefore, have lower values. Coal finer than 44 microns is difficult to dewater to below 35%–40% moisture with existing mechanical dewatering technologies. The high moisture content of coal fines is of serious concern to coal producers due to stringent moisture specifications required by consumers. Further, the cost of cleaning fine coal is three to four times higher than for cleaning coarse coal.

In the absence of appropriate separation technologies to remove ash-forming minerals and water, many companies discard coal fines to impoundments and/or inject them into old underground mine workings. At present, the U.S. coal industry discards annually 70–90 million tons of fine refuse to slurry impoundments, according to a recent NRC report. Approximately 30–40 million tons of the refuse may be recoverable coals, worth approximately $1.5–$2 billion based on the average price of $51.5/ton for U.S. bituminous coal in 2008, according to the U.S. Energy Information Administration.

Over the years, 2.5–3 billion tons of fine coal have been discarded to numerous impoundments in the United States, mostly in Appalachia. CAST has been focusing on the development of advanced fine coal cleaning technologies over the years. A series of advanced technologies has already been developed, which includes the Microcel^{TM} flotation column, dewatering aids, and hyperbaric centrifuge, all of which are marketed commercially under appropriate license agreements. The hyperbaric centrifuge was tested at pilot scale in 2009, and successful test results were reported in DOE's February 9, 2009 Fossil Energy Techline report. Encouraged by the test results, a first full-scale unit was recently tested successfully in February 2010 in Alabama, and the results were presented at the XVI International Coal Preparation Congress and at the 13th Australian Coal Preparation Conference.

Most of the technologies developed to date by CAST are designed to maximize the efficiency of cleaning fine coal at operating plants and, thereby, help companies minimize the amounts of coal being discarded. Therefore, they are not ideally suited for recovering coal from existing impoundments. Typically, fine coal recovery projects can have life spans of three to eight years, for which a large capital investment is difficult to justify. A solution to this problem would be to develop new technologies that could be implemented as a mobile unit, which can be moved to another site after completion of one project. The Microcel columns developed previously are too large (4–5 m diameter with 8–10 m height) to be installed in a mobile unit. Further, a large number of the columns may need to be used as their throughput capacities decrease with decreasing particle size.

More recently, CAST has developed a novel process that is ideally suited for recovering ultrafine coal (<44 µm) with high throughput. Further, the process can dewater both the clean coal and refuse products. Preliminary test results, as disclosed in a recent patent application, show that moisture contents can be reduced to less than 5% by weight of coal. These results are as good as obtainable by thermal drying, which is costly and less environmentally acceptable because of air quality issues. It is necessary, however, that the new technology be further developed before it can be used commercially. The project team is in the process of designing and building a bench-scale continuous unit. This technology should also be useful for addressing the issues concerning ash ponds near power plants.

At present, CAST is also studying the basic mechanism of gas hydrate formation. It is well known that the kinetics of hydrate formation include slow methods of extracting methane (CH_4) from the gas hydrate resources at the continental margins of the United States; sequestering CO_2 as hydrate; transporting and storing Marcellus shale gas as hydrate; and separating one type of gas (e.g., CO_2) from another (e.g., nitrogen and hydrogen) by selectively forming hydrates. In addition, CAST is helping FLSmidth Salt Lake City, Inc. to design more efficient flotation machines that can be used to upgrade coal and minerals. During the last two years, the company has provided more than $1.5 million of research funding for CAST. As part of the Asia Pacific Partnership (APP) for Clean Development and Climate, the U.S. Department of State has been funding CAST to help India clean coal without using water. In addition, CAST is in the final stages of negotiations to design advanced fine coal cleaning plants for Coal India Limited, the largest coal producer in the country, and Dengfeng Power Plant in Henan Province, China.

19: FC26-06NT42804

Project Number	**Project Title**			
FC26-06NT42804	Long-Term Environmental and Economic Impacts of Coal Liquefaction in China			
Contacts	**Name**	**Organization**	**Email**	
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Stage of Development				
__ Fundamental R&D	_X_ Applied R&D	__Prototype Testing	__Proof of Concept	_Demonstration

Technical Background

This project was developed following a meeting on July 21, 2002 of Yuzhuo Zhang (then president of the China Shenhua Coal Liquefaction Company Ltd. [CSCLCL], now CEO of the Shenhua Group), Jerald J. Fletcher, and Qingyun Sun of West Virginia University (WVU). At that meeting, Dr. Zhang expressed an interest in developing a better understanding of the environmental and economic consequences associated with implementing a coal liquefaction plant in Inner Mongolia, China using direct liquefaction technologies. Many of the technologies incorporated into the plant design were developed in the United States with DOE support. To develop a better understanding of the potential for WVU cooperation, Dr. Zhang visited the WVU campus on October 24, 2002, presented a seminar on the current CSCLCL plans and the potential for future cooperation, and met with a variety of researchers and administrators from both WVU and NETL. Given the influence that NETL had in the development of many of the key technologies, the potential to observe implementation was of interest to a number of those attending from NETL.

Based on the potential to develop improved relations with China in the area of fossil fuels and an interest in the development of a commercial coal liquefaction sector, NETL provided initial support to WVU for collaborative activities with CSCLCL beginning September 1, 2003, through the CTC support contract. (This initial support was replaced by the current cooperative agreement in May 2006.)

Discussions with Shenhua representatives continued. Based on mutual WVU and CSCLCL interests, a Memorandum of Understanding (MOU) was signed in December 2003 to (1) promote joint research on the economic and environmental impacts of coal liquefaction in China and (2) encourage technical collaboration on coal and energy projects between WVU and CSCLCL. This MOU provided the basis for the current project and a pathway to develop programs as part of Annex II under The Protocol for Cooperation in the Field of Fossil Energy Technology

Development and Utilization Between the Department of Energy of the United States of America and the Ministry of Science and Technology (MOST) of the People's Republic of China (PRC), known as the US-China Fossil Energy Protocol. The specific issues addressed under the MOU were in line with WVU capabilities in economic analysis and environmental assessment. The activities met CSCLCL concerns related to the economic and environmental consequences that operation of such a facility could have on the region. An expanded MOU between WVU and CSCCL was developed and signed in September 2009 to explicitly include carbon management and geological storage of the carbon dioxide (CO_2) from the direct coal liquefaction (DCL) plant as well as other coal conversion plants in the Erdos Basin. During the next phase of the research, the scope of potential geological CO_2 storage will be expanded and research related to the potential for the storage capacity of the Erdos Basin will be developed, including explicit consideration of the interactions with the produced CO_2 stream with the water in deep saline aquifers.

Research has also been expanded to include other companies in China. A MOU with the Lu'an Group was signed in August 2009. Research plans are now being developed to work on the efficiency of alternative catalysts for coal conversion to liquid fuels using the indirect Fischer-Tropsch process. The Lu'an Group has provided test equipment and will collaborate on research in this area.

The project is in line with programs within the Office of Sequestration, Hydrogen and Clean Coal Fuels in the Office of Fossil Energy. This project provides information on clean coal technology utilization in China. In addition, while the US-China Fossil Energy Protocol was signed by DOE and MOST, Annex II is an agreement between the DOE Office of Fossil Energy and the National Energy Administration (NEA) of the PRC (initially the National Development and Reform Commission [NDRC]). NEA and MOST are quite different agencies. The first activities under Annex II were facilitated by the cooperative work between WVU and CSCLCL along with informal discussions with NDRC officials; these continue with NEA. Annex II was renewed in China in 2009 and a successful meeting was held on the Fossil Energy Protocol in San Francisco in August 2010 that extended all of the other Annexes under the Protocol and added additional tasks.

Relationship to Program

This project supports important advances in coal liquefaction and the co-production with coal and biomass within the Coal and Biomass to Liquids Research focus of the NETL Advanced Fuels Program. The primary benefit to the United States and DOE has been access to additional information on the status of many aspects of the energy sector in China. Project presentations by high-level officials from the Shenhua Group, the NDRC, and the NEA on the CSCLCL coal-to-liquids plant and the relationship of that project to developments in the overall energy sector in China have been of greater depth and detail than information from other current sources. This project has provided the primary information on current clean coal activities in China including the range of coal-to-liquids, coal-to-chemicals, coal-to-methanol, and other technologies. Recent efforts have expanded the number of Chinese companies involved and developed relationships with a number of provincial government officials in the energy sector as well.

There are other benefits to the United States. Current work to develop a large scale project to store the CO_2 produced by the CSCLCL coal-to-liquids plant in geologic formations can influence the adoption of such carbon management alternatives in China. As initially designed, the purity of the CO_2 stream produced was not sufficient to support economical geological storage options as currently understood. The project team identified the issue and provided guidance to the CSCLCL research team. They were subsequently able to redesign aspects of the system to provide a CO_2 stream with 95%+ purity that can be stored without additional capture costs. During a recent visit to the facility, the Chinese said that they now plan to upgrade the facility to produce food-grade CO_2—indicating a sufficient market potential to justify such an additional expenditure for the current facility.

The project has also supported the development of additional lines of communication between private sector businesses in the United States and China, which resulted in increased trade and commerce.

The primary long-term benefits for China relate to potentially improved environmental quality if the project identifies environmental issues that were not expected or not previously addressed. They also gain access to firms interested in developing and implementing coal conversion facilities in the United States. Successful implementation of a carbon storage project for the DCL plant has implications for carbon management for clean coal projects not only in China but throughout the world.

Primary Project Goal

The initial project goal was to better understand the development and implementation of direct coal liquefaction and related clean coal technologies in the PRC through joint research efforts with CSCLCL. These technologies are closely related to the production of hydrogen-intensive fuels in general. Knowledge of the experience gained by the Chinese is expected to aid in the transition to new generations of clean coal technologies in the United States.

This goal has been expanded in two ways. One is to better understand current clean coal conversions projects being developed in China. The second is to better understand and assist the Chinese in implementing subsurface carbon storage projects. The availability of highly concentrated CO_2 streams from large coal conversion facilities makes the development of carbon storage projects in China much more economical than in the United States, where approximately 75% of the project costs are expected to be needed for CO_2 capture (concentration of exhaust gases to 95% CO_2 or greater). It is important to the United States and other developed countries that the initial CO_2 storage projects be successfully implemented to alleviate concerns related to human health and welfare and subsurface water quality.

Objectives

The overall objective of this effort is to describe and quantify the environmental and economic impacts associated with the development of a coal liquefaction sector in the People's Republic of China (China). This has been more broadly defined to include the impacts of new technologies and carbon management with emphasis on geologic carbon storage.

Within the context of this overall objective, there are six tasks listed in the latest statement of project objectives: four specific research tasks, a communication and collaboration activity, and an explicit project management task. The objective of the first research task is to describe and quantify the environmental impacts expected from the world's first commercial DCL plant now operating in Inner Mongolia. The objective of the second research effort is to describe and quantify the economic impacts that the DCL plant has had and is expected to have in the future on the local region. The third objective is to develop an understanding of the potential and actual processes of alternative clean coal utilization in China with emphasis on coal conversion processes. The fourth research effort focuses on carbon management with special emphasis on CO_2 geologic storage options for the DCL plant and other coal conversion facilities in the Erdos Basin. The communication and collaboration activity directly supports DOE Office of Fossil Energy activities under Annex II and economic development objectives related to the coal sector in China. The third and fourth research tasks support the first two research efforts as well as communication and collaboration activities.

APPENDIX F: LIST OF ACRONYMS AND ABBREVIATIONS

Acronym or Abbreviation	**Definition**
%vol	percent volume
°C	degrees Celsius
Ag	silver
Al_2O_3	aluminum oxide
ALK	alkylation
Ar	argon
ARI	Adsorption Research Inc.
ASME	American Society of Mechanical Engineers
ASU	air separation unit
Au	gold
BCC	body-centered cubic
BCY	$BaCe_{0.8}Y_{0.2}O_{3-\delta}$
BE	binding energy
BET	Brunauer-Emmett-Teller
BRTD	ASME Board on Research and Technology Development
B.S.	bachelors of science
C_2H_6	ethanol
CAER	Center for Applied Energy Research
CBTL	coal/biomass to liquid
CCC	Copyright Clearance Center
CCS	carbon capture and storage
CDH	catalytic dehydrogenation
CDP	congressionally directed project
cermet	ceramic metal
CFFS	Consortium for Fossil Fuel Science
CH_4	methane
CO	carbon monoxide
Co	cobalt
CO_2	carbon dioxide
COS	carbonyl sulfide
CRTD	ASME Center for Research and Technology Development
CSM	Colorado School of Mines
CSTR	continuous stirred tank reactor
Cu	copper
DHY	dehydrogenation
DME	dimethyl ether
DMFC	direct oxidation methanol fuel cell technology
DOE	U.S. Department of Energy
EDTA	ethylenediaminetetraacetic acid

EERC	Energy & Environmental Research Center at the University of North Dakota
FCC	fluid catalytic cracking
Fe	iron
FE	Office of Fossil Energy
FEED	Front End Engineering and Design
FT	Fischer-Tropsch
ft	feet
FTS	Fischer-Tropsch synthesis
FY	fiscal year
GE	General Electric
GHG	greenhouse gas
H_2	hydrogen gas
H2A	Hydrogen Analysis Project
H_2O	water
H_2S	hydrogen sulfide
HCN	hydrogen cyanide
He	helium
HTM	hydrogen transport membrane
HYC	hydrocracking
IGCC	integrated gasification combined cycle
INL	Idaho National Laboratory
Ir	iridium
K	potassium
kDa	kiloDaltons
lb	pound
LHI	Loker Hydrocarbon Research Institute
LTI	Leonardo Technologies, Inc.
M.B.A.	master of business administration
MMM	mixed-matrix membranes
Mo	molybdenum
MoF_6	molybdenum fluoride
MoO_3	molybdenum trioxide
MPa	millipascal
M.S.	master of science
N_2	nitrogen
Na	sodium
NAFTC	National Alternative Fuels Training Consortium
NASA-JPL	National Aeronautics and Space Administration - Jet Propulsion Laboratory
Nb	niobium
NCHT	National Center for Hydrogen Technology
NETL	National Energy Technology Laboratory
NH_3	ammonia
Ni	nickel
nm	nanometer

NO_x	nitrogen oxides
O_2	oxygen
OCC	Office of Clean Coal
OMB	Office of Management and Budget
Os	osmium
ORD	Office of Research and Development
OSAP	Office of Systems, Analyses, and Planning
OSU	Ohio State University
OTM	oxygen transport membrane
P&ID	process & instrumentation design
P+E	Power+Energy Inc.
PBI	polybenzimidazole
Pd	palladium
Pd_4S	palladium sulfide
PGM	platinum group metals
PECVD	plasma-Enhanced Chemical Vapor Deposition
PEM	Polymer Electrolyte Membrane
PFD	Process Flow Diagrams
Ph.D.	doctor of philosophy
PI	principal investigator
PMG	platinum metal group
ppmv	parts per million volume
PSA	pressure swing adsorption
psi	pounds-force per square inch
psia	pounds-force per square inch absolute
psig	pounds-force per square inch gauge
PSS	porous stainless steel
Pt	platinum
PxCSM	Praxair and the Colorado School of Mines
Q&A	question and answer
R&D	research and development
RD&D	research, development, and demonstration
RF	Radio frequency
RGA	residual gas analyzer
Rh	rhodium
RTI	Research Triangle Institute
Ru	ruthenium
S	sulfur
scfh	standard cubic feet per hour
SEM	scanning electron microscope
SO_x	sulfur oxides
STP	standard temperature and pressure
syngas	synthesis gas
Ta	tantalum
TGA	thermal gravimetric analysis

TOC	total overnight cost
TPC	total plant cost
tpd	tons per day
TPR	temperature-programmed reaction
TRDU	transport reactor development unit
UK	University of Kentucky
UOP	Universal Oil Products LLC
USC	University of Southern California
UTRC	United Technologies Research Center
V	vanadium
VCR	vacuum coupling radiation
w/w	weight per weight
WF_6	tungsten fluoride
WGCU	warm-gas cleanup
WGS	water-gas shift
WPI	Worcester Polytechnic Institute
XRD	x-ray diffraction
Y_2O_3	yttrium (III) oxide
ZIF	zeolitic imidazolate frameworks
Zr	zirconium
ZrO_2	zirconium dioxide