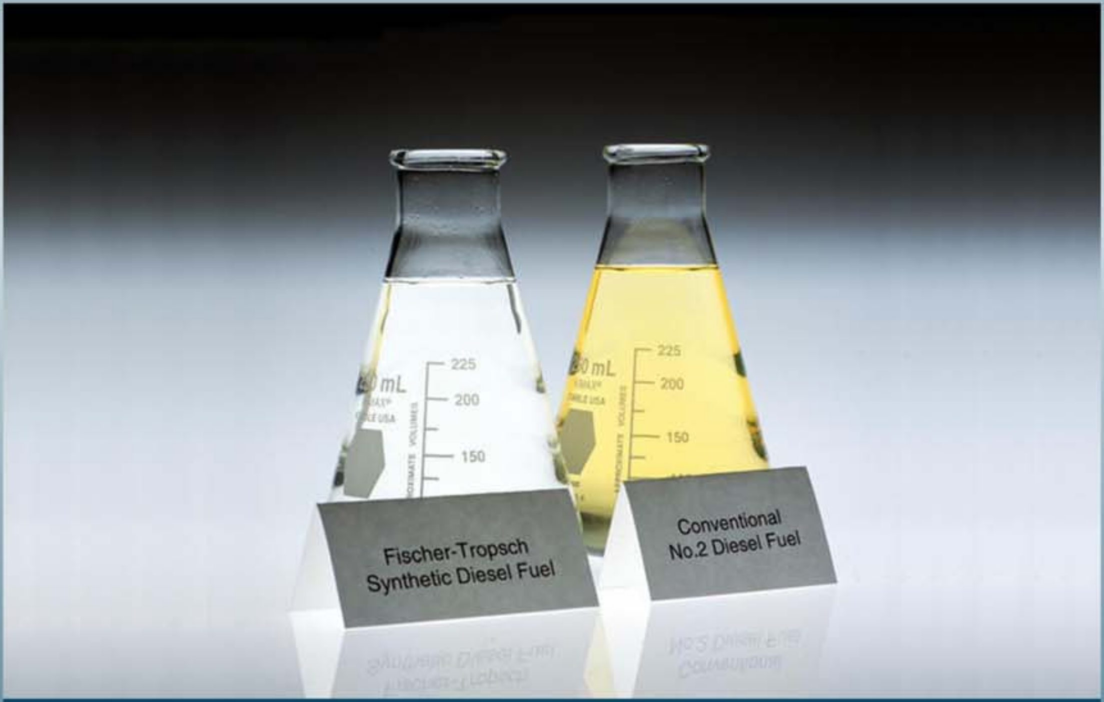
Final Report
Strategic Center for Coal
Hydrogen and Clean Fuels Program
2009 Fuels Peer Review Meeting



MEETING SUMMARY AND RECOMMENDATIONS REPORT

Pittsburgh, Pennsylvania
February 23 – February 27, 2009

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

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FINAL REPORT
STRATEGIC CENTER FOR COAL
HYDROGEN AND CLEAN FUELS PROGRAM
2009 FUELS PEER REVIEW MEETING

Pittsburgh, Pennsylvania
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MEETING SUMMARY AND RECOMMENDATIONS REPORT

José D. Figueroa
NETL Project Manager and Meeting Coordinator
(412) 386-4966

Meeting Host Organization

Technology & Management Services, Inc.
Steven T. Ostheim
(412) 386-6485

Review Panel

AMERICAN SOCIETY OF MECHANICAL ENGINEERS
Daniel J. Kubek, Chair, Peer Review Panel
Richard Laudenat, Chair, Peer Review Executive Committee
Michael Tinkleman, Director, Research
ASME Center for Research and Technology Development
(202) 785-7394

Meeting Facilitator and Final Report

Ross Brindle, Energetics Incorporated
(410) 953-6239

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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 emissions), abundant, low-cost domestic energy from coal to fuel economic prosperity, strengthen energy security, and enhance environmental quality. The OCC is organized into eight technology programs and an international program. The OCC Fuels technology program is administered by the DOE Office of Fossil Energy's National Energy Technology Laboratory (NETL). The Mission of the NETL Hydrogen & Clean Fuels Program is to develop advanced and novel energy technologies, through joint public and private R&D, which will facilitate the use of our nation's abundant coal resources to produce, deliver, and utilize affordable hydrogen in an environmentally clean manner.

In compliance with requirements from the Office of Management and Budget (OMB), 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 2009 Fuels Peer Review Meeting with independent technical experts to assess ongoing research projects and, where applicable, to make recommendations for improvement.

In cooperation with Technology & Management Services Inc., the American Society of Mechanical Engineers (ASME) convened a panel of eleven leading government, academic, and industry experts on February 23–27, 2009 to conduct a five-day Peer Review of selected Hydrogen and Clean Fuels Program research projects supported by NETL.

Overview of Office of Fossil Energy Hydrogen and Clean Fuels Program Research Funding

The total funding for these 17 projects, over the duration of the projects, is $62,509,155. Of this amount, $48,404,335 (77.4%) comes from DOE and the remaining $14,104,820 (22.6%) comes from project partner cost sharing.

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

TABLE ES-1 HYDROGEN AND CLEAN FUELS PROGRAM PROJECTS REVIEWED

Reference Number	Project No.	Title	Lead Organization	Principal Investigator	Total Funding^{A}		Project Duration^{A}	
					DOE	Cost Share	From	To
01	ORD-09-220661	Computational Studies of the Initial Mechanistic Steps in Fischer-Tropsch Synthesis	National Energy Technology Laboratory	Dan Sorescu	$191,290	$0	10/01/2008	09/30/2009
02	OSAP CBTL	Affordable, Low-Carbon Diesel Fuel from Domestic Coal and Biomass	National Energy Technology Laboratory	Thomas Tarka	$255,000	$0	03/12/2008	01/14/2009
03	NT42449	Production of High-Hydrogen Content Coal-Derived Liquids	Integrated Concepts & Research Corporation	Steve P. Bergin	$2,779,168	$698,326	03/30/2006	06/30/2010
04	NT0006368	Sensitivity of FT and Water-Gas Shift Catalyst to Poisons from Gasification of Biomass and Coal/Biomass Mixtures	University of Kentucky – Center for Applied Energy Research	Burtron Davis	$1,088,066	$285,850	10/01/2008	09/30/2011
05	OSAP - 401.01.08.002	Technical, Economic, and Environmental Assessment of a Commercial Scale Fischer-Tropsch Liquids Plant Using a Dry-feed Gasifier with Carbon Capture	National Energy Technology Laboratory	Erik P. Shuster	$50,000	$0	05/20/2008	10/31/2009
06	NT42456	Production and Storage of Hydrogen from Coal Using C1 Chemistry	University of Kentucky – Consortium for Fossil Fuel Science	Gerald P. Huffman	$6,000,000	$1,500,000	06/02/2005	06/30/2009
07	NT43024	Catalytic Processes for the Synthesis of Ethanol from Coal-Derived Syngas	Louisiana State University	James J. Spivey	$1,779,899	$904,579	10/01/2006	03/31/2010
08	NT06523	Demonstration of a Piston Driven Plug Feed System for Feeding Coal/Biomass Mixtures Across a Pressure Gradient for Application to Commercial CBTL Systems	Southern Research Institute	A. John Rezaiyan	$1,053,894	$571,435	10/01/2008	02/28/2010
09	NT0006305	Product Characterization for Entrained Flow Coal/Biomass Co-Gasification	GE Global Research	Boris Eiteneer	$838,913	$209,728	10/01/2008	09/30/2010
10	ORD-09-220662	Next Generation, Sinter-Resistant, Catalysts for Syngas Conversion	National Energy Technology Laboratory	Christopher Matranga	$429,000	$0	07/31/2007	09/30/2009
11	FWP49601	Development of Mixed-Conducting Dense Ceramic Membranes for Hydrogen Separation	Argonne National Laboratory, Illinois	U. Balachandran	$5,884,000	$0	03/31/1998	09/30/2009
12	NT43027	Investigation of Hydrogen-Fueled Internal Combustion Engine Durability	Electric Transportation Engineering Corporation	Garrett Paul Beauregard	$1,322,844	$567,117	02/15/2007	07/14/2010
13	NT42759	Development of a Hydrogasification Process for Co-Production of Substitute Natural Gas (SNG) and Electric Power from Western Coals	Arizona Public Service	Raymond S. Hobbs	$15,709,770	$6,015,805	04/01/2006	08/30/2013
14	NT41874	An Industrial Based Consortium to Develop Premium Carbon Products from Coal	Pennsylvania State University – Office of Sponsored Programs	Bruce G. Miller	$3,949,023	$1,503,557	09/30/2003	09/30/2009
15	NT42439	Development of Nanocrystalline Doped Ceramic Enabled Fiber Sensors for High Temperature In-Situ Monitoring of Fossil Fuel Gases	New Mexico Institute of Mining and Technology	Hai Xiao	$527,942	$175,981	06/21/2005	06/30/2009
16	NT41873	Development of Continuous Solvent Extraction Processes for Coal-Derived Carbon Products	West Virginia University Research Corporation	Elliot B. Kennel	$5,045,297	$1,279,203	09/30/2003	06/30/2009
17	NT42804	Long-Term Environmental and Economic Impacts of Coal Liquefaction in China	West Virginia University Research Corporation	Jerald J. Fletcher	$1,500,229	$393,239	08/15/2006	12/31/2009
				TOTALS	$48,404,335	$14,104,820		

Note: A: Funding amounts and project durations obtained from project summaries submitted by the Principal Investigator.

HYDROGEN & CLEAN FUELS PROGRAM OVERVIEW

The use of coal—the nation’s largest domestic fossil energy resource—offers the potential for producing abundant, economically attractive hydrogen and hydrogen-rich liquid and gaseous fuels to provide both increased energy security and reduced levels of carbon dioxide (CO_2) emissions. The Hydrogen and Clean Fuels Program, consisting of a portfolio of laboratory and field R&D projects focused on technologies which advance the production of synthetic fuels, enables and promotes efforts toward realizing this potential.

Mission

The Mission of the NETL Hydrogen & Clean Fuels Program is to develop advanced and novel energy technologies, through joint public and private R&D, which will facilitate the use of our nation's abundant coal resources to produce, deliver, and utilize affordable hydrogen in an environmentally clean manner. The program will help reduce environmental concerns associated with energy use in automotive and stationary power applications through clean production of hydrogen from coal in tandem with carbon management, and will ensure the availability of hydrogen in sufficient volumes for advanced power generators and vehicles. The Hydrogen & Clean Fuels Program is divided into four program areas: Central Hydrogen Production; Alternate Hydrogen Production; Delivery & Infrastructure; and System Studies.

Program Area: Central Hydrogen Production

Purpose:

To develop technologies and supporting capabilities that maximize hydrogen production and separate hydrogen from coal-derived synthesis gas, including efforts that reduce processing steps, combine functions, and significantly improve efficiency.

Goal:

By the end of 2016, to prove the feasibility of a 60 percent efficient, near-zero emissions, coal fueled hydrogen and power co-production facility that reduces the cost of hydrogen by 25 percent compared to current coal-based technology.

Program Area: Alternate Hydrogen Production

Purpose:

To develop processes to produce high hydrogen content hydrocarbons and hydrocarbon reforming technologies that enable hydrogen to be produced efficiently near the point of use.

Goal:

By the end of 2014, optimize, integrate, and make available an alternative economic and environmentally responsive hydrogen production pathway and reforming system to produce decentralized hydrogen.

Program Area: Utilization

Purpose:
To modify and optimize conventional and advanced engine types to operate on hydrogen or hydrogen-natural mixtures and demonstrate the performance of these engines in vehicles or in stationary applications.

Goal:
Complete the small-scale development of hydrogen and/or hydrogen-natural gas mixture engine modifications and operations.

Program Area: System Studies

Purpose:
To develop centralized, coal-based facilities employing modern and advanced techniques to inexpensively produce both hydrogen and electric power.

Goal:
Achieve a $2–$3 cost of hydrogen per gallon of gasoline equivalent.

Overview of the Peer Review Process

NETL requested that ASME assemble a Peer Review Panel of recognized technical experts to provide recommendations on how to improve the performance, management, and overall results from each individual research project. In advance of the Peer Review Meeting, each project team prepared for the Review Panel an 11-page Project Information Form containing an overview of the project's purpose, objectives, and achievements. At the meeting, each research team made a 45-minute presentation that was followed by a 30-minute question-and-answer session with the reviewers and a 40-minute closed-session discussion of each project. ASME developed a set of agreed-upon review criteria to be applied to the projects under review by the Review Panel at this meeting.

Based on lessons learned from prior Peer Reviews and the special circumstances associated with fuels research, both the principal investigator (PI) presentations and question-and-answer sessions with the ASME Review Panel were held as closed sessions, limited to the ASME Review Panel and DOE/NETL personnel. The closing of these sessions ensured frank and open discussions between the PIs and the Review Panel.

Each Panel member then individually evaluated the 17 projects based on a predetermined set of review criteria and provided written comments and recommendations. 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 reviewers occasionally had divergent views of certain projects, particularly when considering criteria "Performance and Economic Factors," "Anticipated Benefits, if Successful," and "Technology Development Pathways." In the extreme, this divergence is reflected in projects receiving both "1" and "5" ratings 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 which are a sign of a diverse peer review. Such diversity is a strength that allows the Panel to review fundamental research, systems studies, and demonstration projects with comparable levels of expertise as a panel. The Panel did, however, have differing views regarding the interpretation of specific criteria, particularly those of an economic nature.

Figure ES-1 shows the overall average score, including all nine review criteria, for all 17 projects.

FIGURE ES-1 OVERALL SCORING AVERAGES – BY PROJECT

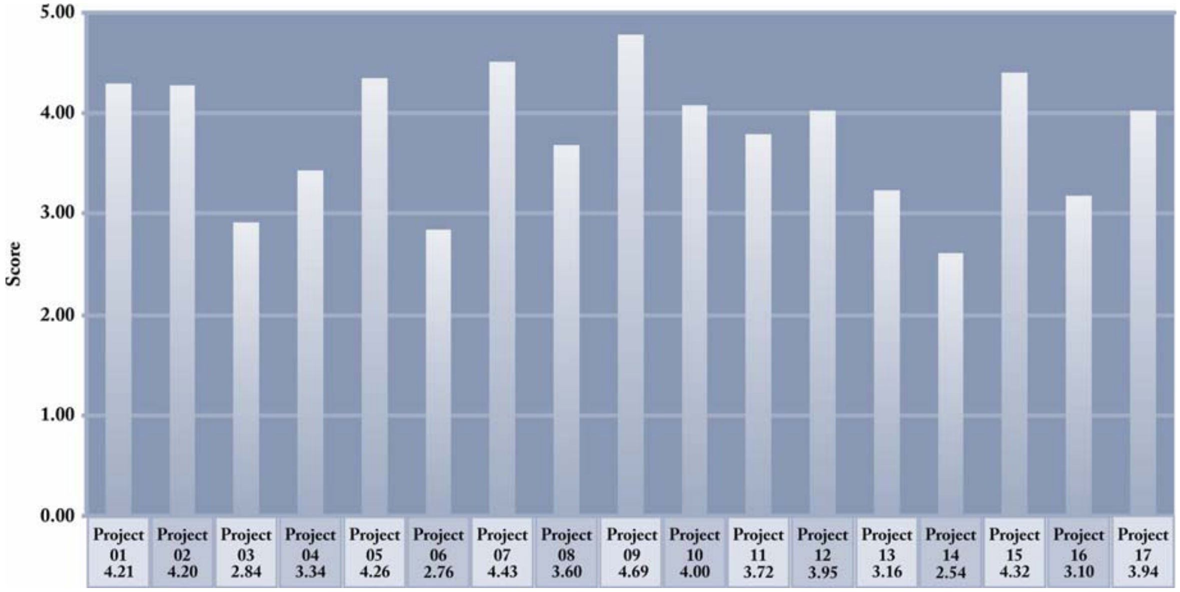


Table ES-2 shows the overall average, highest project average, and lowest project average given for each review criterion across all 17 projects reviewed.

TABLE ES-2 SCORES BY REVIEW CRITERION

Criterion	Average	Highest Project Average	Lowest Project Average
1. Scientific and Technical Merit	4.0	5.0	2.6
2. Existence of Clear, Measurable Milestones	3.8	4.9	2.3
3. Utilization of Government Resources	3.9	4.8	2.7
4. Technical Approach	3.8	4.9	2.6
5. Rate of Progress	3.8	4.7	2.6
6. Potential Technology Risks Considered	3.4	4.7	2.2
7. Performance and Economic Factors	3.3	4.5	2.0
8. Anticipated Benefits, if Successful	3.9	4.8	2.8
9. Technology Development Pathways	3.5	4.7	2.6

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

Projects are also categorized based on their stage of development to assist the review panel in determining the level of effort appropriate for a particular project toward the development of economic and developmental data for proper scoring of the “Performance and Economic Factors” and “Technology Development Path” criteria. Table ES-3 describes the various stages of research.

TABLE ES-3 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 indicative of a long-term commercial installation.
Major Demonstration	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 Project Manager, José D. Figueroa, at (412) 386-4966 or Jose.Figueroa@netl.doe.gov.

I. INTRODUCTION

In 2009, the American Society of Mechanical Engineers (ASME) was invited to provide an independent, unbiased, and timely peer review of selected projects within the U.S. Department of Energy (DOE) Office of Fossil Energy Hydrogen and Clean Fuels Program (a program administered by the Office of Fossil Energy's National Energy Technology Laboratory [NETL]). On February 23–27, 2009 ASME convened a panel of eleven leading government, academic, and industry experts to conduct a five-day peer review of selected Hydrogen and Clean Fuels Program research projects supported by NETL. This report contains a summary of the findings from that review.

Compliance with OMB 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 Hydrogen and Clean Fuels Program was designed to comply with requirements from the Office of Management and Budget (OMB).

Overview of the Peer Review Process

ASME was selected as the independent organization to conduct a five-day Peer Review of 17 Hydrogen and Clean Fuels Program projects. ASME performed this project review work as a subcontractor to Technology & Management Services Inc. (TMS), a NETL prime contractor. NETL selected the 17 projects, while ASME organized an independent Review Panel of eleven leading government, academic, and industry fuels technology experts. Prior to the meeting, principal investigators (PIs) submitted an 11-page written summary (Project Information Form) of their project's purpose, objectives, and progress. At the meeting, each research team made a 45-minute oral presentation that was followed by a 30-minute question-and-answer session with the reviewers and a 40-minute review panel discussion of each project. Each Panel member then individually evaluated the project presented based on a predetermined set of review criteria and provided written comments and recommendations. This document (*Meeting Summary and Recommendations Report*), prepared by ASME, provides a general overview of findings from the Peer Review and is available to the public.

Based on lessons learned from prior peer reviews and the special circumstances associated with fuels research, both the PI presentations and question-and-answer sessions with the ASME Review Panel for the ASME DOE Fuels Peer Review were held as closed sessions, limited to the Review Panel and DOE/NETL personnel. The closing of these sessions ensured frank and open discussions between the PIs and the Review Panel.

ASME Center for Research and Technology Development (CRTD)

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 selecting all Review Panel members and ensuring there are no conflicts of interest within the panel or the review process. In consultation with NETL, ASME was responsible for formulating the review meeting agenda, for providing information advising the PIs and their colleagues on how to prepare for the review, for facilitation of the review session, and for preparing a summary of the results. A more extensive discussion of the ASME peer review methodology used for the Fuels Peer Review Meeting is provided in Appendix A. A copy of the meeting agenda is provided in Appendix B, and an introduction to the Peer Review Panel members is provided in Appendix C.

Peer Review Criteria and Peer Review Criteria Forms

ASME developed a set of agreed-upon review criteria to be applied to the projects under review at this meeting. The review criteria were provided to the Review Panel and PIs 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, completing the review criteria forms in closed sessions. 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 Fuels Peer Review Meeting and are organized as follows:

II. Summary of Projects Reviewed in 2009 Fuels Peer Review

A list of the 17 projects reviewed and the selection criteria.

III. An Overview of the Evaluation Scores in 2009

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 2009 FUELS PEER REVIEW

NETL selected the projects that were reviewed by the independent ASME Review Panel for the Fuels Peer Review. Selected projects were key projects within the Hydrogen and Clean Fuels Program as well as related projects being conducted in NETL's Office of Research and Development (ORD) and Office of Systems Analysis and Planning (OSAP).

PROJECTS REVIEWED

01: ORD-09-220661
Computational Studies of the Initial Mechanistic Steps in Fischer-Tropsch Synthesis
National Energy Technology Laboratory

02: OSAP CBTL
Affordable, Low-Carbon Diesel Fuel from Domestic Coal and Biomass
National Energy Technology Laboratory

03: DE-FC26-06NT42449
Production of High-Hydrogen Content Coal-Derived Liquids
Integrated Concepts & Research Corporation

04: DE-NT0006368
Sensitivity of FT and Water-Gas Shift Catalyst to Poisons from Gasification of Biomass and Coal/Biomass Mixtures
University of Kentucky Center for Applied Energy Research

05: OSAP-401.01.08.002
Technical, Economic, and Environmental Assessment of a Commercial-Scale Fischer-Tropsch Liquids Plant Using a Dry-Feed Gasifier with Carbon Capture
National Energy Technology Laboratory

06: DE-FC26-05NT42456
Production and Storage of Hydrogen From Coal Using C1 Chemistry
University of Kentucky Consortium for Fossil Fuel Liquefaction Science

07: DE-FC26-06NT43024
Catalytic Processes for the Synthesis of Ethanol From Coal-Derived Syngas
Louisiana State University

08: DE-FC26-08NT0006523
Demonstration of a Piston Driven Plug Feed System for Feeding Coal/Biomass Mixtures Across a Pressure Gradient for Application to Commercial CBTL Systems
Southern Research Institute

09: DE-NT0006305
Product Characterization for Entrained Flow Coal/Biomass Co-Gasification
GE Global Research

10: ORD-09-220662
Next Generation, Sinter-Resistant Catalysts for Syngas Conversion
National Energy Technology Laboratory

11: FWP49601
Development of Mixed-Conducting Dense Ceramic Membranes for Hydrogen Separation
Argonne National Laboratory, Illinois

12: DE-FC26-07NT43027
Investigation of Hydrogen-Fueled Internal Combustion Engine Durability
Electric Transportation Engineering Corporation

13: DE-FC26-02NT42759
Development of a Hydrogasification Process for Co-Production of Substitute Natural Gas (SNG) and Electric Power from Western Coals
Arizona Public Service

14: DE-FC26-05NT41874
An Industrial Based Consortium to Develop Premium Carbon Products from Coal
Pennsylvania State University – Office of Sponsored Programs

15: DE-FC26-05NT42439
Development of Nanocrystalline Doped Ceramic Enabled Fiber Sensors for High Temperature In-Situ Monitoring of Fossil Fuel Gases
New Mexico Institute of Mining and Technology

16: DE-FC26-03NT41873
Development of Continuous Solvent Extraction Processes for Coal-Derived Carbon Products
West Virginia University Research Corporation

17: DE-FC26-06NT42804
Long-Term Environmental and Economic Impacts of Coal Liquefaction in China
West Virginia University Research Corporation

A short summary of each of the above projects is presented in Appendix E.

III. AN OVERVIEW OF THE EVALUATION SCORES IN 2009

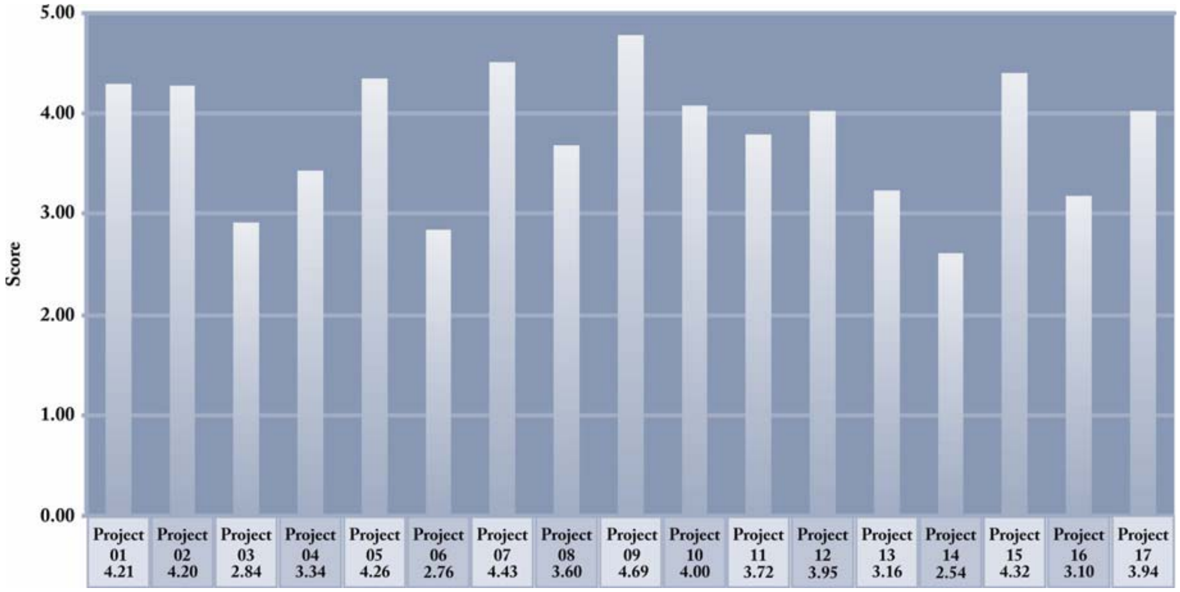
The ASME team, in cooperation with NETL and with input from the Peer Review Panel, continues to enhance and refine the peer review process. A copy of the Peer Review Criteria Form and a detailed explanation of the process are provided in Appendix D.

For each of the nine review criteria, an 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)

Figure 1 shows the average score for the nine review criteria for each of the 17 projects reviewed in the Hydrogen and Clean Fuels Program. The panel viewed most of the projects favorably, giving the projects presented an average score of 3.7—indicating that overall, the projects were well above an "Adequate" score of 3.0. The project with the lowest overall average score earned a 2.5, halfway between "Ineffective" and "Adequate," while the project with the highest overall average score earned a 4.7, very close to a perfect "Effective" score of 5.0. Three projects scored below a score of 3.0 ("Adequate"), while seven projects scored at or above a score of 4.0 ("Moderately Effective"), with seven scoring between 3.0 and 4.0.

FIGURE 1 OVERALL SCORING AVERAGES - BY PROJECT



It can also be beneficial to look at the average scores for all projects across the nine review criteria. The combined average scores for all review criteria are shown in Table 1. The group of projects received the highest average score for the "Scientific and Technical Merit" criterion, with an average score across all projects of 4.0. This reflects a continuing effort by DOE to ensure the highest standards in R&D.

TABLE 1 SCORES BY REVIEW CRITERION

Criterion	Average	Highest Project Average	Lowest Project Average
1. Scientific and Technical Merit	4.0	5.0	2.6
2. Existence of Clear, Measurable Milestones	3.8	4.9	2.3
3. Utilization of Government Resources	3.9	4.8	2.7
4. Technical Approach	3.8	4.9	2.6
5. Rate of Progress	3.8	4.7	2.6
6. Potential Technology Risks Considered	3.4	4.7	2.2
7. Performance and Economic Factors	3.3	4.5	2.0
8. Anticipated Benefits, if Successful	3.9	4.8	2.8
9. Technology Development Pathways	3.5	4.7	2.6

A sample copy of the Peer Review Criteria Form is provided in Appendix D.

IV. SUMMARY OF KEY FINDINGS

This section offers a summary of key findings from across all of the 17 individual projects evaluated.

General Project Strengths

In general, reviewers found the projects to be sound, applauding DOE for presenting a high quality, diverse portfolio. All but three projects had scores that averaged above "Adequate." The reviewers found that many of the projects provided great value for their level of funding and were extremely timely, fitting into an overall energy strategy and providing concrete answers to questions of energy production, energy security, and environmental stewardship that are of vital importance to the nation. One reviewer went so far as to say that the Hydrogen and Clean Fuels Program is absolutely essential to the improvement of developing technologies and to informing national policy. In general, the Panel found that projects focusing on fundamental research had a greater potential for success than more mature projects and found that the more developed projects would have benefited greatly from earlier review. In general, the Panel found project leadership and management of the projects impressive and found most teams responsible for these projects to be competent in and passionate about their areas of expertise.

The seven highest-scoring projects (01, 02, 05, 07, 09, 10, and 15) averaged a 4.0 or better across all criteria. The overall average scores of four criteria in particular are impressive: the average scores for the criteria "Scientific and Technical Merit" and "Utilization of Government Resources" were 4.7 overall, while the average scores for "Existence of Clear, Measurable Milestones" and "Rate of Progress" were 4.5. These scores clearly demonstrate that the responsible use of funding has allowed nearly half of the projects reviewed to quickly and effectively achieve their goals.

The highest-rated project was Project 09, "Product Characterization for Entrained Flow Coal/Biomass Co-Gasification," conducted by General Electric Global Research. This project averaged 4.7 out of 5.0 across all criteria and earned a 5.0 for the "Scientific and Technical Merit" criterion.

The reviewers found that projects that brought together academics and industry were significantly better focused and more productive. This academic and industrial collaboration demonstrated a better bridge to commercialization than projects that had little collaboration.

The reviewers were impressed by projects developing baseline process, performance, and/or cost information, noting that the papers being produced are "very important" and "extremely strong." The Panel stated that the importance of these baseline studies could not be overemphasized and urged DOE to continue to produce and update baseline studies to maintain consistency in technology analysis.

The reviewers found that most of the projects were being conducted by capable and enthusiastic personnel, often going beyond requirements in pursuit of their goal. The Panel applauded these extended efforts and recognized the large skill base being developed in the area of Hydrogen and Clean Fuels.

General Project Weaknesses

The Panel found several of the projects to have an unjustified focus on particular materials, typically catalysts. Often this was because the material, even if successfully used, would be far too expensive for commercial purposes. The Panel also occasionally found that projects were focusing on materials and reactions that already had been sufficiently studied, to the point of finding the current research to be redundant, or in some cases, the Panel stated that research into an alternative, lesser known material would be more beneficial. Examples include projects using palladium and rhodium for catalyst formulations, projects exploring the effects of sulfur contaminants, and projects attempting to improve water-gas shift. The Panel suggested that other areas of focus could yield a much larger impact.

The “Performance and Economic Factor” criterion had lowest average score (3.3) across all projects—a score closer to a rating of “Adequate” than “Moderately Effective.” Though many of the projects explicitly considered the potential economic impact of the technology being researched, many of these projects failed to justify their assumptions or provide reliable economic data. There were also several projects that failed to provide sufficient cost and performance data for “Performance and Economic Factors,” earning a score lower than 3.0. Overall, the reviewers thought that there was considerable opportunity for improvement in this area, and hope that, in the future, even the most fundamental of research projects will be performed with knowledge of a sound economic basis.

The “Potential Technology Risks Considered” criterion had the next-lowest average score (3.4) across all projects—a score between “Adequate” and Moderately Effective.” The Panel found that many of the projects did not adequately identify and plan for the mitigation of factors that could lead to the failure of the technology to be developed and commercialized. The Panel rated four of the projects below 3.0 in this area, indicating that, for these projects to be acceptable, the project teams must examine and plan for potential risks.

The Panel found that many of the projects were reliant on the development of modular (or otherwise standardized) small-scale plants, which have proven to be far less economically viable than mid- to large-scale plants. The reviewers suggested that the program would better benefit from focusing on large-scale operations, allowing for competition with more traditional sources of fuel.

Issues for Future Consideration

On the whole, the reviewers were impressed by the technical expertise, knowledge, and productivity of the researchers. However, the reviewers found that many projects should have conducted early modeling to complement the experiments conducted. The Panel noted that a large area for exploration exists in performing projects that are similar to those being conducted but examine different materials and/or maintain different assumptions. The Panel also expressed that many of the projects could benefit from the use of less idealized operating conditions to achieve more realistic predictions of performance, especially in terms of potential contaminants in the gas stream.

The reviewers viewed the early economic analysis and early consideration of commercial implementation, two of the weakest performing criteria, as areas where general improvement can be made. The Panel did not find the specification of “Performance and Economic Factors” and “Technology Development Pathways” by stage of project development to be particularly helpful, often generating more discrepancies among the panel ratings, as the panel suggested that many of the fundamental research projects could not fulfill or should not be asked to fulfill the criteria outlined. Some reviewers proposed adding a rating of “Not Applicable” for appropriate programs, while others strongly argued that the inclusion of such a rating should not be allowed, as even fundamental research needs to be cognizant of economic concerns. This should be a process consideration for future reviews.

Several of the projects appeared to the Panel to be a loose association of what could effectively be considered separate projects. The Panel recommended providing some mechanism for each of these subprojects to be rated independently, because attempting to rate the sum of these projects was a difficult task.

V. PROCESS CONSIDERATIONS FOR FUTURE PEER REVIEWS

Both the Review Panel members and DOE/NETL managers involved in the peer review offered constructive comments on the review process and possible modifications for the future. Comments were provided at the conclusion of the Peer Review Meeting. The following is a brief summary of ideas recommended for use in planning future project review sessions.

General Process Comments

All involved agreed unanimously that the current Peer Review process is excellent and requires little or no modification. There was high praise both for the facilitation of the meeting and the superb work of the support staff. Panel members found the computerized score tabulation method effective and beneficial, as it allowed for quick display of a project's average score.

The Review Panel preferred the downtown venue selected for the review to a venue in a more isolated area, such as the airport.

Hydrogen and Clean Fuels Program and Projects Reviewed

The presentation and question-and-answer periods were held in closed sessions consisting only of DOE/NETL and ASME personnel and their contractors; the Review Panel; and the project team, allowing for candid discussion of the material. However, several Panel members thought that the PIs could have presented more details on certain aspects of these projects without disclosing proprietary information. For a small number of projects, the Panel felt that the PI did not effectively present the content of the project and in some cases was not able to respond effectively to the Panel's questions. The Panel suggested that a shared project presentation including the other partners would help address the issue.

The reviewers felt that many of these more developed projects would have greatly benefited from early, expert review with the aim to assess and augment project goals and activities.

Meeting Agenda

The Panel agreed that the information in the DOE roadmap presentation at the beginning of the review should be reinforced briefly at the beginning of each PI presentation. Many reviewers at times felt that they lacked context for a project, which prevented them from seeing how the project related to the Hydrogen and Clean Fuels Program as a whole. As a result, the panel found it necessary to direct programmatic questions to NETL staff during the first two days. Briefly presenting how each project fits within the overall Hydrogen and Clean Fuels Program, before each PI presentation, would address this issue and should be considered for future reviews.

The meeting agenda was unanimously found to provide the perfect amount of time for presentations, questioning, and subsequent discussion, allowing adequate time for the PI to present the project, for the Panel to have its questions answered, and for the Panel to discuss the project's strengths and weaknesses without feeling rushed or overburdened. Members of the Review Panel were appreciative of the diverse areas of expertise of the panel members, which allowed other reviewers to gather needed insight on various topics during discussion so as to be able to provide more accurate and comprehensive ratings and comments. The Panel agreed that a similar schedule should be used in future reviews.

Presentations and Evaluations

The Panel found that several of the presenters were ill-prepared for the review, failing to present adequate, relevant data for examination and evaluation by the panel. The reviewers proposed that an enhanced basic template, with examples, be provided to the PIs to assist them in providing the necessary information. The Panel also suggested that further orientation to the review process would prove beneficial to the PIs, especially if it would allow them to treat the review as a learning experience and an opportunity to gain expert insight into their project, rather than a simple evaluation.

As stated above, reviewers did not find the specification of “Performance and Economic Factors” and “Technology Development Pathways” by stage of project development to be particularly helpful. The Panel felt that many of the fundamental research projects could not fulfill or should not be asked to fulfill the criteria outlined, some reviewers going so far as to propose the addition of a rating of “Not Applicable” for appropriate programs, which others strongly opposed, arguing that even fundamental research needs to be cognizant of economic concerns. This issue should be examined more closely for future reviews to reach consensus on and present clearly to the reviewers what is to be required of fundamental research projects.

Review Panel

The panel thanked DOE for the opportunity to participate in this Peer Review, citing it as an enjoyable and educational experience.

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 has developed a standardized approach to reviewing research projects. The purpose of this section is to give a brief overview of the review procedure established for the U.S. Department of Energy (DOE)/National Energy Technology Laboratory (NETL) 2009 Fuels Peer Review.

ASME Knowledge and Community (K&C) Sector

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

Center for Research and Technology Development (CRTD)

The mission of the CRTD is to effectively plan and manage the collaborative research activities of ASME to meet the needs of the mechanical engineering profession as defined by the ASME members. The center is governed by the Board on Research and Technology Development (BRTD). The BRTD has organized more than a dozen research committees in specific technical areas. 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 review panel, provides facilitation of the actual review meeting, and prepares all summary documentation.

Board on Research and Technology Development (BRTD)

The BRTD governs the activities of the CRTD. 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 BRTD and to function as liaisons between BRTD and the appropriate ASME sectors, boards, and divisions.

Fuels Peer Review Executive Committee

For each set of projects to be reviewed, the BRTD convenes a Peer Review Executive Committee to oversee the review process. The Executive Committee is responsible for: seeing that all ASME rules and procedures are followed; reviewing and approving the qualifications of those asked to sit on the Review 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, and those members must have experience relevant to the program being reviewed. Members of the 2009 Fuels Peer Review Executive Committee were as follows:

- **Richard T. Laudenat, Chair.** Mr. Laudenat is the 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**, of Sargent and Lundy. Mr. Stenzel is a former chair of the ASME Power Division and past member of the ASME Energy Committee.
- **William Worek**, of the 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.

Fuels Peer Review Panel

The Fuels Peer Review Executive Committee accepted résumés for proposed Fuels Peer Review Panel members from CRTD, from a limited call to ASME members with relevant experience in this area, and from the DOE/NETL program staff. From these sources, the ASME Peer Review Executive Committee selected an eleven-member 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. The Review Panel members needed experience in several subject matters, including: hydrogen and alternative fueled vehicles; field tests; hydrogen storage; third party performance testing; emissions testing; durability; alloys and composites; corrosion protection; economic analysis; risk assessment; hydrogen production; reactor design; ethanol purity; reformability synthesis; catalytic conversion of syngas; catalyst selection; Fischer-Tropsch synthesis; coal-derived syngas; coal-derived carbon products; coal liquefaction; plant scale and electricity production; computational simulation; mathematical models; C-1 chemistry; advanced separation; and membranes.

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 including project goals, purpose, accomplishments to date, etc. A standard set of specifications for preparing this document was provided by CRTD. These Project Information Forms were collected and sent to the Peer Review Panel for background reading prior to the meeting.

Also in advance of the review meeting, CRTD gave project teams a standard presentation format and complete set of instructions for the oral presentations to the review panel. All presentations were created in PowerPoint format, and reviewers were also given hard-copy handouts of these slides.

Project Presentations, Evaluations, and Discussion

At the Fuels Peer Review Meeting, presenters were held to a time limit of 45 minutes to allow sufficient time for all presentations within the five-day meeting period. After each presentation, the project team participated in a question-and-answer session with the Review Panel for 30 minutes.

Following each presentation and Q&A, the Review Panel 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 reviewers 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, TMS provided reviewers with laptop computers that were pre-loaded with Peer Review Criteria Forms for each project. After scoring the projects on these criteria, the Panel members provided written comments about each project. The Review Panel then discussed the project for the purpose of defining: project strengths, project weaknesses, recommendations for other possible activities, and a list of action items that the team must address.

APPENDIX B: MEETING AGENDA

U.S. Department of Energy - Office of Fossil Energy - National Energy Technology Laboratory

2009 Fuels Peer Review

Sheraton Station Square

February 23 - 27, 2009

AGENDA

Monday, February 23, 2009 - Brighton I, II, & III

8:00 - 9:00 a.m.	Registration - 2ND Floor Foyer
9:00 - 9:45 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 - Meeting logistics/completion of forms - Charles Schmidt/Nicole Ryan/Justin Strock, TMS - Role of NETL - José Figueroa, NETL
9:45 - 10:30 a.m.	Overview - Open to NETL and ASME staff only - Hydrogen and Clean Fuels Program Technology Manager - Daniel Cicero
10:30 - 10:45 a.m.	**BREAK - Brighton III**
10:45 - 11:30 a.m.	***Project # ORD-09-220661*** - Computational Studies of the Initial Mechanistic Steps in Fischer-Tropsch Synthesis - *Dan Sorescu*, **National Energy Technology Laboratory**
11:30 - 12:00 p.m.	Q&A
12:00 - 12:40 p.m.	Discussion, evaluation, and written comments
12:40 - 1:40 p.m.	**Lunch (on your own)**
1:40 - 2:25 p.m.	***Project # OSAP CBTL*** - Affordable, Low-Carbon Diesel Fuel from Domestic Coal and Biomass - *Thomas Tarka*, **National Energy Technology Laboratory**
2:25 - 2:55 p.m.	Q&A
2:55 - 3:35 p.m.	Discussion, evaluation, and written comments
3:35 - 3:50 p.m.	**BREAK - Brighton III**
3:50 - 4:35 p.m.	***Project # 42449*** - Production of High-Hydrogen Content Coal-Derived Liquids - *Steve Bergin*, **Integrated Concepts & Research Corporation**
4:35 - 5:05 p.m.	Q&A
5:05 - 5:45 p.m.	Discussion, evaluation, and written comments

2009 Fuels Peer Review

Sheraton Station Square

February 23 - 27, 2009

Tuesday, February 24, 2009 - Brighton I, II, & III

7:00 - 8:00 a.m.	Registration - 2ND Floor Foyer
8:00 - 8:45 a.m.	***Project # 6368*** **-** Sensitivity of FT and Water-Gas Shift Catalyst to Poisons from Gasification of Biomass and Coal/Biomass Mixtures - *Burtron H. Davis*, **University of Kentucky - CAER**
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 - **Brighton III**
10:10 - 10:55 a.m.	***Project # OSAP-401.01.08.002*** **-** Technical, Economic, and Environmental Assessment of a Commercial Scale Coal to Fischer-Tropsch Liquids Plant Using a Dry-feed Gasifier with Carbon Capture - *Erik P. Shuster*, **National Energy Technology Laboratory**
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.	***Project # 42456*** **-** Production and Storage of Hydrogen From Coal Using C1 Chemistry - *Gerald P. Huffman*, **University of Kentucky - CFFS**
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 - **Brighton III**
3:15 - 4:00 p.m.	***Project # 43024*** - Catalytic Processes for the Synthesis of Ethanol From Coal-Derived Syngas - *James J. Spivey*, **Louisiana State University**
4:00 - 4:30 p.m.	Q&A
4:30 - 5:10 p.m.	Discussion, evaluation, and written comments

Wednesday, February 25, 2009 - Brighton I, II, & III

7:00 - 8:00 a.m.	Registration - 2ND Floor Foyer
8:00 - 8:45 a.m.	***Project # 6523*** - Demonstration of a Piston Driven Feed System for Feeding Coal/Biomass Mixtures Across a Pressure Gradient for Application to Commercial CBTL Systems - *A. John Rezaiyan*, **Southern Research Institute**
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 - **Brighton III**

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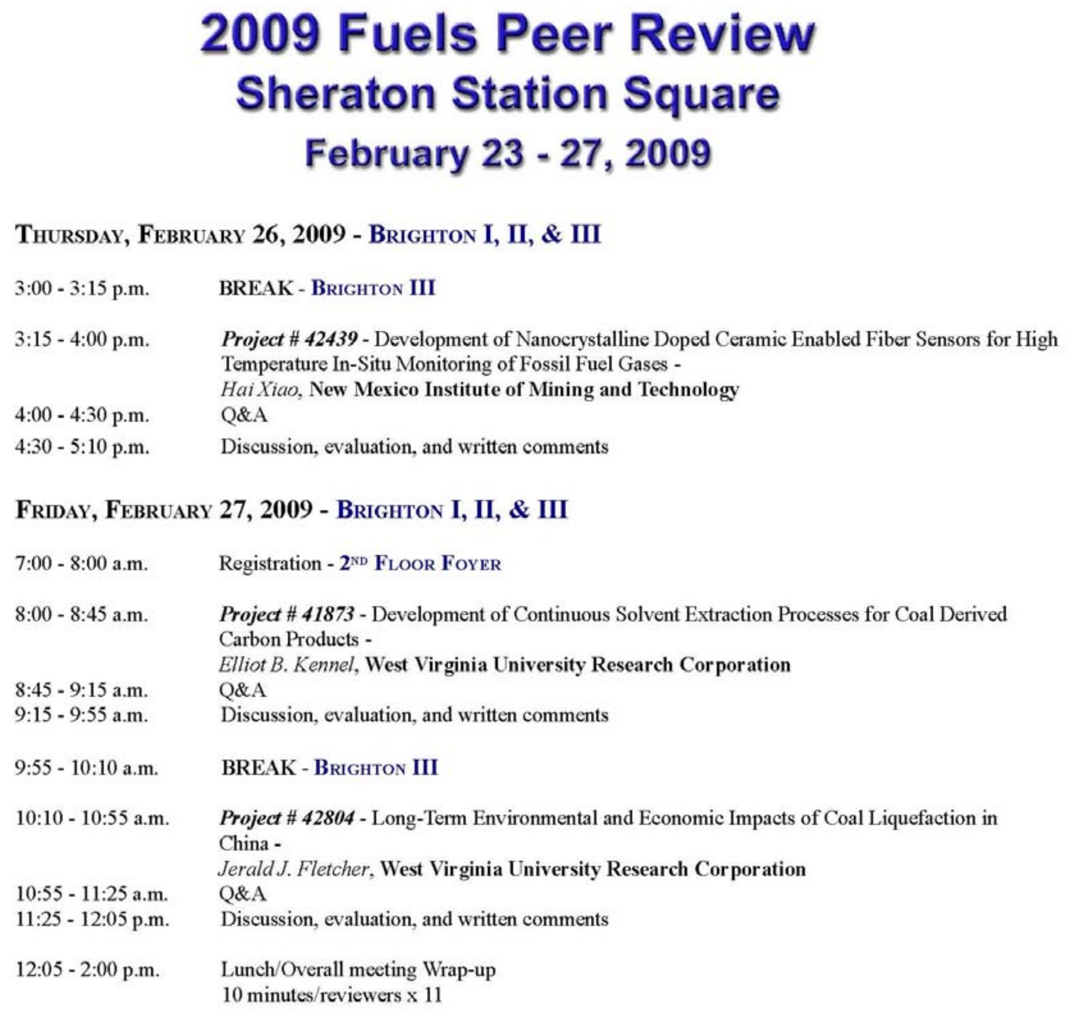
U.S. Department of Energy - Office of Fossil Energy - National Energy Technology Laboratory

WEDNESDAY, FEBRUARY 25, 2009 - BRIGHTON I, II, & III

10:10 - 10:55 a.m.	***Project # 6305*** - Product Characterization for Entrained Flow Coal/Biomass Co-Gasification - *Boris N. Eiteneer*, **GE Global Research (GEGR)**
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.	***Project # ORD-09-220622*** - Next Generation, Sinter-resistant, Catalysts for Syngas Conversion - *Christopher Matranga*, **National Energy Technology Laboratory**
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 - BRIGHTON III**
3:15 - 4:00 p.m.	***Project # FWP-49601 -*** Development of Mixed-Conducting Dense Ceramic Membranes for Hydrogen Separation - *U. Balachandran*, **Argonne National Laboratory-IL (ANL)**
4:00 - 4:30 p.m.	Q&A
4:30 - 5:10 p.m.	Discussion, evaluation, and written comments

THURSDAY, FEBRUARY 26, 2009 - BRIGHTON I, II, & III

7:00 - 8:00 a.m.	Registration - **2ND FLOOR FOYER**
8:00 - 8:45 a.m.	***Project # 43027*** - Investigation of Hydrogen-Fueled Internal Combustion Engine Durability - *Garrett Paul Beauregard*, **Electric Transportation Engineering Corporation**
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 - BRIGHTON III**
10:10 - 10:55 a.m.	***Project # 42759*** - Development of a Hydrogasification Process for Co-Production of Substitute Natural Gas (SNG) and Electric Power from Western Coals - *Raymond S. Hobbs*, **Arizona Public Service**
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.	***Project # 41874*** - An Industrial Based Consortium to Develop Premium Carbon Products from Coal - *Bruce G. Miller*, **Pennsylvania State University - OSP**
1:50 - 2:20 p.m.	Q&A
2:20 - 3:00 p.m.	Discussion, evaluation, and written comments



2009 Fuels Peer Review
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THURSDAY, FEBRUARY 26, 2009 - BRIGHTON I, II, & III

3:00 - 3:15 p.m.	BREAK - BRIGHTON III
3:15 - 4:00 p.m.	***Project # 42439*** - Development of Nanocrystalline Doped Ceramic Enabled Fiber Sensors for High Temperature In-Situ Monitoring of Fossil Fuel Gases - *Hai Xiao*, **New Mexico Institute of Mining and Technology**
4:00 - 4:30 p.m.	Q&A
4:30 - 5:10 p.m.	Discussion, evaluation, and written comments

FRIDAY, FEBRUARY 27, 2009 - BRIGHTON I, II, & III

7:00 - 8:00 a.m.	Registration - 2ND FLOOR FOYER
8:00 - 8:45 a.m.	***Project # 41873*** - Development of Continuous Solvent Extraction Processes for Coal Derived Carbon Products - *Elliot B. Kennel*, **West Virginia University Research Corporation**
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 - BRIGHTON III
10:10 - 10:55 a.m.	***Project # 42804*** - Long-Term Environmental and Economic Impacts of Coal Liquefaction in China - *Jerald J. Fletcher*, **West Virginia University Research Corporation**
10:55 - 11:25 a.m.	Q&A
11:25 - 12:05 p.m.	Discussion, evaluation, and written comments
12:05 - 2:00 p.m.	Lunch/Overall meeting Wrap-up 10 minutes/reviewers x 11

APPENDIX C: PEER REVIEW PANEL MEMBERS

After reviewing the scientific areas and issues addressed by the 17 projects to be reviewed, the CRTD staff and the ASME Peer Review Executive Committee, in cooperation with the NETL project manager, identified the following areas of expertise that the 2009 Fuels Peer Review Panel would need to possess:

- Hydrogen and alternative fueled vehicles
- Hydrogen storage
- Alloys and composites
- Corrosion protection
- Economic analysis and risk assessment
- Hydrogen production
- Reactor design
- Catalytic conversion of synthetic natural gas
- Fischer-Tropsch synthesis
- Coal-derived carbon products
- Computational simulation and mathematical modeling
- Basic and C-1 chemistry

It was also important that the Peer Review Panel represent the distinctly different perspectives of academia, industry, government, and nonprofit sectors.

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 form of Peer Review Meeting, a number of new submissions both from DOE, and those resulting from a limited call to ASME members with relevant experience. It was determined that six individuals who had served on prior ASME Review Panels were well qualified to serve on the Fuels Peer Review Panel.

Appropriate résumés were then submitted to the Fuels Peer Review Executive Committee for review. The following eleven members were selected for the 2009 Fuels Peer Review Panel:

- Daniel J. Kubek, consultant – Panel Chair
- Dr. Calvin H. Bartholomew, Brigham Young University
- Dr. Brian Gleeson, University of Pittsburgh
- Dr. J. Stephen Herring, Idaho National Laboratory
- Dr. James R. Katzer, Consultant
- Dr. William R. Owens, Princeton Energy Resources International
- Dr. Ravi Prasad, Helios-NRG, LLC
- Dr. Gregory M. Shaver, Purdue University
- James C. Sorensen, Consultant
- Martin Van Sickels, Consultant
- Dr. Michael R. von Spakovsky, Virginia Polytechnic Institute and State University

Panel members reviewed pre-presentation materials and spent five days 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.

2009 Fuels Peer Review Panel Members

Daniel J. Kubek – Panel Chair

Mr. Kubek is a consultant specializing in synthesis gas and natural gas purification and separation. His clients include the Electric Power Research Institute (EPRI) – CoalFleet, for whom he provides technical guidance on integrated processes for gasification projects; and the Gasification Technologies Council (GTC), where he serves as an advisor on technical issues related to gasification, particularly in the areas of H_2S removal and CO_2 capture and sequestration. Prior to this, Mr. Kubek was with Universal Oil Products (UOP) for 18 years as senior technology manager. His primary work was for UOP's solvent absorption, molecular sieve adsorption, and H_2 processing technologies as applied to natural gas and synthesis gas processing. He was the process manager responsible for all process design packages for multiple gasification projects and served as development manager for their gas processing business. In 2005, Mr. Kubek was awarded UOP's Don Carlson Award for Career Technical Innovation. Before joining UOP, he spent 17 years with Union Carbide. Mr. Kubek received a B.S. degree in chemical engineering from Rutgers University and earned a M.S. in chemical engineering from Purdue University.

Calvin. H. Bartholomew, Ph.D.

Dr. Bartholomew is a professor of chemical engineering and the founder and head of the Catalysis Laboratory at Brigham Young University. The courses he teaches cover topics on kinetics, catalysis, catalyst deactivation, air pollution control, creativity, and engineering materials. He has over 38 years of research experience in the areas of catalysis and combustion and has been principal or co-investigator on over 60 grants and contracts. Dr, Bartholomew has authored or co-authored five books and 120 peer-reviewed papers and reviews with emphases on catalyst design, catalyst deactivation, chemisorption, syngas production/conversion catalysis, and selective catalytic reduction of NO_x; and has consulted with over 40 companies on problems related to catalysis and air pollution. He was appointed Pope Professor of Chemical Engineering from 1997 through 2002, and in 2006, received a lifetime achievement award from colleagues and former students.

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. 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. He is the editor of the international journal *Oxidation of Metals.* 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.

J. Stephen Herring, Ph.D.

Dr. Herring is the technical director for the High Temperature Electrolysis, DOE Nuclear Hydrogen Initiative at the Idaho National Laboratory (INL). He originated concepts and formed a team for the development of solid oxide electrolytic cells. His research has grown to include the use of nuclear heat and electricity for the production of synthetic diesel; jet fuel and gasoline; and the recovery and upgrading of unconventional fossil fuels such as oil sands, oil shale, and heavy crude. Dr. Herring's previous responsibilities at INL include the evaluation of nuclear designs in conjunction with electrolytic and thermochemical processes for the production of elemental hydrogen and other hydrogen-transport compounds. Dr. Herring received B.S. degrees with distinction in both mechanical and electrical engineering from the Iowa State University and a Ph.D. in nuclear engineering at the Massachusetts Institute of Technology.

James R. Katzer, Ph.D.

Dr. Katzer is an independent energy consultant and member of the National Academy of Engineering. He has recently worked on several panel studies at the National Research Council, including "Resource Needs for Fuel Cell and Hydrogen Technologies" and "Alternative Liquid Transportation Fuels." As a visiting scholar at Massachusetts Institute of Technology (MIT) (2004 to 2007), he was the executive editor/director of the MIT study on "The Future of Coal in a Carbon Constrained World." In 2003, he retired from his position as manager of Strategic Planning and Performance Analysis for the ExxonMobil Research and Engineering Company, where he was responsible for technology planning and analysis activities. During his career, Dr. Katzer also served as vice president of Technology for Mobil Oil Corporation and vice president of Planning & Finance for the Mobil Research & Development Corporation. Dr. Katzer has more than 80 publications in technical journals, holds several patents, co-authored and edited several books, and developed the Center for Catalytic Science and Technology at the University of Delaware with Professor B. C. Gates. He has also received two awards from the Catalysis Club of Philadelphia, a B.S. degree from Iowa State, and a Ph.D. in Chemical Engineering from MIT.

William R. Owens, Ph.D.

Dr. Owens is vice president of fossil energy projects at Princeton Energy Resources International. He has extensive experience in system engineering principles, cost estimation, project economics, environmental control technologies, project management, and project control of power generation systems including conventional and emerging technologies. This experience includes fuel cells, turbines, gasifiers, fluidized bed combustors, etc. Dr. Owens's experience includes systems with bituminous coal, anthracite coal, and subbituminous western coals. He has worked with alternate fuel systems, including natural gas, hydrogen, gasifier fuel-gas, oil, and oil-shale systems. Dr. Owens has provided DOE with detailed support in outreach programs, deregulation of the electric utility industry, and international programs. 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 a former corporate fellow of Praxair Inc., has 60 U.S. patents and broad industrial experience in developing and commercializing new technologies, launching technology programs ($2–$50MM), supporting business development, building cross-functional teams, and setting up joint development alliances. He was a founding member of an alliance involving Praxair, British Petroleum, Amoco, Phillips Petroleum, Statoil, and Sasol to develop ceramic membrane syngas technology for gas-to-liquid processes. He established and led programs for ceramic membrane oxygen technology; co-developed proposals to secure major DOE programs worth $35MM in syngas and $20MM 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, aerospace business opportunities; and developed implementation plans resulting in a new R&D center in Shanghai. Dr. Prasad has a B.S. in mechanical engineering from the Indian Institute of Technology in Kanpur, India, and a M.S. and Ph.D. in mechanical engineering and chemical engineering from the State University of New York, Buffalo, New York.

Gregory M. Shaver, Ph.D.
Dr. Shaver is an assistant professor of mechanical engineering at Purdue University, studying and developing advanced powertrain solutions. His research interests include work in modeling and control of novel combustion methodologies, utilization of environmentally friendly alternative fuels, and incorporation of advanced internal combustion (IC) engines on hybrid powertrains. He has written for multiple journals, including the *International Journal of Engine Research*; the *ASME Journal of Dynamic Systems*, *Measurement, and Control*; and the *IFAC Journal on Control Engineering Practice*, writing on such subjects as the physics-based modeling and control of residual-affected homogenous charge compression ignition (HCCI) engines and the modeling of cycle-to-cycle coupling and mode transition in HCCI engines with variable valve actuation. He is the editor of the 2007 International Federation of Automatic Control (IFAC) Symposium on Advances in Automotive Control. He received a B.S. in mechanical engineering from Purdue University and an M.S. and Ph.D. from Stanford University.

James C. Sorensen
Mr. Sorensen is a consultant specializing in the conception and development of clean coal and other energy programs with a focus on integrated gasification combined cycle (IGCC), oxy-fuel combustion, gas-to-liquids (GTL), and air separation and hydrogen/syngas technology. Prior to this, he worked for Air Products and Chemicals both as director of new markets and as director of gasification and energy conversion. While in these positions, his achievements included developing and selling a $26 million ultra clean fuels technology development program that was selected by DOE, selling a $30 million single train separation facility for a 250 MW IGCC power plant, proposing and developing a $22.5 million fossil fuel R&D program selected by DOE, and leading Air Products' effort on a multiteam proposal selected by DOE for a $180 million Clean Coal Technology award. Mr. Sorensen is the founding chairman of the Gasification Technologies Council. He received a B.S. degree in chemical engineering from the California Institute of Technology and earned a M.S. in chemical engineering from Washington State University. Mr. Sorensen also earned a M.B.A in general management from Harvard Business School.

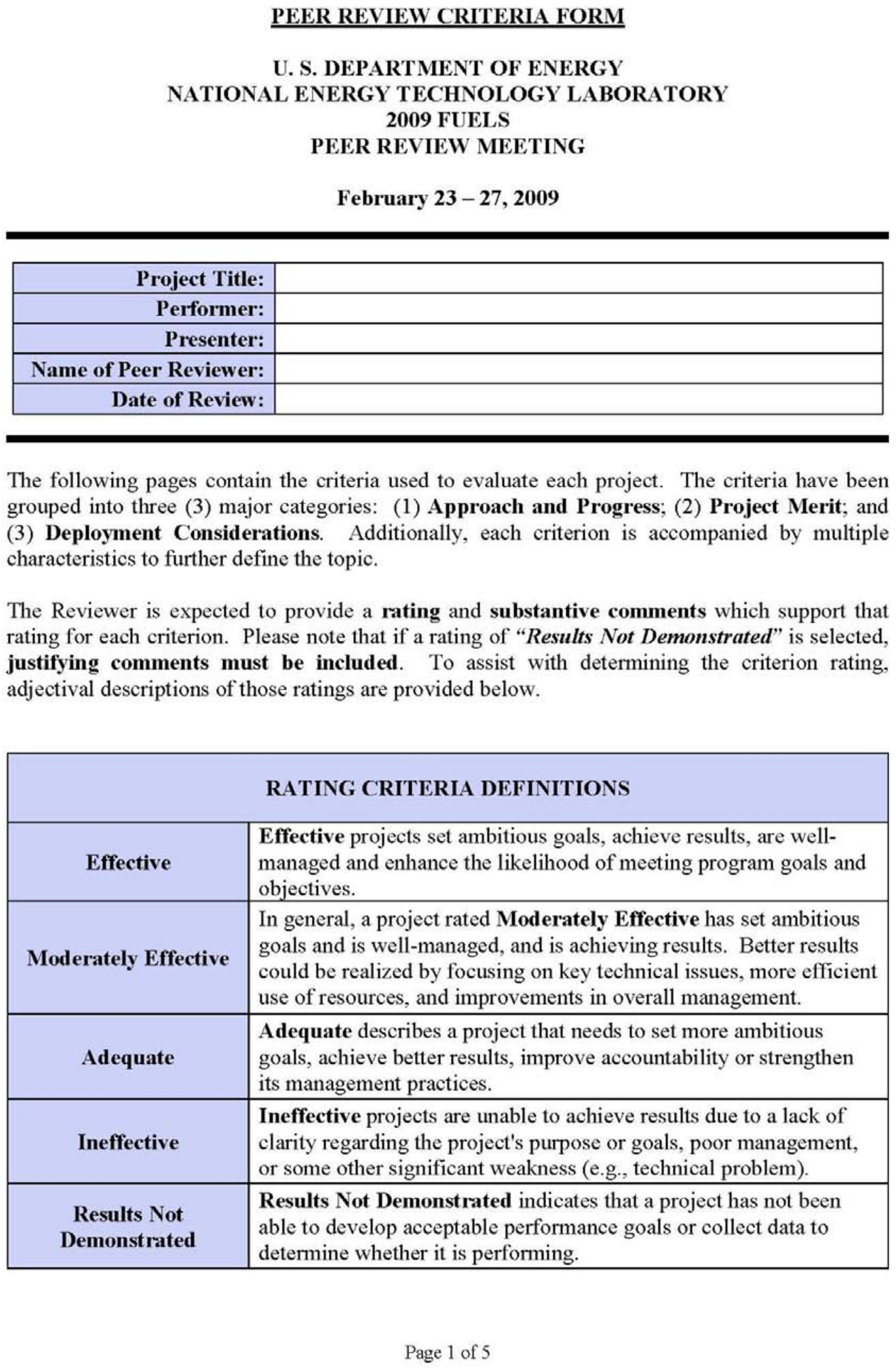
Martin J. Van Sickels

Mr. Martin Van Sickels, president of MVS Consulting LLC, has been in the process and engineering construction business for over 42 years. During a 30-year career with Kellogg Brown & Root, Inc. (KBR), he was responsible for all research and development programs, including onshore, offshore, operations and maintenance, and infrastructure. He led the development of a ranking methodology for all R&D activities to fully align them with KBR's strategic and business plans, was a member of the inquiry review and pricing committees, and was chairman of the technology screening and patent committees. His last position at KBR was vice president and chief technology officer, a member of the executive committee. His duties in this position included worldwide responsibility for the management, marketing, and development of all KBR proprietary and licensed technologies (chemicals, fertilizers, olefins, petroleum refining, and coal gasification) and special execution technologies (liquid-nitrogen gas, gas-to-liquid, gas processing, and offshore technology). He received a B.S. in chemical engineering from the City College of New York and a M.S. in chemical engineering from New York University.

Michael R. von Spakovsky, Ph.D

Dr. von Spakovsky is a professor of mechanical engineering and director of the Center for Energy Systems Research at the Virginia Polytechnic Institute and State University. He teaches undergraduate and graduate level courses in thermodynamics, kinetic theory, fuel cell systems, and energy system design. His research interests include computational methods for modeling and optimizing complex energy systems; methodological approaches for integrated synthesis, design, operation, control, and diagnosis of such systems; and fuel cell applications for both transportation and distributed power generation. He is associate editor for the *ASME International Journal of Fuel Cell Science and Technology* and an ASME Fellow. He is also editor-in-chief of the *International Journal of Thermodynamics* as well as chairman of the Executive Committee of the International Center for Applied Thermodynamics. He received 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
2009 FUELS
PEER REVIEW MEETING

February 23 – 27, 2009

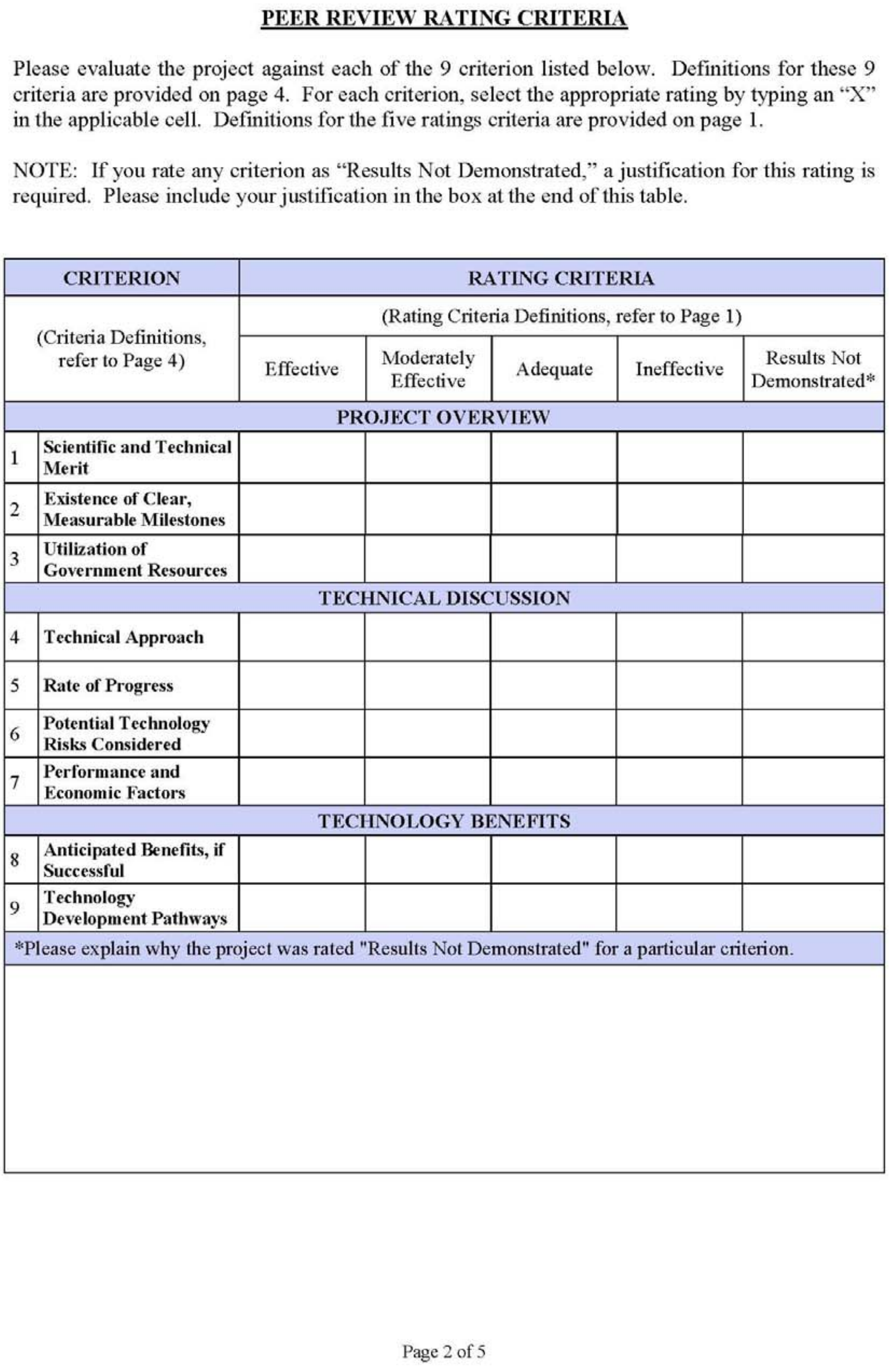
Project Title:	
Performer:	
Presenter:	
Name of Peer Reviewer:	
Date of Review:	

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

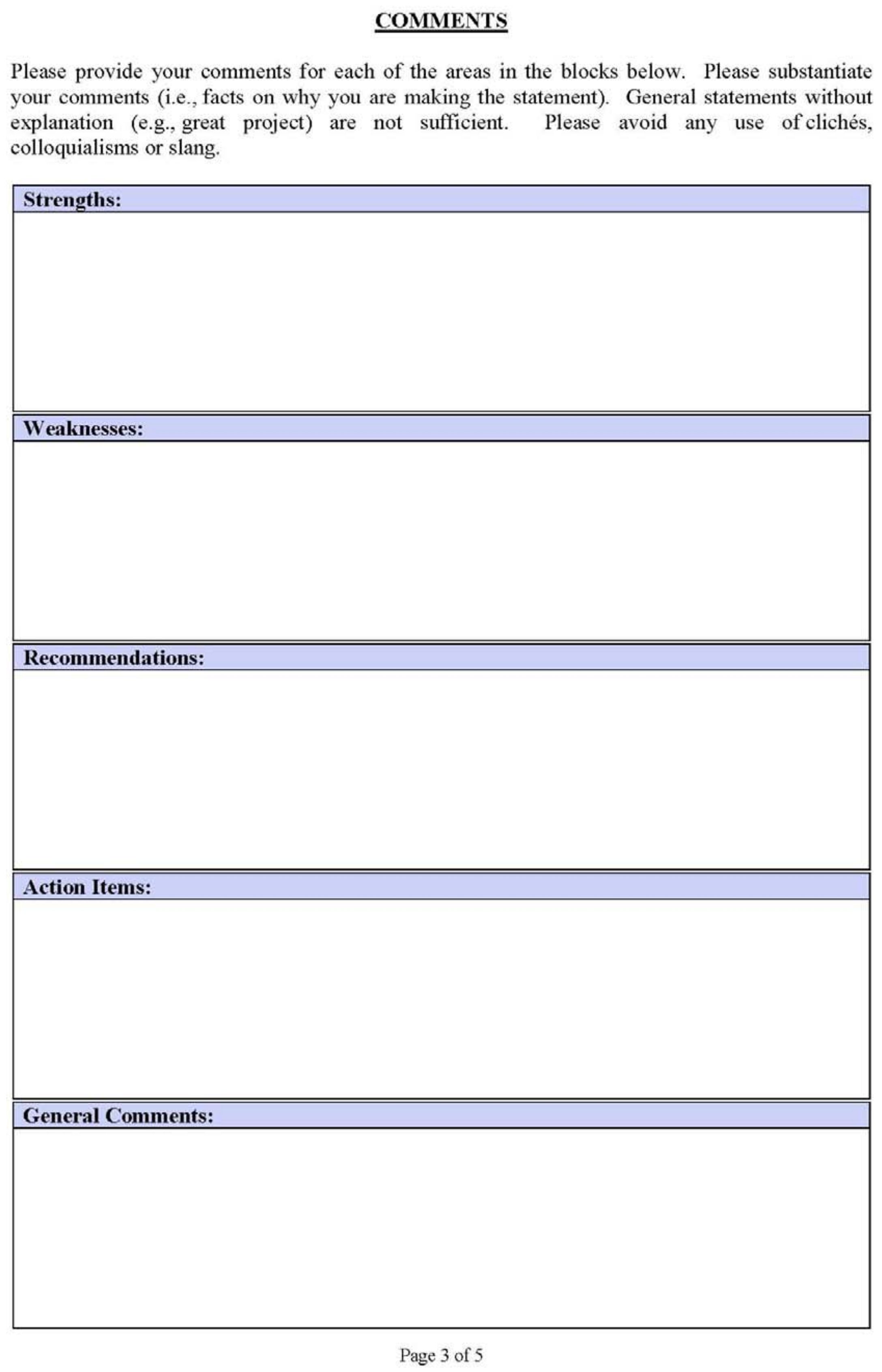


PEER REVIEW RATING CRITERIA

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				
(Criteria 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:

Page 3 of 5

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.

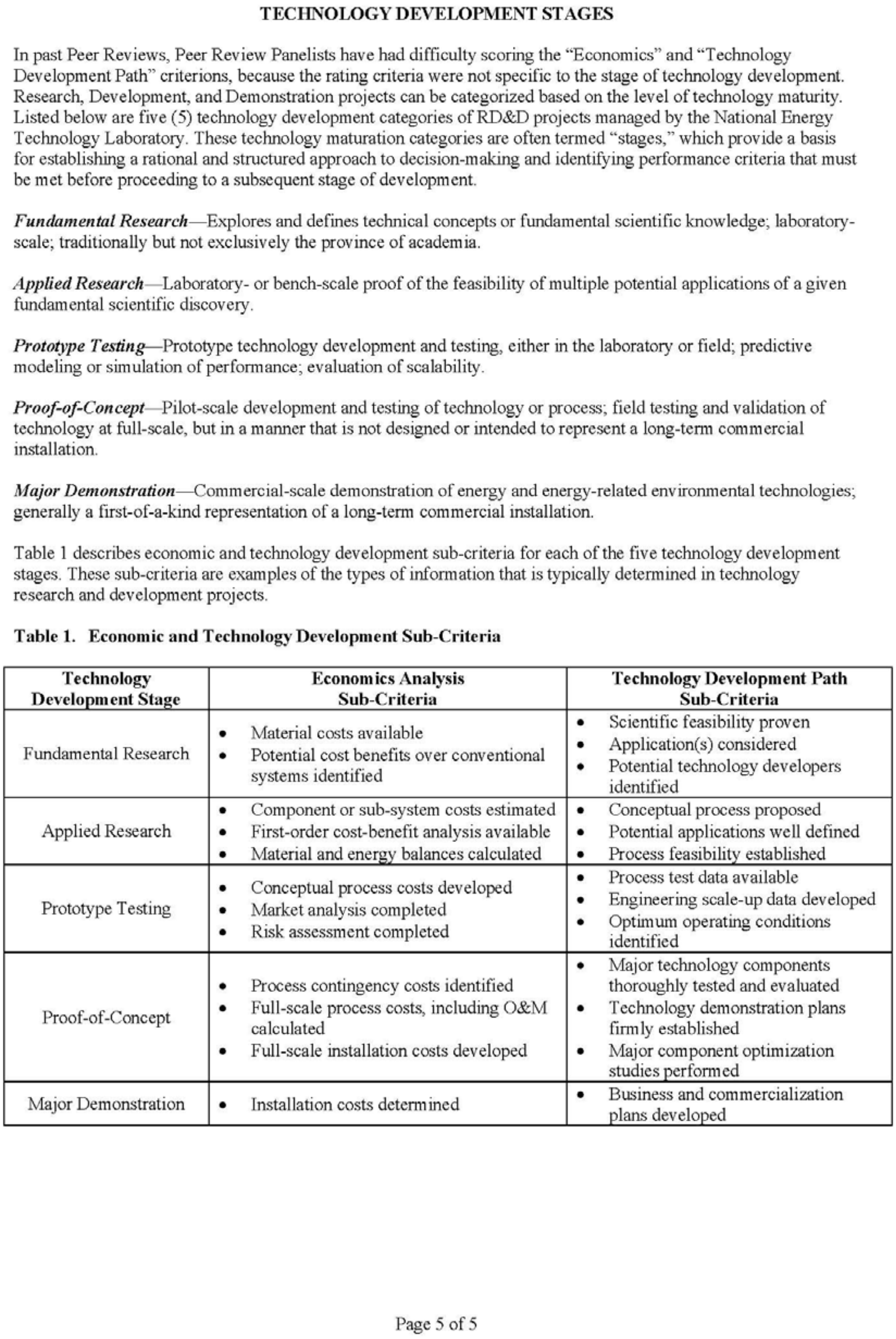
TECHNOLOGY BENEFITS

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.



TECHNOLOGY DEVELOPMENT STAGES

In past Peer Reviews, Peer Review Panelists have had difficulty scoring the "Economics" and "Technology Development Path" criterions, because the rating criteria were not specific to the stage of technology development. Research, Development, and Demonstration 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 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.

Table 1. Economic 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

APPENDIX E: HYDROGEN AND CLEAN FUELS PROGRAM PROJECT SUMMARIES

Presentation ID Number	Project Number	Title
01	ORD-09-220661	Computational Studies of the Initial Mechanistic Steps in Fischer-Tropsch Synthesis and Kinetic Monte Carlo Simulations
02	OSAP CTL	Affordable, Low-Carbon Diesel Fuel from Domestic Coal and Biomass
03	DE-FC26-06NT42449	Production of High-Hydrogen Content Coal-Derived Liquids
04	DE-NT0006368	Sensitivity of FT and Water-Gas Shift Catalyst to Poisons from Gasification of Biomass and Coal/Biomass Mixtures
05	OSAP-401.01.08.02	Technical, Economic, and Environmental Assessment of a Commercial Scale Fischer-Tropsch Liquids Plant Using a Dry-feed Gasifier with Carbon Capture
06	DE-FC26-05NT42456	Production and Storage of Hydrogen from Coal Using C1 Chemistry
07	DE-FC26-06NT43024	Catalytic Processes for the Synthesis of Ethanol from Coal-Derived Syngas
08	DE-FC26-08NT06523	Demonstration of a Piston Driven Plug Feed System for Feeding Coal/Biomass Mixtures Across a Pressure Gradient for Application to Commercial CBTL Systems
09	DE-NT0006305	Product Characterization for Entrained Flow Coal/Biomass Co-Gasification
10	ORD-09-220662	Next Generation, Sinter-Resistant, Catalysts for Syngas Conversion
11	FWP-49601	Development of Mixed-Conducting Dense Ceramic Membranes for Hydrogen Separation
12	DE-FC26-07NT43027	Investigation of Hydrogen-Fueled Internal Combustion Engine Durability
13	DE-FC26-02NT42759	Development of a Hydrogasification Process for Co-Production of Substitute Natural Gas (SNG) and Electric Power from Western Coals
14	DE-FC26-03NT41874	An Industrial Based Consortium to Develop Premium Carbon Products from Coal
15	DE-FC26-05NT42439	Development of Nanocrystalline Doped Ceramic Enabled Fiber Sensors for High Temperature In-Situ Monitoring of Fossil Fuel Gases
16	ORD-07-220611	Development of Continuous Solvent Extraction Processes for Coal-Derived Carbon Products
17	DE-FC26-06NT42804	Long-Term Environmental and Economic Impacts of Coal Liquefaction in China

01: ORD-09-220661

Project Number ORD-09-220661	**Project Title** Computational Studies of the Initial Mechanistic Steps in Fischer-Tropsch Synthesis			
Contacts DOE/NETL Project Mgr.	**Name**	**Organization**	**Email**	
Principal Investigator	Dan Sorescu	NETL – ORD	Dan.Sorescu@netl.doe.gov	
Partners				
Stage of Development				
X Fundamental	__Applied	__ Proof of Concept	__ Prototype Testing	__ Demonstration

Technical Background:

Implementation of the FutureGen program and of the congressional mandates Coal-to-Liquid Fuel Promotion Act of 2007; Clean, Affordable, and Domestic Fuels for Energy Security Act of 2007; and Clean Coal-Derived Fuels for Energy Security Act of 2008 will be highly dependent on further development of new materials and processes able to solve some of the demanding conditions imposed on the use of coal fossil fuels by new environmental standards for the reduction of carbon dioxide (CO_2) emissions and the achievement of carbon-neutral technologies. Specifically, these demands require the continued development of catalysts for the conversion of coal-derived synthesis gas (syngas) to liquid fuels and the optimization of the corresponding products obtained by Fischer-Tropsch (F-T) synthesis. Such objectives can only be achieved through a comprehensive scientific approach, starting with an atomistic understanding of the physical and chemical transformations of the catalysts under realistic Fischer-Tropsch process conditions, followed by process optimization at larger scales, and leading to process optimization at the plant scale, where demonstration and commercialization tasks play the central role.

As one of the various research initiatives coordinated by NETL in the area of fossil fuels, this project emphasizes the use of computational chemistry methods to obtain unique information about the structural and electronic properties of the catalysts, while also contributing to the description of key reactions involved in the F-T process on iron-based (Fe-based) catalysts. This computational effort complements experimental investigations and is correlated to additional research projects existent in the Computational Chemistry Group at NETL, including catalyst development, solid membranes for gas separation, nanostructured materials for gas storage and separation, and development and optimization of sorbent systems for CO_2 separation applications.

In the particular case of coal-to-liquids technologies, it is well documented that iron-based catalysts can be used effectively in F-T synthesis for conversion of syngas (containing carbon monoxide [CO] and hydrogen gas [H_2]) to liquid fuels. Relative to other F-T catalysts such as cobalt or ruthenium, the advantages of iron (Fe) catalysts include a relatively low cost, flexibility in product distribution, and suitability to convert low H_2/CO-ratio syngas obtained from coal or biomass feedstocks.

In practical applications, the α-Fe_2O_3 (hematite) oxide is generally used as the starting catalyst. As this phase is (almost) inactive for F-T synthesis, the catalyst is subject first to an activation treatment that can be done in different reducing atmospheres such as H_2, CO, or syngas. The oxide reduction was found to take place in two steps. The first one corresponds to a facile reduction of α-Fe_2O_3 to Fe_3O_4 (magnetite) and does not depend on the activation gas used. The second one is a slow reduction of Fe_3O_4 to either metallic iron (H_2 reduction) or to iron carbide phases (under CO or syngas treatment). In particular, under F-T synthesis conditions, several carbide phases such as ε-Fe_2C, ε'-$Fe_{2.2}C$, χ-Fe_5C_2, and θ-Fe_3C have been detected. There seems to exist some consensus that among various carbide phases, the active phase in F-T synthesis is the monoclinic Hägg iron carbide (χ-Fe_5C_2) phase. As a result, characterization of the surface properties of the χ-Fe_5C_2 surface, previously indicated as the “true Fischer-Tropsch catalyst,” is of utmost importance for the understanding and further optimization of the F-T process on Fe-based catalysts. Despite its importance, a detailed experimental characterization at the atomic level of the surface properties of the χ-Fe_5C_2 phase is not yet available.

Correlated to structural and chemical transformations of the catalyst properties, characterization of the elementary surface reactions (i.e., adsorption, diffusion, and dissociation reactions of various atomic and molecular species such as H, CO, CH_x, and C_xH_y) represents a second essential research direction that can help in further optimization of the F-T process. In the particular case of syngas F-T conversion, generically represented as $CO+(1+n/2)H_2 \rightarrow CH_n+H_2O$, adsorption and dissociation of CO on iron and iron carbide surfaces followed by hydrogenation, chain growth reactions, and formation of hydrocarbon and water species are of paramount importance. Additionally, understanding the nature of the deposited carbon and oxygen species is also essential, as significant transformations of the iron surface by carburization can take place. In all of these instances, some of the key scientific questions are the identification of the active surface sites, the nature of the adsorbed molecular and atomic species, and the description of the barrier heights for different surface reactions. Understanding these processes is essential in order to determine the relationship between the intrinsic catalyst surface structure and the corresponding catalytic activity. Additionally, essential data related to the reaction mechanism for adsorption and dissociation of the elementary gases on iron carbide surfaces is currently lacking.

The computational approach to be used in this project is based on plane-wave density functional theory (DFT) calculations in conjunction with periodic slab models. For the treatment of exchange and correlation, the generalized gradient approximation and the Perdew, Burke, and Ernzerhof (PBE) functional are used together with the spin interpolation for the correlation energy introduced by Vosko-Wilk-Nusair (VWN). The calculations are spin polarized to account for the magnetic properties of iron. The surface and the interaction of adsorbate species to the surface are represented using slab models with periodic boundary conditions. This computational approach is very effective and has proven accuracy for description of the adsorption properties of the molecular and radical species on different surfaces and for description of the diffusion and dissociation reactions. The computation method used in this work represents the state of the art given the size of the systems involved. The corresponding results are highly accurate, and no fitting of the experimental data is involved in these calculations. As a result, the information generated can be used, for example, for further parameterization of larger-scale simulation methods.

Relationship to Program:

This project will support important F-T catalyst advances within the alternate hydrogen production pathway focus area of the Hydrogen and Clean Fuels Program. The proposed theoretical work will directly complement the experimental investigations to be done on iron carbide catalysts by the Surface Science group in NETL's Chemistry and Surface Science Division. In concerted efforts with this group, this project will be able to provide a comprehensive picture of the atomistic mechanism involved in the adsorption and dissociation processes of CO on the active F-T phase on Fe catalysts. This project supports NETL goals because if it succeeds, it will place NETL at the forefront of scientific research, as no other group to date has been able to provide this information on the atomic scale.

The proposed work will help to improve the understanding of the performances of Fe-based F-T catalysts. Specifically, this research will determine fundamental thermochemical data related to elementary surface reactions, and in particular, data for the adsorption, diffusion, and activation energies of CO on various surfaces of Fe and Fe_5C_2 carbide at the atomic scale. This information will then be extended to other types of reactions, such as hydrogenation or carbon-carbon coupling reactions. Such topics are not covered in literature, specifically for the case of the Fe_5C_2 carbide phase, despite the fact that this phase is known to be active in F-T synthesis.

Additionally, in the case of the Fe surface, the studies in this project were the first to provide a systematic analysis of the adsorption and reaction properties on different Fe crystallographic surfaces at the atomic scale. These investigations will lead to the identification of the optimal crystallographic orientations among various flat, stepped, or kinked surfaces, information that catalyst developers can further use to develop Fe-based F-T catalysts with significantly increased catalytic activity. Additionally, the stability and activation data determined in this project can be further used in performing simulations at large scales, in process optimizations, or to achieve a better correlation to experimental data.

Primary Project Goal:

Given the importance of the Fe and iron carbide (Fe_5C_2) phase in the F-T process, this project proposes to characterize the adsorption and reaction properties of the elementary gas-phase species on representative types of iron and iron carbide surfaces using first-principle DFT calculations. The main emphasis in this case will be to identify the correlation between chemical activity and the electronic and structural properties of different crystallographic surfaces of both iron and iron carbide phases.

Additionally, in the case of the Fe_5C_2 phase, another goal of this project is to determine the structural and stability properties of different surfaces of this phase, information that is not currently available experimentally. Following this computational step, the project team will then characterize the set of elementary chemical reactions starting with adsorption and dissociation properties of CO molecular species.

The ensemble of atomistic data to be determined in this project will allow for creation of an essential database of structural, electronic, energetic, and thermodynamic properties against which further studies can be performed. Such studies can involve, for example, multiscale simulations or parameterization of such methods. Additionally, the results obtained can be used as a reference to study the influence of other important parameters in F-T processes, such as the role of the promoter or poisoning species.

Objectives:

The objectives of this project are divided into the following phases:

I. Stability properties of different crystallographic surfaces of the Fe_5C_2 phase—The first objective of the project team's calculations is to determine the stability properties of different low-index Miller surfaces. This information is essential to identify the most stable surface orientations. As the bulk structure of Fe_5C_2 is monoclinic with C2/c symmetry, the investigation of stability properties will require the analysis of a large number of crystallographic surface orientations, such as (001), (010), (100), (101), (110), (011), and (111). The main outcome of this computational step will be the identification of the most thermodynamically stable surfaces of Fe_5C_2.

II. Adsorption properties of CO on the most stable Fe_5C_2 surfaces—For the set of the most stable surface orientations, this research will then determine the adsorption properties of CO at different surface sites. It is expected that different types of binding configurations will be identified, involving either Fe atoms or mixed Fe and C atoms. Significant differences in binding properties are expected to be seen among these sites. Besides the geometric and energetic (binding energies) properties, the vibrational properties for the adsorbate species will be determined. Such data can be measured experimentally and can be used for further correlation with theoretical results.

III. Activation and dissociation properties of CO on Fe_5C_2 surfaces—The activation and reaction energies for dissociation of $CO(a) \rightarrow C(a)+O(a)$ on the most stable Fe_5C_2 surfaces will be determined using the climbing image nudged elastic band method. This computational step is essential, as it will determine the activation energies of CO on iron carbide—one of the first steps involved in the F-T process. Additionally, the research will provide a direct comparison of the CO activation properties on bare Fe, relative to Fe_2C_5 surfaces. The project team emphasizes that, to date, no other experimental or theoretical studies have determined this information on the atomic scale, despite the fact that the iron carbide phase is the active phase in F-T synthesis.

Additionally, the results of the current work continue the following fiscal year 2008 computational activities:

I. Characterization of the adsorption, diffusion and dissociation properties of CO on stepped Fe surfaces—The focus of this activity was to determine the preferential adsorption sites of CO in the case of surfaces with different types of steps. The variation of the binding properties with coverage for either molecular (CO) or atomic (C, O) species was also investigated. Additional studies were done to map the diffusion barriers among different local minima at the steps or on the terraces of Fe surfaces.

II. Analysis of dissociation properties of CO on a comprehensive set of crystallographic Fe surfaces—The focus of this task was to identify the adsorption and dissociation properties of CO on a large set of Fe crystallographic surfaces ([110], [100], [211], [107], [310], and [111]) in order to identify those surfaces with the smallest activation energy for CO dissociation. Additionally, this information has been used to obtain a direct correlation between the apparent activation energy of dissociation and the rebonding energy of the non-interacting products of reaction.

02: OSAP CBTL

Project Number OSAP CBTL	**Project Title** Affordable, Low-Carbon Diesel Fuel from Domestic Coal and Biomass			
Contacts DOE/NETL Project Mgr.	**Name** Thomas J. Tarka	**Organization** NETL – OSAP	**Email** Thomas.Tarka@netl.doe.gov	
Principal Investigator	Thomas J. Tarka	NETL – OSAP	Thomas.Tarka@netl.doe.gov	
Partners	Noblis, Inc.			
Stage of Development				
__ Fundamental	X Applied	__ Proof of Concept	__ Prototype Testing	__ Demonstration

Technical Background:

This study evaluates the conversion to diesel fuel of bituminous coal, switchgrass, and various mixtures of those two feedstocks via Fischer-Tropsch synthesis. Conversion facilities, configured for fuels production, produce a minimum of excess power in plant sizes ranging from 5,000 barrels per day (BPD) to 50,000 BPD based on feedstock availability. This study supplements several existing NETL studies and includes new process configurations which build upon existing technologies used in power and fuels production applications.

This study is of particular value at present because of the nation's dependence on oil imports for transportation fuel, the current economic crisis, and the desire to produce fuels with reduced climate change impacts. Abundant domestic resources, including coal and biomass, can be leveraged effectively to address these concerns. This study provides an in-depth assessment of the impact of different feedstock pairings and plant configurations on product cost and greenhouse gas (GHG) emissions.

The plants evaluated in this study were found to have the following potential benefits to the nation:

- The ultra-low-sulfur diesel fuel produced by coal-to-liquids (CTL) and coal-and-biomass-to-liquids (CBTL) plants is Section 526 compliant, having a life-cycle GHG emission level that is 5%–63% lower than the petroleum-derived fuels.
- CTL and CBTL plants that blend up to 15% biomass (by weight) are economically feasible (i.e., achieve a 20% internal rate of return) when crude oil is priced between $80 and $95 per barrel and carbon is priced between $0 and $45 per metric ton carbon dioxide (CO_2)-equivalent. Producing diesel fuel exclusively from biomass, without the economies of scale provided by coal, is not economically feasible unless crude oil prices are very high—between $170 and $240 per barrel.
- CTL and CBTL plants offer a very inexpensive opportunity to demonstrate the geologic sequestration of CO_2, which is necessary to enable the nation to continue use of its most abundant and secure energy resource in a carbon-constrained world. Because the capture of CO_2 is an inherent part of the CTL process, sequestering over 90% of the CO_2 emissions from a CTL plant is inexpensive (adding only 7¢ per gallon to the product cost).
- If CO_2 captured from CTL/CBTL plants is used for enhanced oil recovery, energy security benefits are increased; up to 1.5 barrels of oil can be recovered for each barrel of CTL/CBTL product.

- A national commitment to building a CTL/CBTL industry would have a positive impact on the economy, creating skilled jobs and improving the balance of trade by reducing the amount of money sent overseas for oil imports, which was valued between $400 and $500 billion in 2008.
- Also, there are opportunities for applied research and demonstrations to improve the economic competitiveness and climate change benefits of this technology, likely resulting in a new, high-tech industry.

Relationship to Program:

This project will support important liquid fuels production advances within the alternate hydrogen production pathway focus area of the Hydrogen and Clean Fuels Program. The study provides technical and economic insight into the economic feasibility and climate change impacts of converting coal, biomass, and coal/biomass mixtures into synthetic diesel fuel. The results of this study will be helpful in determining what type of plant best provides a balanced energy solution, simultaneously addressing energy security, economic sustainability, and climate change, in the area of transportation fuels.

The whole of this report builds on the following studies published by or for NETL:

- *Assessment of Technologies for Co-Converting Coal and Biomass to a Clean Syngas*
- *Development of Baseline Data and Analysis of Life Cycle Greenhouse Gas Emissions of Petroleum-Based Fuels*
- *Characterization of Biomass Feedstocks*
- *Baseline Technical and Economic Assessment of a Commercial Scale Fischer-Tropsch Liquids Facility*
- *Cost and Performance Baseline for Fossil Energy Power Plants study, Volume 1: Bituminous Coal and Natural Gas to Electricity*

Primary Project Goal:

The primary goal of this project is to provide a comprehensive techno-economic assessment of the production of diesel fuel from domestic coal and biomass using Fischer-Tropsch synthesis, highlighting impacts on energy security, economic sustainability, and climate change.

Objectives:

The main objective of this project is to provide detailed conceptual plant designs to evaluate the economic feasibility and climate change impacts of the conversion of CTL, CBTL, and biomass to liquids (BTL). These plant designs are to be modeled using the AspenPlus process modeling software, and the resultant systems will include component descriptions, process flow diagrams, heat and mass flow balances, estimates of capital and operating costs, and economic data that can be used to evaluate the financial feasibility of the CTL/CBTL/BTL plants relative to petroleum-based fuels.

Care will also be taken to evaluate the greenhouse gas emissions, which occur over the life cycle of the fuel and to determine how this may affect economic feasibility.

These plant designs will then be used to inform policy makers and technology developers regarding options for the use of coal and biomass for liquid fuels production, including the economic, climate change, and energy security impacts of these fuels.

03: DE-FC26-06NT42449

Project Number DE-FC26-06NT42449	**Project Title** Production of High-Hydrogen Content Coal-Derived Liquids			
Contacts DOE/NETL Project Mgr.	**Name** Daniel Driscoll	**Organization** Fuels Division	**Email** daniel.driscoll@netl.doe.gov	
Principal Investigator	Steve P. Bergin	Integrated Concepts and Research Corporation (ICRC)	sbergin@icrcsolutions.com	
Partners	EnviRes LLC University of Kentucky Center for Applied Energy Research (CAER) University of Alaska Fairbanks			
Stage of Development				
__ Fundamental	__ Applied	__ Proof of Concept	X Prototype Testing	__ Demonstration

Technical Background:

This project evaluates the potential advantages of a cobalt (Co) Fischer-Tropsch (F-T) catalyst with coal-derived synthesis gas (syngas), an alternative to the iron (Fe) catalyst systems that have been used by virtually all coal-based F-T plants to date. Iron F-T catalysts are relatively cheap and are more tolerant of low hydrogen gas (H_2) to carbon monoxide (CO) syngas ratios. Additionally, Fe can simultaneously catalyze water-gas shift and F-T synthesis.

Cobalt F-T catalyst systems, on the other hand, are more expensive than Fe systems and are generally less tolerant. Cobalt requires that the syngas H_2 to CO ratio be boosted to about 2:1, increasing the processing cost. Cobalt systems may require expensive syngas cleaning because Co is more sensitive to impurities than Fe. However, Co is perceived as a viable F-T catalyst option because Co-based fuel products may be superior to Fe-based fuel products, which will require less expensive upgrading than Fe catalyst systems to obtain high hydrogen-content coal-derived liquid fuels.

The project was awarded to Integrated Concepts and Research Corporation (ICRC) on March 30, 2006 in partnership with Syntroleum Corporation, a provider of both F-T technology and the project’s required 20% cost share. Due to financial difficulties, Syntroleum Corporation ceased project activity in December 2006. NETL managers decided to continue the project as had been planned with Syntroleum, if possible, encouraging ICRC to find a new partner (or partners), such as the University of Kentucky Center for Applied Energy Research (CAER), to replace Syntroleum. This was successfully done, and the kickoff meeting for the revised ICRC project in partnership with EnviRes and CAER was held in November 2008.

Relationship to Program:

This project will support important F-T catalyst advances within the alternate hydrogen production pathway focus area of the Hydrogen and Clean Fuels Program. The project will provide real-world data and will evaluate the comparative advantages and disadvantages of Co and Fe catalyst systems for the synthesis of F-T fuels with coal-derived syngas.

Primary Project Goal:

The primary goal of this project is to evaluate and compare intrinsic differences between Co and Fe catalysts for F-T synthesis using coal-derived synthesis gas.

Objectives:

The objectives of this project include the evaluation of the following specific parameters:

- 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
- The raw product upgrading requirements to produce high hydrogen-content coal-derived liquids

F-T fuel will be produced from actual coal-derived syngas and will be demonstrated in mobile and stationary diesel engines. The following assessments of the following components will also be made:

- The use of existing industrial facilities in Alaska to produce coal-derived military F-T jet fuel
- Permits required from state and local authorities to build and operate a commercial-scale coal-to-liquid fuels plant, including carbon-capture strategies, related environmental issues, and the effects of environmental compliance on plant economics

04: DE-NT0006368

Project Number DE-NT0006368	**Project Title** Sensitivity of FT and Water-Gas Shift Catalyst to Poisons from Gasification of Biomass and Coal/Biomass Mixtures			
Contacts DOE/NETL Project Mgr.	**Name** Donald Krastman	**Organization** Fuels Division	**Email** donald.krastman@netl.doe.gov	
Principal Investigator	Burtron Davis	University of Kentucky, Center for Applied Energy Research	davis@caer.uky.edu	
Partners	Rentech			
Stage of Development				
__ Fundamental	X Applied	__ Proof of Concept	__ Prototype Testing	__ Demonstration

Technical Background:

Coal synthesis gas (syngas) cleaning contributes approximately half the total cost of the production of syngas for the Fischer-Tropsch (F-T) synthesis process. To date, little data is available on the extent that syngas must be cleaned in order for the presence of potential catalyst poisons to not limit the catalyst lifetime. To optimize the syngas cleaning part of the overall process, data is needed that enables one to relate the rate of catalytic activity loss to the level of the catalyst poison in the syngas. To date, little reliable data is available to define the level of a catalyst poison that can be tolerated before the catalyst lifetime becomes an economic problem. The present studies are designed to develop reliable data that quantifies the detrimental effects that a specific level of a catalyst poison has on the decline in catalytic activity for Fischer-Tropsch (F-T) and water-gas shift (WGS) catalysts. These catalysts will be commercial catalysts, or will be similar to them.

In order to poison the F-T catalysts uniformly during use, the experiments will be conducted using continuous stirred tank reactors (CSTRs), so that all catalyst particles will be exposed to the same concentration of catalyst poison. Thus, a cobalt and an iron catalyst will be utilized in parallel tests: one of the tests will utilize very pure syngas, and the other will contain a known quantity of a potential catalyst poison as identified in the proposal. After a baseline aging curve is established in the poisoning run, the catalyst will be exposed to a known concentration of a potential catalyst poison and the impact, if any, that this level of poison has on the catalytic activity will be determined. These studies will allow identification of the highest level of catalyst poison that the catalyst can tolerate while remaining active. After this level is determined, another run will be made that exposes the catalyst to a level of catalyst poison that is slightly higher than the maximum level that does not cause catalyst activity to decline. In this manner, a reliable measure of the rate of decline in catalytic activity will be determined for two or three levels of catalyst poison in the syngas feed. The tail gas will be analyzed so that the fraction of the poison that is retained by the catalyst can be determined, and the accuracy of these measurements will be evaluated by analyzing the aged catalyst for the content of the poison. The nature of the catalyst poison on the catalyst will be defined by analyzing the aged catalyst via a variety of experimental techniques, such as extended x-ray absorption fine structure (EXAFS), which will be conducted at Brookhaven National Laboratory.

The WGS poisoning studies will be similar to those conducted for the F-T catalysts, except that the poisoning effect will be evaluated using fixed-bed reactors rather than the CSTRs. This will make the definition of the impact of the catalyst poison on the catalytic activity more difficult, but this choice was made because it is likely that fixed-bed reactors will be utilized for the WGS reaction at the commercial scale. This makes it more likely that the poison will not deposit uniformly along the length of the catalyst bed, and therefore, catalyst withdrawn from different lengths along the catalyst bed will have to be analyzed in order to define a measure of poison retention by the catalyst under realistic operating conditions. The ability to expose all F-T catalyst particles to the same level of catalyst poison during long-term catalyst testing is a unique condition of the F-T catalyst poisoning experimental test.

The data generated in the proposed studies will provide, for the first time, quantitative information on the aging rate of commercial-type catalysts under reaction conditions that are comparable to those met in a commercial operation.

Relationship to Program:

By quantifying the extent to which syngas must be cleaned in order for the presence of potential catalyst poisons to not limit the catalyst lifetime, this project will support important catalyst advances within the alternate hydrogen production pathway focus area of the Hydrogen and Clean Fuels Program.

If successful, the project will identify the following:

- Quantitative measure of a given level of catalyst poisons in a syngas on the rate of catalyst aging
- Quantitative measure of the fraction of the catalyst poison in the syngas that is retained by the catalyst under realistic commercial reaction conditions
- Definition of the state in which a chemical poison is retained in the aged catalyst and the potential for catalyst regeneration to remove the catalyst poison
- Impact of catalyst poisons unique to syngas derived from biomass on the aging of F-T catalysts
- Impact of catalyst composition, especially for an iron catalyst, on the catalyst lifetime

Primary Project Goal:

The broad objective of this project is to quantify the impacts of alkali halides, hydrogen sulfide, and ammonia on the performance parameters of conventional WGS and F-T catalysts, to define the nature of these poisons that are retained by the catalysts, and to define unique impacts (if any) of potential poisons in a syngas that is partially derived from biomass.

Objectives:

The project will be delineated by three phases, each with a primary objective:

1. Catalyst performance parameters, including carbon monoxide conversion, product distribution, and deactivation rate, will be evaluated after subjecting batches of the same catalyst to synthesis with a pure syngas and with a syngas that contains selected alkali halides (e.g., potassium chloride and sodium chloride). The activity of each catalyst decays during its usage even with exceptionally pure syngas. The Center for Applied Energy Research has developed some of this data using very pure syngas and will develop additional data during the course of this three-year contract. The impact of the alkali and the halide components will be decoupled by separately adding the alkali bicarbonate and the halide acid.

2. Catalyst performance tests with added poisons (sulfur compounds, ammonia, hydrogen cyanide and hydrogen fluoride), conducted similarly to the tests of the alkali halides (Objective 1).
3. To assess the effects of poisons on the structure-function relationships of the catalysts, characterization of both fresh and used catalyst samples will be performed on samples retrieved from testing under both clean and chemically contaminated conditions.

05: OSAP-401.01.08.002

Project Number OSAP-401.01.08.002	**Project Title** Technical, Economic, and Environmental Assessment of a Commercial Scale Coal to Fischer-Tropsch Liquids Plant Using a Dry-feed Gasifier with Carbon Capture			
Contacts DOE/NETL Project Mgr.	**Name** Erik Shuster	**Organization** NETL – OSAP	**Email** Erik.Shuster@netl.doe.gov	
Principal Investigator	John Haslbeck	RDS	John.Haslbeck@PP.netl.doe.gov	
Partners	RDS			
Stage of Development				
__ Fundamental	X Applied	__ Proof of Concept	__ Prototype Testing	__Demonstration

Technical Background:

This study will revise and update the April 2007 NETL report, *Baseline Technical and Economic Assessment of a Commercial Scale Fischer-Tropsch Liquids Facility*.

The baseline plant to be assessed will be designed to produce 50,000 barrels of Fischer-Tropsch (F-T) liquids per day from Illinois No.6 coal while capturing and sequestering carbon dioxide.

Relationship to Program:

This project will support important liquid fuels production commercialization advances within the alternate hydrogen production pathway focus area of the Hydrogen and Clean Fuels Program.

This baseline plant data is essential because it establishes the key environmental and economic benchmarks that new alternative fuel technologies must surpass in order to justify the investment required for their development. Comparing projected or measured performance against the baseline data allows research managers to efficiently screen out less-promising concepts while quantifying the benefits of technology breakthroughs. The baseline data is also critical for informing energy policy decisions that relate to the cost and performance of the current generation of transportation fuel production facilities.

Primary Project Goal:

The primary goal of this project is to establish the baseline cost and performance for a state-of-the-art coal-to-liquids facility fueled with bituminous coal that utilizes F-T synthesis.

Objectives:

The specific objectives of this project include the estimation of the following technical performance metrics:

- Efficiency
- Air emissions (including greenhouse gas emissions)
- Water usage

The study will also estimate the following economic metrics:

- Capital cost
- Operating costs
- Internal rate of return
- Required selling price
- Crude-oil-equivalent required selling price

06: DE-FC26-05NT42456

Project Number DE-FC26-05NT42456	**Project Title** Production and Storage of Hydrogen from Coal Using C1 Chemistry			
Contacts DOE/NETL Project Mgr.	**Name** Donald Krastman	**Organization** Fuels Division	**Email** donald.krastman@netl.doe.gov	
Principal Investigator	Gerald P. Huffman	University of Kentucky - CFFS	huffman@engr.uky.edu	
Partners	Auburn University University of Pittsburgh University of Utah West Virginia University			
Stage of Development				
_X_ Fundamental	__Applied	__ Proof of Concept	__ Prototype Testing	__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, University of Utah, and University of Pittsburgh. For over 20 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 fuels and hydrogen. The project team's most recent DOE contracts have focused on the development of novel technology for producing and storing hydrogen and for converting coal and biomass to liquids.

Relationship to Program:

This project will support coal and biomass to liquids and hydrogen production advances within the alternate hydrogen production pathway focus area of the Hydrogen and Clean Fuels Program. Ultimately, coal and biomass should become the primary source of our liquid fuels, chemicals, plastics, and hydrogen. The project team believes that their research program can contribute significantly to achieving this goal. Former graduate students and postdoctoral students from the CFFS participating universities are expected to make significant contributions to this program in the future. Many former students now hold important positions in both industry and academia, which is perceived by CFFS as just as important as the research results CFFS has obtained.

Primary Project Goal:

The primary goal of this project is to develop viable technology for the production of clean liquid fuels and hydrogen from coal and other available hydrocarbons. This goal is an important component of the national goal to relieve U.S. dependence on foreign oil imported from unstable parts of the world.

Objectives:

In the initial three years of the subject contract, the research was focused entirely on the production and storage of hydrogen, with primary emphasis on production. During the fourth year of the contract, rising oil prices and the need to limit carbon dioxide emissions, led managers at NETL and members of the CFFS to jointly decide on a switch from the development of novel technologies for the production and storage of hydrogen from coal to a potentially more beneficial program emphasis on sustainable transportation fuels from coal and biomass with low carbon dioxide emissions.

The project is subdivided into these two initiatives, each with its own main objectives:

Development of Novel Technologies for the Production and Storage of Hydrogen from Coal

1. Develop novel approaches to produce hydrogen from coal with breakthrough technology potential—Catalytic dehydrogenation of hydrocarbons is a one-step method of producing pure hydrogen. Research on this topic will emphasize development of a continuous reactor for the dehydrogenation of light alkanes to produce hydrogen and carbon nanotubes. Catalytic dehydrogenation of Fischer-Tropsch (F-T) liquids will be investigated with the goal of developing a simpler method of producing hydrogen for fuel cell-based auxiliary power units or other vehicular applications. Several projects will address the water-gas shift (WGS), a critical reaction for production of hydrogen from coal-derived synthesis gas (syngas). One approach will use a novel aqueous reaction sequence using potassium carbonate and formate that is equivalent to the WGS and could yield >98% hydrogen at relatively low temperatures. Other WGS projects will employ conventional reaction conditions but use novel catalysts; these will include several metals (copper [Cu], gold, etc.) supported on ceria aerogels and iron (Fe)-based spinels containing various secondary elements (chromium, cobalt [Co], etc.) to control active site population. Several projects will explore novel approaches for reforming methanol and ethylene glycol, which are widely available liquids that can be produced from coal, to produce hydrogen at low temperatures. Two very novel approaches will employ supercritical fluids (SCF) and electrolysis. Supercritical water (SCW) will act as both a reformant and a solvent to produce hydrogen from methanol, methane, and other sources. Electrochemical production of hydrogen will be investigated using slurries of fine coal or other forms of carbon, which can supply electrons for electrolysis at low potentials.

2. Develop new materials with the potential to solve the very difficult problem of hydrogen storage—Three research tasks will focus on hydrogen storage in several novel solid materials: (i) chemical hydrides doped with titanium or other metal catalysts; (ii) silica nanobubbles produced under SCF conditions; and (iii) stacked-cone carbon nanotubes (SCNT) subjected to acid intercalation and thermal expansion. Catalytic dehydrogenation and rehydrogenation of F-T fuels, which are promising liquid hydrogen carriers, will be explored under both normal and supercritical conditions.

3. Explore catalytic dehydrogenation of hydrogen-rich carrier liquids as an alternative to reforming—An array of analytical techniques will be used to determine the molecular structure and microstructure of catalysts and reaction products developed in this program.

Sustainable Transportation Fuels from Coal and Biomass with Low Carbon Dioxide Emissions

1. Auburn University has recently partnered with the Gas Technology Institute (GTI, Chicago) to design and construct a high-pressure gasifier. This unit will be used to gasify coal and biomass feeds (3–30 lbs/hr) and will be coupled with a SCF F-T reactor downstream of the syngas production and cleanup portions of the facility. It will provide a unique testing facility for novel F-T catalysts and concepts developed in the CFFS.

2. Various biomass feedstocks (lignin, cellulose, hemicellulose, etc.) and binary mixtures of biomass and coal will be tested for hydrogen production by reforming in SCW. This will provide high-pressure hydrogen to optimize the syngas composition from coal and biomass at H_2:CO (hydrogen gas:carbon monoxide) ratios >2:1 for SCF F-T synthesis of middle distillates.

3. Lignocellulosic materials are the preferable biomass source for fuels since they are not food feedstocks. They have low carbon content and high oxygen content compared to coal. Therefore, both acidic catalysts that facilitate carbon-carbon bond cleavage and hydrogenation catalysts that promote carbon-oxygen bond cleavage are needed. A major objective of this work is to develop a catalyst that is effective in breaking both types of bonds.

4. A laboratory-scale gasifier will be designed and built to co-process coal and biomass into syngas with an adjustable ratio of H_2/CO. The gasifier will be designed to operate in either a static batch (Lurgi) mode or a fluidized bed mode. The experiments will focus on mixtures of low-rank coal (lignite or subbituminous) and hardwood sawdust, chosen because of the major hardwood lumber industry in Kentucky, West Virginia, and Pennsylvania.

5. Detailed characterization of the structural and thermal properties of sawdust will be conducted to complement gasification and co-processing research. Structural characterization will include using x-ray diffraction (XRD), electron magnetic resonance (EMR), C near-edge x-ray absorption fine structure (NEXAFS) spectroscopy, and carbon-13 nuclear magnetic resonance (NMR). Thermal analyses will include thermal gravimetry analysis and differential scanning calorimetry.

6. The effect on the product stream of varying H_2/CO ratios, typical of syngas derived from coal and biomass, on the F-T product stream using a simple Fe/Co catalyst will be investigated. Then, the effect of catalyst additives and reaction conditions (temperature and pressure) will be studied. Finally, the effect of process impurities will be determined.

7. Bimetallic carbides of the form X_6W_6C, with X = Co or nickel (Ni) and W is tungsten, have been shown to be effective and robust catalysts for the WGS reaction. The catalysts will be tested for the low-temperature WGS using syngas of compositions appropriate for gasification of coal and biomass.

8. 2,5-dimethylfuran (DMF) is potentially an attractive substitute for ethanol, having a higher octane rating, boiling point, and energy density, as well as a lower water solubility. A new approach for the conversion of glucose to DMF will be investigated using redox targeting to prepare Cu-based catalysts with precious metal promoters (ruthenium, palladium, and platinum) on xerogel as well as more traditional supports. The structure of the catalysts will be determined by x-ray absorption fine structure (XAFS), XRD, and transmission electron microscopy (TEM).

9. Incomplete gasification of biomass can lead to the presence of undesirable polycyclic aromatic hydrocarbons. To avoid this problem, Ni-based steam reformation catalysts that are “redox-targeted” by appropriate transition metals will be developed. Calcium or magnesium oxides prepared by sol-gel techniques will be used as supports.

10. Approximately monosized Fe-Co nanoparticles will be synthesized and dispersed onto several supports, including SCNTs and several xerogels. The F-T synthesis of clean liquid fuels from syngas typical of that derived from coal and biomass will then be investigated as a function of the Fe/Co ratio, nanoparticle size, and the support.

11. The CFFS analytical team will provide a wide range of spectroscopic (XAFS, Mössbauer, NMR, EMR) and microscopic (TEM/scanning electron microscopy) techniques; XRD; thermal activity; and magnetic measurements for thorough characterization of catalyst structures and reactions.

12. Integrated system engineering strategies for modeling, integration, and optimization of fuels production from coal and biomass will be developed. Such models will optimize process conditions resulting in appropriate synthesis gas compositions for subsequent F-T synthesis and other fuel production strategies.

07: DE-FC26-06NT43024

Project Number DE-FC26-06NT43024	**Project Title** Catalytic Processes for the Synthesis of Ethanol From Coal-Derived Syngas			
Contacts DOE/NETL Project Mgr.	**Name** Daniel Driscoll	**Organization** Fuels Division	**Email** daniel.driscoll@netl.doe.gov	
Principal Investigator	James J. Spivey	Louisiana State University	jjspivey@lsu.edu	
Partners	Clemson University Conoco Phillips Oak Ridge National Laboratory			
Stage of Development				
X Fundamental	__Applied	__ Proof of Concept	__ Prototype Testing	__ Demonstration

Technical Background:

The overall process for the synthesis of ethanol from coal (Fig. 1) begins with a coal-fed gasifier, which produces coal-derived synthesis gas (syngas). After cleanup and any necessary adjustment of syngas composition (e.g., shift, not shown), the syngas is converted to ethanol, with the following as the primary reaction of interest:

$$2\ CO + 4\ H_2 \rightarrow C_2H_5OH + H_2O$$

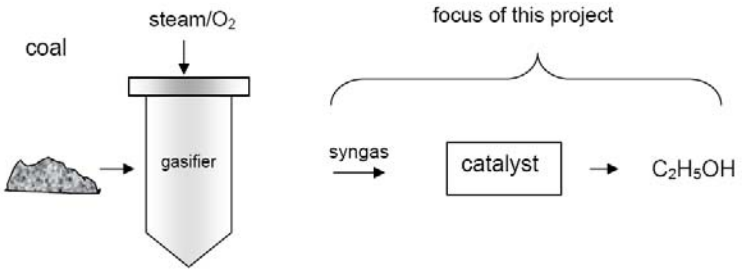


Figure 1 Conversion of coal to ethanol using catalytic conversion of syngas

The literature shows that commercially practical selectivities to ethanol can be obtained over several catalysts, but only at impractically low conversions—net yields are typically well below 10%. The thermodynamically favored product is methane, which is undesirable in this process.

This project seeks to maximize ethanol yield using several approaches. In addition to a conventional approach in which catalysts shown to be active/selective for this reaction are modified to maximize ethanol yield, this project uses first-principles computational methods to identify catalysts that will surpass yields achieved to date. A key element of this approach is the inclusion of novel approaches to catalyst synthesis (e.g., electrodeposition and emulsion methods) so that catalysts identified computationally can at least be approximated in the lab. A final element of the project team's approach is an economic/process analysis carried out by Conoco-Phillips, the commercial partner. This analysis helps to guide the research, pointing out the impacts of process parameters (e.g., catalyst cost, selectivity, and conversion) on the economics of ethanol synthesis.

Relationship to Program:

This project will support coal-to-ethanol fuel production advances within the alternate hydrogen production pathway focus area of the Hydrogen and Clean Fuels Program. At present, the primary focus of ethanol fuel production is on biochemical routes, based principally on enzymatic hydrolysis of corn. Despite the advantages of high selectivity and domestically available feedstocks, these processes are characterized by low reaction rates, relative to conventional thermochemical processes, and by costly product separation. Some studies show that corn-to-ethanol is energetically inefficient and may be less environmentally innocuous than first thought. Even assuming an optimistic 86% of theoretical energy efficiency in the overall process of producing ethanol (2.3 gallons [gal] ethanol/bushel corn), more fossil energy is consumed in producing ethanol than the energy content of the ethanol product, and at least 30 gal of water are needed to produce 1 gal of ethanol. (Note that more favorable conclusions can be drawn if different assumptions are made).

Under the assumption that ethanol from syngas is at least as energy efficient as that from corn, there is more potential for large-scale ethanol production from coal than from corn, with the potential for greater economy of scale. In 2004, 3.6 billion gal of ethanol were used as a fuel additive in the United States, corresponding to an equivalent fuel energy of about 2.5 billion gal of gasoline, roughly 2% of domestic consumption. Under certain assumptions, a single 2,500 measurement tons per day integrated-gasification-combined-cycle unit could produce roughly 450 million gal ethanol/yr. Eight such plants could therefore produce as much fuel ethanol as is currently being produced nationwide. This suggests that coal-based ethanol could provide a substantial portion of the future demand for ethanol. (Note: coal-based technology should be viewed as complementary to biological routes to ethanol. The availability of both technologies will allow market competition and maximize efficiency.)

Another advantage of the processes developed in this project is that because gasification technology can be easily modified to use biomass and/or other carbon sources, the catalytic conversion of syngas to ethanol could be readily adapted to future feedstocks. Finally, the raw product of the catalytic conversion step will inevitably include a range of products (e.g., methanol and higher oxygenates). This product can be separated into an ethanol-rich liquid that can be used as a hydrogen carrier, neat fuel, or fuel blending stock. This raw product could also be fractionated into custom blends for use in other processes. This provides a degree of flexibility in preparing the final, saleable product.

Primary Project Goal:

The primary project goal is to develop an economically viable catalytic process for the selective conversion of coal-derived synthesis gas to ethanol.

Objectives:

The project will be delineated by three phases, each with its own objectives:

I. Conduct initial process simulations to quantify performance targets for catalysts; conduct computational catalytic simulations to identify active/selective catalysts; and prepare catalysts.

II. Carefully characterize catalysts; carry out experiments to quantify ethanol yields; and synthesize improved catalysts based on experiments and detailed characterization.

III. Complete conceptual process design and material/energy balances, along with preliminary economics; and complete long-term studies on optimal catalysts.

08: DE-FC26-08NT0006523

Project Number DE-FC26-08NT0006523	**Project Title** Demonstration of a Piston Driven Plug Feed System for Feeding Coal/Biomass Mixtures Across a Pressure Gradient for Application to Commercial CBTL Systems			
Contacts DOE/NETL Project Mgr.	**Name** Steven M. Seachman	**Organization** Fuels Division	**Email** Steven.Seachman@NETL.DOE.gov	
Principal Investigator	A. John Rezaiyan	Southern Research Institute	Rezaiyan@SouthernResearch.org	
Partners	TK Energi			
Stage of Development				
__ Fundamental	__ Applied	__ Proof of Concept	X Prototype Testing	__ Demonstration

Technical Background:

The incorporation of biomass feedstocks in large-scale gasification and liquids production processes partially mitigates negative carbon dioxide (CO_2) emission impacts associated with the production of coal-derived liquid fuels. With CO_2 sequestration, coal-and-biomass-to-liquids (CBTL) processes may even be carbon negative.

Previous studies have demonstrated the ability to co-gasify biomass in entrained-flow (EF) gasifiers, the dominant technology for large-scale gasification and future CBTL systems. However, several challenges related to biomass utilization have been observed: a primary challenge related to biomass utilization in large-scale commercial CBTL is the ability to reliably feed a variety of biomass feedstocks to the gasifier as biomass-coal mixtures. Southern Research Institute and its partner TK Energi A/S of Denmark have identified an approach to feeding coal/biomass blends that is based on a proven, existing biomass feed system.

Relationship to Program:

This project will support important advances in CBTL processes within the alternate hydrogen production pathway focus area of the Hydrogen and Clean Fuels Program. This project could result in the development and demonstration of an advanced coal-biomass feed system for high-pressure, EF gasifiers, leading to a commercial offering for CBTL projects which will help to overcome the barrier to the development of large-scale CBTL technology. Additionally, the use of CBTL processes can also reduce CO_2 emissions.

Primary Project Goal:

The goal of this project is to design and demonstrate the operability of a coal and biomass pretreatment and coal-biomass co-feed system for high-pressure, commercial-scale EF gasification systems utilized in future large-scale CBTL facilities.

Objectives:

The specific objectives of this project include the following:

- Specifying an appropriate biomass pretreatment process
- Demonstrating the ability of an existing feed system design to feed a variety of biomass and coal mixtures into a high-pressure environment
- Evaluating the engineering and economic viability of the proposed feed system and large-scale CBTL processes

09: DE-NT0006305

Project Number DE-NT0006305	**Project Title** Product Characterization for Entrained Flow Coal/Biomass Co-Gasification			
Contacts DOE/NETL Project Mgr.	**Name** Donald Krastman	**Organization** Fuels Division	**Email** donald.krastman@netl.doe.gov	
Principal Investigator	Boris Eiteneer	GE Global Research	boris.eiteneer@ge.com	
Partners				
Stage of Development				
__ Fundamental R&D	_X Applied R&D	__ Proof of Concept	__ Prototype Testing	__ Demonstration

Technical Background:

Biomass is considered a renewable energy source because carbon dioxide (CO_2) emissions caused by its use are absorbed during biomass growth. Only biomass offers the possibility of producing nearly carbon-neutral liquid transportation fuels that provide feasible alternatives for the transportation sector in the foreseeable future. This issue is particularly relevant today, as transportation is responsible for a large part of global CO_2 emissions. The portion of energy used by transportation in the world's total energy consumption is increasing, especially in developing countries.

Common barriers to biomass utilization at scales large enough to make a noticeable contribution to global energy production include biomass variability, availability, seasonality, and low energy density. The influence of these factors can be substantially mitigated if biomass is used synergistically with the most abundant fossil fuel resource—coal. The worldwide efforts to develop and commercialize coal/biomass co-combustion and co-gasification technologies have intensified over the last several years. The feasibility of co-combusting or co-gasifying small quantities of biomass (typically less than 10% by weight) had been demonstrated in many projects. For example, the Tampa Electric Company integrated gasification combined cycle (IGCC) project, located at Mulberry, Polk County, Florida demonstrated that a fuel blend of coal, petroleum coke, and eucalyptus grove (1.2% biomass by weight) could be successfully gasified to produce electricity using the IGCC system, without an adverse impact on the biomass availability and plant performance. However, successful long-term utilization of larger biomass quantities, exceeding 30% by weight, still remains to be achieved.

Air-blown circulating fluidized bed (CFB) gasifiers are widely considered to be well suited for small-scale biomass gasification. However, nitrogen dilution, high costs, high tar concentrations in the product gas, and the need for subsequent gas cleanup suggest that CFB gasifiers are not the most cost-effective option for large-scale gasification. High-temperature, high-pressure entrained flow (EF) oxygen-blown gasification, with its high efficiency and ability to provide the coal-derived synthesis gas (syngas) at pressures required for downstream Fischer-Tropsch (F-T) synthesis without additional compression steps, offers the best commercial potential for large-scale conversion of coal/biomass mixtures to liquid fuels.

Co-gasification of coal and biomass in the EF gasifiers presents several technical challenges, including the following:

- Reliable feeding into the pressurized gasifier

- Unknown effects of coal and biomass compositions on the solid, liquid (if any), and gaseous products of co-gasification
- Effects of syngas impurities on downstream equipment such as water-gas shift and F-T catalysts

Entrained flow oxygen-blown coal gasification typically yields a product gas that contains hydrogen gas (H_2), carbon monoxide (CO), CO_2, water (H_2O), small quantities of methane, sulfur (S) compounds (such as hydrogen sulfide [H_2S], carbonyl sulfide [COS], and carbon disulfide), nitrogen (N) compounds (such as ammonia [NH_3] and hydrogen cyanide [HCN]), halides, alkali and trace metals, small particles of soot and ash, and trace concentrations of organic and hetero-organic components [including S, N, and oxygen (O)]. Ash-forming components, including the inorganic mineral matter present in the feedstock, melt inside the gasifier and are typically removed as a liquid slag. The quality of the raw product gas is insufficient to meet the feed specifications for downstream processes, such as F-T. The typical catalysts used in these processes are extremely sensitive to small amounts of impurities in the raw product gas. As a result, these catalysts are regenerated or replaced on a regular basis in an attempt to maintain the reactor's productivity and optimal catalyst performance in F-T synthesis. Feed gas specifications for these processes are determined based on an economic trade-off between increased capital and operating expenditures for gas cleanup and decreased reactor yields due to catalyst poisoning.

Due to differences in fuel properties, co-gasification of biomass with coal in an entrained flow reactor (EFR) is expected to affect the product gas composition. While the main gasification products for both fuel types comprise H_2, CO, CO_2, and H_2O, albeit in varying concentrations, the makeup of minor components of the syngas can change dramatically depending on chemical compositions of both coal and biomass, as well as process conditions.

In addition to the major elements (carbon, hydrogen, O, N, and S), minor elements (aluminum, calcium [Ca], iron, potassium [K], magnesium [Mg], sodium [Na], phosphorus [P], silicon [Si], and titanium) and trace elements (arsenic [As], barium [Ba], cadmium [Cd], cobalt [Co], chromium [Cr], copper [Cu], mercury [Hg], manganese [Mn], molybdenum [Mo], nickel [Ni], lead [Pb], antimony [Sb], thallium, vanadium [V], and zinc [Zn]) are also present in biomass fuels. These inorganic constituents can significantly affect the behavior of biomass during thermal processing, directly influencing the quality and conversion during pyrolysis, combustion, and gasification. Many of the inorganic components are retained in the char and can influence the combustion or gasification of the solid residue.

In particular, the higher alkali metal content of biomass, relative to coal, poses a serious operational problem because these metals can easily vaporize at the high temperatures encountered in commercial EF gasifiers. The condensation of volatile metals can form sticky deposits on heat exchangers and downstream gas cleanup equipment. The problems associated with deposit formation during combustion of biomass and co-combustion of biomass with coal have been investigated by many researchers in bench-scale and full-scale facilities. Substantially less is known about the mechanistic and chemical aspects of deposit formation during gasification of coal and biomass mixtures, especially following the exposures to high temperatures and pressures characteristic of EF gasifiers.

In contrast to combustion under oxidizing conditions, the thermodynamic modeling predicts a much higher proportion of the alkali in the gas phase under reducing conditions during gasification. Alkali species in coal are mostly associated with mineral matter and are not easily volatilized during gasification. For example, in bituminous coals, they are present mainly in the mineral components, such as in the mineral matrix itself (e.g., feldspar and muscovite) or as sodium chloride or potassium chloride inclusions. For lignite coals, they are mainly found bound to phenolic hydroxyl and carbonate groups in the organic structure. In contrast, biomass materials contain Na and K largely in water-soluble forms in vacuoles but also as constituents of organic structures. These forms are readily accessible for release during combustion or gasification, resulting in subsequent chemical reactions to form gas-phase and condensed-phase metal species. The gas-phase alkali species formed in the gasification process are predominantly chlorides and hydroxides, whereas the condensed-phase metal species consist mainly of silicates. The critical control variables that affect the formation of the gas-phase alkali species include the concentrations of sulfur, silicon, and particularly chlorine, and gasification conditions such as pressure, temperature, and the oxygen/fuel ratio. Alkali gas-phase species may exacerbate the problems associated with deposit formation on cooled walls or heat exchanger tubes. The deposition of submicron alkali-rich particles or condensation of alkali vapors on the heat exchanger surface may create a sticky layer that promotes particle retention and the growth of the deposit layer, leading to increased thermal resistance, reduced efficiencies, and high maintenance costs.

While debarked wood is a relatively clean fuel with low ash content, herbaceous biomass feedstocks typically have a higher content of ash and heteroatoms, especially K and chlorine (Cl), which are needed as catalysts for the faster metabolism. Chlorine concentrations in certain types of biomass residues (e.g., straws, cereals, and grasses) can be substantial and can lead to the formation of hydrogen chloride, which causes high-temperature corrosion in the gasifier. Chlorides can also contribute to the production of low pH conditions in the syngas quenching and scrubbing operations. In the presence of chlorine, alkali chlorides become the most thermodynamically stable gas-phase alkali species at the high temperatures that are typical in EF gasifiers. Additionally, experiments and thermodynamic modeling show that under both combustion and gasification conditions, alkali volatilization can be significantly enhanced by chlorine.

For the biomass feedstocks of interest in this program, the concentrations of S and N species in the product gas from biomass gasification are expected to be lower, compared to those from coal gasification. The complex interaction of S, Cl, and alkali species is primarily driven by temperature and species concentrations and can lead to the formation of corrosive alkali salts downstream of the gasifier. Additional cleaning steps, such as control of chloride concentration in the process water, may be required to mitigate these issues.

In addition to posing operational difficulties, N, S, alkali, and Cl species (including H_2S, COS, NH_3, HCN, chlorides, and particulates) act as severe poisons to commercial F-T catalysts. Sulfur is an irreversible poison for the typical F-T catalysts. The tolerance for S contaminants in the F-T feed gas is low, and deep cleaning is required. The typical specifications for N, alkali, S, and Cl compounds for F-T synthesis are on the order of 10 parts per billion (ppb), requiring cleaning efficiencies exceeding 99.9%.

The configuration and operating requirements of the cleanup system will be to a large extent dictated by the syngas cooling method (direct quench or dry cooler). While the direct quench may provide some benefits (such as additional scrubbing of undesirable species), making it attractive in the short term, the dry syngas cooling in combination with hot or warm syngas cleanup will be more attractive in the long term, driven by efficiency requirements and consistent trends toward zero plant discharge and minimization of water requirements. The study of syngas cleaning requirements resulting from the dry syngas cooling suggested in this program is aligned with the long-term trends of gasification technology development. Additionally, because concentrations of impurities resulting from dry syngas cooling might be higher than those resulting from a direct quench, this program will provide relevant data for the downstream cleaning equipment under a more challenging scenario of dry syngas cooling.

The trace metal composition of biomass fuels differs significantly from that of coals. While the metal constituents of coal fuels have been studied in detail, data on the trace element composition of biomass is limited. The differences in the concentrations of some trace species between coal and biomass can often exceed several orders of magnitude. In addition, the modes of occurrence of these elements in coal and biomass are substantially different. The possible forms of occurrence of heavy metals in coals include pyrite, sulfides, carbonates, clays, or organic matter. In biomass, most metals play some role in enzymes, but predominantly they appear to be bound to organic groups, organic acid groups, or associated with inorganic ions such as carbonates, oxalates, and phosphates in aqueous solution. In coal, many trace elements are mostly associated with mineral matter, are not easily volatilized, and tend to be relatively inert during gasification. However, in biomass, many trace elements are associated with the organic matrix and are readily released during gasification. If the formation of solid phase is thermodynamically favorable, the released trace elements may recondense immediately on existing solid particles. Because recondensation may be kinetically constrained at typical gas residence times observed in EF gasifiers, part of the volatilized trace elements will exit the reactor with the syngas. The behavior of the individual trace elements during gasification depends not only on their concentrations and on their modes of occurrence in the fuel, but also on other factors such as the concentrations of minor elements (Na, K, Ca, S, Cl, and P). Predicting the trace element partitioning in the gasification products using thermodynamic equilibrium models is very complex due to the large number of species involved and the incomplete thermodynamic data for some of them. Modeling results often contradict experimental observations, in part due to kinetic limitations. Careful analysis of model assumptions and predictions is required to obtain meaningful results.

The trace metals that are of primary concern due to their volatility and toxicity (As, Cd, Hg, and selenium) are present in plant residue biomass at significantly lower concentrations than in coal, while Pb concentrations are comparable between the two fuel types. The trace toxic metal emissions have upper specification limits that are regulated by the U.S. Environmental Protection Agency under the Clean Air Act. While it is expected that these toxic metal emissions may be mitigated in some cases due to the reduction of the overall concentration resulting from utilization of biomass, such assumptions must be experimentally verified because the relative partitioning of heavy metals in gasification products might differ from the coal-only case.

The elements of intermediate concern include Cr, Cu, Ni, V, and Zn. The V content of biomass fuels is significantly lower than that of coal. The concentrations of Ni and Cr are comparable between the two fuel types, while the concentrations of Cu and Zn present in biomass exceed those of coal by as much as an order of magnitude. The measurements of Ni, Cr, and Mn can be complicated by possible contamination resulting from abrasion and erosion of the stainless steel components of the gasifier and sampling system. The elements Ba, beryllium (Be), Co, Mn, Mo, and Sb are of somewhat lesser concern due to their lower volatility.

During gasification, some of the minor and trace components of the fuel will be volatilized (K, Na, S, Cl, Zn, Pb, Cd, Ca, Mg, and Si) and released to the gas phase. Reducing conditions characteristic to gasification can substantially increase the volatility of some trace elements compared to oxidizing conditions typical to combustion. Subsequent syngas cooling will lead to nucleation and condensation of these volatiles to form fine aerosol particles with sizes between 1 nanometer (nm) and 1 (micrometer) µm. The nonvolatile compounds will form, by coalescence or melting, ash particles with a wide range of compositions, shapes, and sizes. These ash particles consist mainly of refractory species, such as Ca, Mg, and Si, as well as of smaller amounts of bound volatile compounds, such as K and Na. During syngas cooling, the vapors of volatilized compounds can also condense or react on the surface of existing solid particles (char, soot, and ash). Due to the much larger specific surface area of the fine particles in comparison to the coarse particles, surface-dependent mechanisms, such as heterogeneous condensation or surface reaction of metal vapor, lead to increased (enriched) concentrations of condensing or reacting trace elements with decreasing particle size. Under assumptions of a purely physical condensation mechanism, if spherical particles with diameters much larger than the gas mean free path and negligible particle size increase due to condensation, the concentration of condensed species in particles is proportional to $1/d^2$, where d is the particle diameter. If the gas-to-particle conversion is controlled by surface chemical reactions and/or pore diffusion in the porous particles, the concentration of condensed species is proportional to 1/d. Both types of behavior were observed in experiments. The smallest particles, substantially enriched in trace elements, due to their size will tend to preferentially penetrate commercial gas-cleaning devices. In fact, most of the particulate control devices exhibit size-dependent collection efficiencies, with minimum efficiencies typically seen for submicron particles with the diameter range of 0.1–1.0 µm. These particles contain neither the mass (momentum) to be removed by impaction nor the high diffusion velocities necessary to migrate to collection surfaces. Because these particles are also more likely to be inhaled, their analysis must be included into the human-health risk assessment.

The minor elements that are present in coal and biomass fuels are of key relevance regarding ash melting, deposit and slag formation, corrosion, and catalyst deactivation effects. The trace elements are of special importance for particulate emissions and environmental assessment for most coal and biomass thermochemical conversion technologies. The specific standard operating procedures for determining these elements in biofuels are rare. Most laboratories determine minor and trace elements in biofuels using in-house methods or standards originally developed for fossil fuels. This often leads to considerable deviations between the results of different laboratories. Most recent studies demonstrated that acid digestion methods, in combination with inductively coupled plasma atomic emission spectroscopy (ICP-AES) and inductively coupled plasma mass spectrometry (ICP-MS), are suitable for analyses of the above-mentioned elements.

Based on the results of the literature studies, as well as the significant expertise in chemical and elemental analysis developed by GE Global Research, the ICP-AES and ICP-MS methods with appropriate sample digestion methods will be applied in this program to determine the minor and trace metal concentrations in the fuel samples and gasification products. Several ICP-AES and ICP-MS instruments are available at GE Global Research's facility in Niskayuna, New York. The samples collected during GE's bench-scale gasifier (BSG) and EFR testing at GE's Irvine, California office during this project will be properly packaged, sealed, and shipped to GE Global Research, Niskayuna for trace metal analysis. The time between sample collection and analysis will be minimized to the extent possible. Due to the significant variations in the elemental compositions of the coal and biomass fuels studied under this program, as well as anticipated partitioning effects of different elements between solid, gas, and possibly liquid components of the raw syngas, it is expected that the analysis methods and sampling procedures will need to be further optimized and validated. These issues are the focus of task 3 of the proposed program and will be addressed in parallel to the BSG and EFR measurements conducted under tasks 2 and 4, respectively.

While coal-gasification products have been studied in the past, data on characterization of the products resulting from biomass and coal/biomass mixture gasification in an EF gasifier are scarce. The product distribution, which results from co-gasification of coal and biomass blends, will depend on the interaction between various components of coal and biomass and cannot be predicted a priori based on the knowledge of product distributions from pure coal and pure biomass gasification. Nonlinear effects due to the possible interaction of inorganic constituents present in biomass with coal char must be verified and experimentally characterized to provide guidance on the development of appropriate cleanup systems. In particular, the amount of volatilization and retention of trace elements during co-gasification will depend on the complex interplay between various components of coal and biomass fuels and must be carefully described for each coal/biomass blend. Moreover, different slag behavior resulting from coal/biomass co-gasification can pose operational problems and affect the refractory-lined walls of the gasifier and the syngas cooler. With uncertainties in gasifier operation and costs associated with gas cleanup systems, complete characterization of coal/biomass co-gasification represents a critical step toward the commercialization of this technology.

To provide an accurate description of the raw syngas composition as a function of operating parameters and fuel mixture characteristics, experimental measurements will be performed using the BSG and EFR gasification facilities, which are uniquely suited to the objectives of the current program. GE has selected the combination of BSG and EFR experiments to ensure high-fidelity quantitative experimental data. This experimental approach offers the following advantages:

1. Both the BSG and the EFR are high-temperature (up to 1600ºC) entrained flow facilities that are capable of achieving fast particle heating rates exceeding 104ºC/s, which are close to those employed by commercial entrained flow gasifiers. The devolatilization process, the first step of fuel conversion, is significantly affected by the heating rate of the fuel particles, and in turn, to a large

extent determines the composition and behavior of volatilized species and solid residues during subsequent gasification steps.

2. Both the BSG and the EFR are designed to operate under plug-flow conditions and provide precisely controlled testing environments that allow for the accurate monitoring of time and temperature histories of gases and particles during the gasification process. The experimental data obtained in BSG and EFR can be directly used to develop and validate predictive gasification models describing commercial gasifiers. In contrast, the direct or slipstream measurements performed in large-scale gasifiers can be affected by flow recirculation and other factors that cannot be accurately determined and controlled. As a result, the data obtained by such measurements are more difficult to interpret and generalize to other types of gasifiers or different operating conditions.
3. A combination of atmospheric pressure data obtained in the BSG with the medium and high pressure (up to 65 bar) data obtained in the EFR will cover the entire spectrum of pressures encountered in commercial EF gasifiers. These data will provide guidance for appropriate gas cleanup systems over a wide range of operating pressures.
4. In addition to providing representative temperatures, pressures, heating rates, and residence times for gasification processes, the EFR is equipped with a sophisticated syngas cooling section that can replicate the time-temperature histories of full-scale gas cooling devices. The cooling process significantly influences the element partitioning as well as physical and chemical properties of syngas components at the outlet of the syngas cooler, and therefore directly affects the downstream gas cleanup system. The measurements at the outlet of the syngas cooling section of the EFR will provide quantitative information that is crucial to the development of the requirements for cleanup of syngas resulting from the gasification of coal and biomass mixtures.

This experimental work will leverage other ongoing GE research and development (R&D) efforts in coal and biomass gasification. The experimental data obtained during this program will be compared with predictions of the advanced gasification model that is currently being developed by GE under an internally funded gasification fundamentals program. Comparing the data obtained in this program with the fundamentals-based model will play an important role in extending the applicability of the program’s findings and will provide guidance on the appropriate cleanup system(s) and operating parameters to coal and biomass combinations beyond those evaluated under this program.

The combination of GE’s vast experience in the research, development, and commercialization of gasification technologies, the design and operation of bench-scale and state-of-the-art EFR experimental gasification facilities, and unique modeling capabilities will achieve the greatest impact on advancing the environmentally sound conversion technologies to produce liquid hydrocarbon fuels from coal/biomass mixtures.

Relationship to Program:

This project will support important coal/biomass gasification and cleanup advances within the alternate hydrogen production pathway focus area of the Hydrogen and Clean Fuels Program.

This program will deliver a comprehensive description of raw syngas compositions resulting from the co-gasification of coal/biomass mixtures. This effort will support R&D on coal-and-biomass-to-liquid (CBTL) syngas cleanup systems and help determine the optimal operating conditions for the co-gasification process. In conjunction with an optimal feeding strategy for biomass and optimized F-T processes, this represents a critical step towards the commercialization of co-gasification technology. Oxy-co-gasification of coal and biomass mixtures with steam presents several advantages over conventional coal gasification technologies, including increased efficiency and reduced greenhouse gas footprint. In addition, this approach mitigates several risks associated with biomass-only gasifiers, including feedstock availability and variability, high specific costs, low efficiency, high tar concentrations in the raw syngas, and potential for shutdown due to biomass shortage.

This program will provide crucial information required to expand the EF gasification technology to coal/biomass mixtures with biomass inputs exceeding 30% by dry weight. At these high biomass utilization levels, the EF coal/biomass co-gasification has the potential to provide a noticeable contribution to reducing the carbon footprint of the global energy production, especially if the CO_2 sequestration option is employed.

Primary Project Goal:

The primary project goal is to perform a complete characterization of the gas, liquid, and solid products that result from the co-gasification of various coal/biomass mixtures (three major coal types with three biomass types) with a focus on biomass concentrations between 30 weight percent (wt%) and 50 wt% to provide guidance on the appropriate gas cleanup systems and optimization of operating parameters for development of future gasification systems.

Objectives:

Under this project, GE Global Research will perform a comprehensive characterization of the gas, liquid, and solid products that result from the co-gasification of various coal/biomass mixtures. This characterization will be performed using both a BSG and an EFR. These data will be essential to provide guidance on the appropriate gas cleanup systems and optimization of operating parameters for development of future gasification systems. To minimize expensive experimentation with the EFR, the BSG will be used initially to map the composition of the gaseous, liquid, and solid products; define their concentration ranges; and optimize product-analysis methods and procedures. The EFR will be used in the second part of the program to perform a focused set of experiments based upon the initial results obtained from BSG. Experiments will be performed on mixtures of the three major types of coal (bituminous, sub-bituminous, and lignite) with three types of biomass (corn stover, wood, and grass). Suggested biomass feedstocks include wood sawdust as a representative wood biomass and switchgrass as a representative grass biomass. Wood sawdust and milled switchgrass are well-suited for experimental testing in the small-scale EF gasification facilities. The main focus of the experiments will be on biomass concentrations between 30 wt% and 50 wt% (dry coal and dry biomass basis).

The following technical objectives will be achieved during the proposed program:

1. Conduct initial experiments using BSG to characterize the product stream.
2. Optimize product analysis methods and procedures based on bench-scale results.
3. Characterize co-gasification products in the EFR using the target test matrix.
4. Identify cleanup requirements for mixtures containing three types of coal (bituminous, subbituminous, and lignite) and three types of biomass (corn stover, wood sawdust, and switchgrass).

5. Evaluate the applicability of the observed trends to a wider range of coal/biomass fuels by comparing the experimental results of this program with the predictions of the fundamentals-based kinetic model developed by GE under a separate program.

Initial BSG experiments

The BSG is an externally heated gasifier that operates in a semicontinuous mode. This system is designed for coal/biomass feed rates up to 20 g/hr and allows for operation at temperatures up to 1400ºC and heating rates exceeding 104ºC/s at atmospheric pressure with gas and particle residence times of up to 5 s. This operation is representative of temperatures and residence times found in commercial EF gasifiers. The complete raw syngas flow will be collected at the outlet of the reactor by a water-cooled probe and will be rapidly quenched by inert gas (N or argon [Ar]) flow. The quenched flow will be subject to particle separation in a cyclone or virtual impactor, fine particle and condensables (soot, aerosols, tars) separation by filtration, and gas analysis. The ratio of quench to syngas flow rates, cyclone operation, and filter fineness and temperature will be independently varied to achieve the desired separation characteristics. The sampling system is configured to separate and collect solid products (char, soot, ash), liquid products (tar), and gaseous products for online and offline analyses. An online measurement system will include continuous emissions monitors (CEMs), a Fourier Transform infrared (FTIR) spectrometer, and a gas chromatograph (GC). Char and ash will be collected by cyclone separation. Tars (if any), condensable aerosols, fine ash, and soot will be collected by filtration.

Samples of bituminous, sub-bituminous, and lignite coals and at least three different types of biomass (corn stover, wood sawdust, and switchgrass) will be procured, ground, sieved to particle sizes that are representative of EFR gasifier feeds (~100–200 µm), and dried as appropriate. At least two different particle size distributions from this range will be evaluated. Various size-reduction equipment (impact mill, jet mill, etc.) as well as sieving and drying equipment is available on-site and can be operated under inert atmosphere, if required, to avoid ambient effects on ground fuel particles before injection into the reactor.

Baseline tests will be performed to establish product compositions and their variation ranges for each of the individual coals (bituminous, subbituminous, and lignite) under at least two different temperatures and oxygen-to-coal ratios. Bench-scale gasification tests will be performed for at least two different biomass concentrations, 30 wt% and 50 wt%, on a dry coal and dry biomass basis for each coal/biomass mixture. Reactor parameters, such as temperature and residence time, will be varied to obtain product distributions at different degrees of conversion. By using these data together with baseline data for each type of coal, the effects of biomass-to-coal mixing ratios on product compositions will be determined and trends established. Additional experiments at other coal/biomass ratios will be performed as needed to describe possible nonlinear and/or synergistic interaction effects between the two types of fuels at higher resolution. A number of replicate tests will be performed to evaluate repeatability and reproducibility of the sampling and analysis systems. Advanced statistical tools will be used to ensure the statistical robustness and establish confidence intervals of the experimental data.

Optimization of product analysis methods and procedures

Solid products, such as char and ash particles larger than 5–10 µm, will be separated by inertial methods (cyclone and/or virtual impactor). Fine particles, such as soot, fine ash, and condensables (tars and aerosols), will be collected on filters (0.1–1.0 µm). Tar will be separated from soot by dissolving it in an organic solvent such as 1-Methyl-2-pyrrolidinone (NMP), and it will be analyzed by gas chromatography-mass spectrometry (GC-MS). Sampling system components, flow rates, and temperatures will be selected and optimized to preserve the sample integrity and minimize sample losses. Solid char samples will be analyzed for elemental composition by standard analysis methods. Morphology of solid char and ash samples will be characterized using a scanning electron microscope (SEM).

The most important nitrogen compounds that must be analyzed downstream of the gasifier are NH_3 and HCN, while the major sulfur compounds are H_2S and COS. Fourier transform infrared (FTIR) and GC analyzers will be used to measure N and S compounds and establish their variation ranges. Mass balance calculations will be performed to verify mass balance closures for elemental N and S.

Analysis of minor (Na, K, Ca, Mg) and trace metals (such as As, Ba, Be, Cd, Co, Cr, Cu, gallium, Ni, Mn, Mo, Pb, Sb, V, Zn, etc.) will be performed separately for char, soot, condensable tar, and aerosol fractions to determine the metal partitioning between solid, liquid, and gaseous product streams and define the requirements for the gas cleanup system(s). The methods and procedures for sample collection, storage, digestion, preparation, and analysis will be verified and optimized to avoid interferences and minimize sampling and analysis errors. In particular, extreme care will be exercised during sample collection, storage, and transportation to avoid sample losses and contamination. Samples will be collected in clean plastic containers, such as disposable centrifuge tubes. Vinyl clean room gloves will be used to minimize contamination. Sample vials will be tightly capped, sealed, and placed in plastic bags. The time between sample collection and analysis will be minimized.

Metal analysis will be performed using ICP-MS and ICP-AES. This equipment is available at the GE Global Research facility in Niskayuna, New York. Additional metal characterization for selected samples will be performed using external vendors, such as independent analytical laboratories, to verify the validity of the sampling and analysis methods.

ICP-AES is an emission spectrophotometric technique proven to be extremely useful for the determination of trace elements in various matrices. The ICP-AES analysis interface requires a sample to be in solution form. Solid samples must be dissolved using either acid digestion or alkaline fusion. High-temperature plasma is produced by inductively coupling radio frequency power into a stream of argon gas. A nebulizer is used to introduce the dissolved samples into the plasma torch, where the respective elements emit their characteristic radiation. By analyzing the spectral information (wavelengths and intensities) of the sample emittance spectra, the elemental composition of the given sample can be quantified relative to a reference standard. The ICP-AES tools available at GE Global Research include two Varian Liberty II instruments and a Perkin Elmer Optima 5300DV instrument.

Statistical analysis of the measurement data will be performed to validate measurement accuracy. Tests will be replicated to evaluate the repeatability and reproducibility of the measurement systems. Optimized sampling and analysis methods and procedures will be developed and documented for subsequent use during EFR testing.

Characterization of co-gasification products using EFR

The completion of bench-scale characterization of compositions, variation ranges, and trend analysis of gasification products for baseline coals and coal/biomass mixtures will define the EFR test regime of interest in conjunction with the validation and optimization of the analytical tools.

The high-temperature, high-pressure EFR will be configured to allow co-feeding of coal and biomass fuels at variable coal/biomass ratios. Both coal and biomass feeders will be located inside a pressure vessel to avoid issues associated with coal and biomass feeding across the pressure gradient. The measurement and sampling equipment will be moved from the BSG to the EFR as required. The amounts of coal and biomass fuels required for testing will be prepared based on feed requirement and test matrix.

A focused series of test matrices will be designed based on the test results from the BSG and validated analytical methods. A test plan will be generated and reviewed before the tests are conducted. The required tests will be performed in the EFR to characterize gasifier operation and complete product stream compositions at high temperatures and pressures relevant to commercial-scale units. Relevant gasifier operating parameters (e.g., temperatures and pressures) will be measured to assess the impacts associated with coal/biomass mixture operation.

The characterization of the main syngas components, such as H_2, CO, CO_2, and steam, can provide a syngas quality assessment for liquid fuel production. The characterization of ash and slag can assess the fate of inorganic species in coal/biomass mixtures and provide guidance needed to define the proper operating parameters for each specific coal/biomass feedstock blend. A comprehensive characterization of the syngas impurities will provide the guidance for the development of appropriate syngas cleanup system(s).

The syngas composition and the impurities makeup and concentrations depend on gasification conditions and downstream processing temperature and pressure. Thermodynamic estimations will be conducted with software such as FactSage and MTDATA to evaluate the possible partitioning and behavior of the elements and compounds through the EFR and to guide the optimization of the sample collection and characterization.

The most important nitrogen compounds of interest that must be analyzed downstream of the gasifier include NH_3 and HCN, while the major sulfur compounds include H_2S and COS. Fourier transform infrared (FTIR) and GC analyzers will be used to measure N and S compounds. Mass balance calculations will be performed to verify mass balance closures for elemental N and S. The analysis of minor and trace metals will be performed separately for each of the ash, char, soot, and condensable tar, if any. The formation of tar is unlikely under the typical high-temperature operation of the EFR. However, the condensable tar will be analyzed separately if it is formed.

The experimental data obtained in BSG and EFR will be combined to provide a comprehensive description of the solid, liquid, and gaseous product compositions from the EF gasification of various coal/biomass combinations. Response mapping and statistical analysis of data will be performed to identify trends, correlations, data uncertainties, and confidence intervals. Experimental data will be compared with the predictions of the fundamentals-based gasification model (developed under a separate GE program) to validate the observed trends and provide recommendations for the future work required to extend the applicability of the proposed program’s findings to coal and biomass combinations beyond those evaluated under this program.

10: ORD-09-220662

Project Number ORD-09-220662	**Project Title** Next Generation Sinter-Resistant Catalysts for Syngas Conversion			
Contacts DOE/NETL Project Mgr.	**Name** Christopher Matranga	**Organization** NETL – ORD	**Email** Christopher.Matranga@netl.doe.gov	
Principal Investigator	Christopher Matranga	NETL – ORD	Christopher.Matranga@netl.doe.gov	
Partners	Nisha Shukla, Carnegie Mellon University Goetz Veser, University of Pittsburgh			
Stage of Development				
_X_ Fundamental	__ Applied	__ Proof of Concept	__ Prototype Testing	__ Demonstration

Technical Background:

The goal of catalytic science is to understand key factors influencing reaction rates and selectivities.

Improvement and control of reactivity and selectivity can significantly reduce the cost associated with industrial-scale processes by reducing reaction temperatures and removing any purification steps needed to remove unwanted products. Many catalysts are transition-metal particles supported on high surface-area microporous or mesoporous oxides, typically prepared by impregnating the oxide support with metallic salts or organometallic compounds which are then reduced to metallic form. In this method of preparation the metal particle size and shape are not controlled.

Since reaction selectivity is highly sensitive to particle size and surface defects, these catalysts result in a heterogeneous environment for reactions. In order to prepare catalysts with high selectivity, it is necessary to prepare catalysts that expose specific active sites for reactions; the ability to control the distribution of active sites is also crucial. The preparation and characterization of such catalysts pose important challenges to be overcome in order to advance the field of catalysis.

The most important design targets for effective catalysts are high activity, high selectivity, and high stability. A highly active catalyst must expose a high active surface area, often requiring the use of small particle sizes. This is especially true for expensive catalytic materials such as noble metals. In order to achieve high selectivity, one would like to prepare catalysts that expose a homogeneous set of active sites or active surfaces. High selectivity requires excellent monodispersity or particles exposing only one type of surface, and thus a homogeneous reaction environment for adsorbed reactants. This control of activity and selectivity can be achieved by controlling either the catalyst particle’s size or shape. Finally, catalysts with controlled size and shape must resist sintering at high temperatures and during the course of a catalytic reaction. Very often these constraints are mutually exclusive, with sintering for size- and shape-selected catalysts occurring at low temperature or after a few catalytic cycles.

The traditional methods of catalyst impregnation do not allow sufficient control of particle size and shape to give truly homogeneous catalyst particles. Fortunately, the chemical synthesis of transition-metal nanoparticles has developed rapidly over the past decade and now offers a route to the preparation of nanoparticulate catalysts with very high surface area and high monodispersity. These synthetic techniques are capable of producing a variety of metal nanoparticles of a specific shape or size dispersed in solution as a colloid. The controlled size of these particles means that catalytically active metals can be produced with an increased surface-to-volume ratio, which should improve reactivity. The controlled shape exposes only one type of crystallographic surface for reaction, which can impart excellent selectivity to a catalytic reaction. Finally, nanoparticulate catalysts prepared by chemical synthesis can be coated with inert porous materials, which can prevent sintering and improve thermal stability. Thus, modern synthetic techniques offer many opportunities to improve catalyst performance; however, they have yet to be exploited to their fullest extent, particularly for fossil-energy applications. Complementing this controlled synthetic approach are more sophisticated growth techniques, like surface growth, in which catalytically active metals are deposited on single-crystal surfaces. These surface-growth methods can produce highly monodisperse catalyst particles whose size, shape, and structural properties can be controlled during the growth step. These surface-grown particles serve as excellent model catalysts for delineating size and shape effects in a well-defined system. They also serve as an ideal complementary system to better understand reactivity studies of catalyst particles made by colloidal synthetic methodologies.

For fossil energy-based catalysis, the improvement of reactivity and selectivity has applications for the conversion of coal-derived synthesis gas (syngas) into liquid fuels. The recently published *Hydrogen from Coal RD&D Plan* (NETL, Sept. 2008) identifies the development of novel catalysts as a key step for addressing technical barriers associated with the efficient production of hydrogen-rich liquids from syngas. In this regard, researchers have long sought to better control the distribution of liquids and waxes produced during the hydrogenation of carbon monoxide (CO) by the Fischer-Tropsch (F-T) process and, more specifically, to be able to tailor the selectivity of the catalyst to produce optimal hydrogen-carrier liquids for reforming. The ability to produce a homogeneous set of active sites on F-T catalysts and to control the interaction strength of CO and hydrogen gas (H_2) with these catalysts should help researchers optimize the process. Furthermore, recent in situ x-ray spectroscopy experiments have pointed to the effect of iron carbide crystallite size on the density of active sites, and thus F-T reaction rate and products. Controlled growth of size- and shape-dependent iron-based catalysts can help researchers better understand and optimize the active phases and sites present on F-T catalysts.

Surface Growth of Model F-T Catalysts

Catalyst particles grown on single crystal surfaces will serve as an ideal system for studying size and shape effects, as the growth of these particles on single crystal surfaces will allow researchers to control particle size and shape by controlling growth temperature, time, and pressure. Model catalyst particles may then be characterized using advanced surface-science methodologies, such as scanning tunneling microscopy (STM), x-ray photoelectron spectroscopy (XPS), and low-energy ion-scattering spectroscopy (LEIS)—techniques which will allow researchers to study size- and shape-dependent catalysis in a manner that cannot be achieved using traditional supported catalysts and associated methodologies for characterizing powdered catalysts. In particular, the STM will allow researchers to evaluate, with atomistic-level resolution, the real-space structure of surface-grown catalysts. Additionally, details regarding edge sites, defects, particle height/size, can be evaluated and correlated with any changes seen in particle reactivity. The atomistic-level data acquired from the STM studies will also provide valuable information for ab initio computational modeling and will provide critical information on the role that precise sites (steps, defects edges, etc.) play on the chemical reactivity of particles.

Initial work has focused on growing iron (Fe), Fe-oxide, and Fe-carbide particles on the reconstructed gold (Au) surface of Miller index 111 (Au [111]). Fe-based materials were chosen since real F-T catalysts tend to be a mixed phase of elemental Fe, Fe-oxides, and Fe-carbides, while the Au (111) surface was chosen as a growth substrate because of the relative inertness of Au to essentially all chemical environments. Recent in situ x-ray spectroscopy studies have followed the reduction and carburization of Fe_2O_3 (iron [III] oxide) F-T catalysts, pointing to promoter effects during activation and crystallite size effects on F-T reactivity and product distributions. Future studies will evaluate cobalt (Co) and Fe-Co alloys.

Recent work by de Jong et al. has already indicated optimal sizes for Co catalyst particles. In addition, it has been shown that changing the Co:Fe ratio in alloy catalysts can dramatically change the product distribution of olefins and paraffin waxes produced during F-T reactions. Our work with these Fe-based systems has been successful in growing Fe particles on the reconstructed Au (111) surface with control over both the size and shape of the Fe particles; particles range from irregular shapes with an approximately 3 nanometer (nm) diameter to ordered arrays of triangular Fe particles with an approximately 8 nm diameter. All particles are one single atomic layer of Fe thick and may be reacted with molecular oxygen (at room temperature) to produce iron-oxide nanoparticles. The size and shape of the iron-oxide nanoparticles can also be controlled.

STM, XPS, and LEIS studies all indicate that the particles are single layers of FeO (iron [II] oxide) terminated by oxygen at the (111) face. The FeO particles are two-dimensional (2-D) in nature, with heights of approximately 1.5 angstroms (Ǻ). Larger FeO particles produce a Moire pattern with the underlying Au (111) substrate, producing a hexagonal superstructure with a 35 Ǻ periodicity. If a stronger oxidizer like nitrous oxide is used, the Fe particles are converted into three-dimensional (3-D) nanoparticles that are approximately 5.5 Ǻ in diameter. STM and XPS studies indicate that these particles are Fe_2O_3 and most likely terminated with oxygen. These growth conditions tend to favor small 3-D particles, and larger particles, as seen for FeO, are not produced. The edges of the Fe_2O_3 are stepped and appear to be composed of irregular edge sites. Current work will focus on better evaluating the structure of these particles; attempts are also being made to activate this oxide to the mixed phases of Fe oxide and Fe carbide believed to be present during active F-T catalytic reactions.

Colloidal Growth of Model F-T Catalysts

Wet chemical techniques will be used to synthesize nanoparticles of a specific size and/or shape. The project will also consider alloy nanoparticles and the effects that alloying has on the structure and stability of the particles. These particles will serve as model heterogeneous catalysts to establish how size, shape, and composition impact optimal catalytic properties. They will also be dispersed on high surface-area supports for spectroscopic study and measurement of catalytic activity and selectivity for reactions relevant to F-T synthesis and other catalytic processes used for fuel synthesis.

Multicomponent and multiphase nanoparticle catalysts can drastically improve performance. Alloy nanoparticles can show greater catalytic activity, selectivity, and resistance to poisoning and sintering than monometallic catalysts. Dramatic improvements in activity and selectivity have been observed by modification of traditional, dispersed metal catalysts with other metals—an increase that is not well understood. Nonetheless, the same enhancements in catalyst properties should be observed in size- and shape-selected nanoparticulate catalysts, but it is not clear how the composition and the phases of multicomponent catalysts impact their selectivity and activity, nor is it easy to find the optimum composition for different catalytic processes. One of the key issues concerning multicomponent nanoparticulate catalysts is how the properties of alloy nanoparticles differ from those of nanoparticles with multiple phases. Multicomponent nanoparticles present additional challenges to those of the traditional catalyst design. These challenges open up a whole new area of research problems which, if solved, can improve catalyst efficiency manyfold.

Controlled synthesis of multicomponent and multiphase nanoparticles is significantly more complex than the synthesis of single-component nanoparticles. In addition to the challenges of controlling size and shape, one is faced with the need to control composition and phase distribution. For example, one can, in principle, make nanoparticles of Fe and platinum (Pt) that are simple Fe_xPt_{1-x} alloys or nanoparticles that contain two pure phases, Fe and Pt, in intimate contact. The approach of this project is to develop wet chemical syntheses of multicomponent and multiphase nanoparticulate catalysts with well-defined size, shape, texture, composition, and phase. The goal of the proposed research is the synthesis of multicomponent and multiphase nanoparticles which expose a single type of catalytic reaction site. This requires that catalytic particles be synthesized with well-defined size, shape, and texture, where “texture” refers to the lack of bulk defects; the particles should be single-crystalline and expose only one crystallographic face (for example, cubic nanoparticles of a face-centric cubic [fcc] crystal that only expose [001] planes). The growth of these nanoparticles has to be controlled such that there are no bulk defects such as dislocations and twins.

Multicomponent and multiphase nanoparticles will be synthesized from a number of metals and alloys of various compositions, with the project’s efforts focused primarily on Fe- and Co-based catalysts because of relevance to F-T reactions. Alloying of Fe and Co to make Fe:Co catalysts will be investigated, as will alloys with other materials, like nickel (Ni) and Pt, which have been shown to improve selectivity and may impart better high-temperature stability. The project will also investigate the use of colloidal techniques to produce h nanoparticles with shells of a second component over the initial metal core (core-shell-type particles). Recent studies have shown that core-shell materials can have improved performance over traditional catalysts or simple alloys of materials. The structural characteristics of these nanoparticles will be examined using high-resolution transmission electron microscope (TEM) methods, x-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), and ultraviolet-visible (UV-vis) spectroscopy. Their physical properties will be studied by adsorption and spectroscopy methods, and ultimately, their catalytic activity and selectivity will be probed for test reactions.

Using this approach, the project has been successful in producing different shapes and sizes of Fe nanoparticles, Co nanoparticles, Ni nanoparticles, and ferrocobalt alloy (FeCo) nanoparticles. In addition, the project has also been able to coat these nanoparticles with silica coatings for catalytic studies. The different shapes of nanoparticles achieved so far are spheres, cubes, hexagons, and rods, in sizes of 3–10 nm. Silica-coated, FeCo, Fe, and Ni nanoparticles all show sinter-resistant properties.

The shapes of nanoparticles are characterized using transmission electron micrographs obtained at a single nanoparticle orientation, and, thus, the shape determination is based on viewing a single cross-sectional profile of the nanoparticle (a full determination of particle shape would require viewing over a range of angles.) Angle-resolved TEM techniques are necessary to view the crystals over a range of orientations and to determine their 3-D shapes, and such imaging of nanoparticles reveals information about nanoparticle shape and orientation on substrates that cannot be determined from single cross-sectional TEM images. Angle-resolved TEM imaging of nanoparticles will be very valuable in catalysis and in the fields in which the shapes of nanoparticles play an important role.

High resolution TEM studies are generally performed using a Technai F20 field emission gun (FEG)/high-resolution transmission electron microscopy (HRTEM)/scanning transmission electron microscopy (STEM) with a Gatan imaging filter and energy dispersive x-ray spectroscopy operating at 200 kiloelectronvolts (keV). To demonstrate the value of nanoparticle rotation in determining 3-D shape, this project has utilized successive TEM images taken of a single nanoparticle that has been rotated in space.

Relationship to Program:

This project will support important F-T catalyst advances within the alternate hydrogen production pathway focus area of the Hydrogen and Clean Fuels Program by providing the following technological developments:

- New catalysts with improved selectivity and efficiency for converting coal and biomass to high hydrogen-content hydrocarbons
- The development of techniques to improve the high-temperature stability of small, metal catalyst particles
- Atomistic-level experimental data on Fe-based model catalysts to aid in interpretation of heterogeneous catalysis results and guide computational modeling

Primary Project Goal:

The primary goal of this project is to develop a highly selective and efficient catalyst for converting coal-and-biomass-derived syngas into liquid fuel.

Objectives:

The objectives of the project include the following:

- The project team seeks to develop methods for growing model Fe, Fe-oxide, and Fe-carbide catalyst particles on single-crystal substrates. Evaporation methods and chemical vapor deposition will be the primary techniques employed.
- Work on this project is aimed toward the development of robust and scalable methods for synthesizing size- and shape-selected metal nanoparticles using colloidal synthetic techniques. A large focus of this work will address developing techniques to improve the high-temperature stability of these nanoparticles so they can be incorporated into real-world catalytic processes.

11: FWP-49601

Project Number FWP-49601	**Project Title** Development of Mixed-Conducting Dense Ceramic Membranes for Hydrogen Separation			
Contacts DOE/NETL Project Mgr.	**Name** Richard Dunst	**Organization** Gasification Division	**Email** Richard.Dunst@netl.doe.gov	
Principal Investigator	U. Balachandran	Argonne National Laboratory-IL	balu@anl.gov	
Partners	National Energy Technology Laboratory, Dr. B. Morreale Georgia Institute of Technology, Prof. M. Liu University of Houston, Prof. K. Salama University of Florida, Prof. E. D. Wachsman Eltron Research, Inc., Dr. M. V. Mundschau			
Stage of Development				
__ Fundamental	__ Applied	X Proof of Concept	__ Prototype Testing	__ 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 has to be produced from fossil and other resources by means of various technologies. During its production, hydrogen has to be separated from gas streams containing other species. The Office of Fossil Energy (FE) at DOE sponsors a wide range of research, development, and demonstration (RD&D) programs to maximize the use of vast domestic fossil resources and to 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. Supported by DOE-FE, Argonne National Laboratory is developing dense hydrogen transport membranes (HTMs) for separating hydrogen from mixed gases, particularly product streams generated during coal gasification. Hydrogen separation with these membranes is non-galvanic (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, making post-separation purification steps are unnecessary.

Materials development for the HTM follows a three-pronged approach. In one approach, single-phase mixed (ionic/electronic) conducting ceramics (perovskites doped on both A and B sites) were investigated. The single-phase membranes gave a low hydrogen flux due to their poor electronic conductivity. In the second approach, ceramic-metal composite (cermet) membranes that contained mixed-conducting ceramics combined with a metallic component were developed. In these cermets, the metal enhanced the hydrogen flux of the ceramic phase by increasing the electronic conductivity of the cermet. In the third approach, a hydrogen transport metal, a metal with high hydrogen permeability (e.g., palladium [Pd], palladium-silver [Pd-Ag], and palladium-copper [Pd-Cu]), was dispersed in a thermodynamically and mechanically stable ceramic matrix (e.g., aluminum oxide [Al_2O_3] or zirconium dioxide [ZrO_2]). The cermets made by the third approach presently exhibit the highest hydrogen flux.

This project involves investigations to identify materials with suitable hydrogen permeability, followed by the development of methods for fabricating thin, dense membranes from such materials. Chemical, mechanical, and thermal stability of the membranes are studied. Because HTMs are expected to contact gas streams containing hydrogen gas (H_2), water, hydrogen sulfide (H_2S), carbon monoxide (CO), methane (CH_4), carbon dioxide (CO_2), etc., in concentrations that are typical of coal-derived synthesis gas (syngas) from coal-based gasifiers, the stability of the HTMs are also studied. Tests have been conducted with HTMs prepared by mixing ~50 volume percent (vol%) Pd with yttrium oxide (Y_2O_3)-stabilized ZrO_2. Using several feed gas mixtures, the project team measured the non-galvanic hydrogen permeation rate, or flux, for the cermet membranes in the temperature range 400°C–900°C. This rate varied linearly with the inverse of membrane thickness and reached ~52 cm^3 (standard temperature and pressure [STP])/min-cm^2 (~100 $ft^3/hr\text{-}ft^2$) at 900°C for a ~20-μm-thick membrane on a porous support structure when the feed gas contained 100% H_2 at ambient pressure.

Because the product streams from coal gasification are corrosive, good chemical stability is critical for HTMs; therefore, the project team evaluated the effect of various contaminants on the chemical stability of cermet membranes. The particularly corrosive contaminant (H_2S) impedes hydrogen permeation through cermet membranes by reacting with them to form palladium sulfide (Pd_4S). To evaluate the chemical stability of the HTMs, Pd/Pd_4S phase boundary was determined in the temperature range ~450°C–900°C in tests using various feed gases that contained 10%–73% H_2 and ~8–400 parts per million (ppm) H_2S. Hydrogen flux measurements at 900°C showed that the cermet membranes are stable for up to 1,200 hours in gases that contain 400 ppm H_2S. Cermet membranes also gave stable performance when they were tested in a gas mixture that contained high concentrations of CH_4, CO, and CO_2 for times that approached ~500 hours, and they were stable in the temperature range of 500°C–800°C in simulated synthesis gas mixtures containing ~21% steam.

To be practical, HTMs must also have good mechanical integrity at high temperature (~900°C) and high pressure (>300 pounds per square inch gauge [psig]). The project team recently constructed a reactor that allows the hydrogen flux of membranes to be measured at temperatures up to 900°C and pressures up to 300 psig. The project team also fabricated and tested small tubular membranes. Preliminary engineering analysis for producing hydrogen from coal using hydrogen separation membranes has been carried out. The results obtained so far indicate that the HTM developed at Argonne may be suitable for long-term, practical hydrogen-separation applications.

The HTM work has resulted in three patents, 24 publications in peer-reviewed international journals, and 26 conference proceedings. A hydrogen-selective membrane developed as part of 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) in 2004. 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.

In its 2004 report on the hydrogen economy, the National Research Council concluded that coal must be a significant component of the research and development (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 CO_2 emissions. The technical targets for hydrogen membranes (*Hydrogen from Coal Multi-Year RD&D Plan*, September 2008) lists a flux of 200 $ft^3/hr/ft^2$/100 psi Δp (the total pressure differential across the membrane reactor) by 2010 and 300 $ft^3/hr/ft^2$/100 psi Δp by 2015. So far, a flux of ~100 $ft^3/hr/ft^2$ has been measured under ambient pressure (i.e., where the hydrogen-containing feed gas and the sweep gas [nitrogen] are both at ambient pressure). High pressure measurements made on an ~0.8-mm-thick HTM and flux data scaled to 20-μm thickness showed flux >200 $ft^3/hr/ft^2$/<20 psi Δp. Because the flux increases with Δp, it is reasonable to expect flux >400 $ft^3/hr/ft^2$/100 psi Δp with Argonne's HTMs. Work is in progress on measuring the flux in thinner membranes at high pressures.

The technical target requires the HTM to be resistant to contaminants (CO and H_2S). Short-term tests have already shown that the HTMs are stable in gas streams with >10% CO and 400 ppm H_2S. Long-term stability experiments in mixed gas streams with various levels of contaminants are planned for the future. The dense membrane's selectivity for hydrogen is theoretically infinite; hence, the membranes developed in this project meet the hydrogen purity target (99.99%). 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, alloys of Pd (Pd-Cu, Pd-Ag) and non-precious metals (niobium, vanadium, and zirconium) will be used.

History/Context Leading to the Hydrogen Transport Membranes Project

During fiscal years 1992–1997, R&D funded by DOE's Office of Fossil Energy was performed on dense ceramic membranes for natural gas-to-liquid fuel conversion. In that work, dense ceramic membranes were developed 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 other side of the membrane, where the oxygen reacted with CH_4 to form syngas (in the presence of a reforming catalyst). 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 CH_4 to syngas by ~35% when compared to steam reforming or partial oxidation processes.

Project research has 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 FY 1998, the OTM project was moved to industries for scale-up and large-scale demonstrations. Two separate consortia, one led by Air Products & Chemicals and the other by Praxair, scaled up the OTMs and are currently demonstrating pilot plants for syngas production, industrial oxygen production for coal gasification, and oxy-fuel combustion. Around December 1997, through the Federal Energy Technology Center (presently NETL), the Office of Fossil Energy continued the project at Argonne with an emphasis shift to develop 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.

Relationship to Program:

This project will support membrane-separation system advances within the central hydrogen production pathway focus area of the Hydrogen and Clean Fuels Program. The Hydrogen and Clean Fuels Program also supports the President's Hydrogen Fuel Initiative, 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.

Cost-effective ceramic membranes will benefit hydrogen-based power production and transportation applications that use pure hydrogen to power fuel cells. Using ceramic membranes to separate hydrogen from a shifted syngas stream will also benefit CO_2-sequestration efforts by producing highly concentrated CO_2 streams. Previous studies have shown that ceramic membranes can potentially increase hydrogen production by 32% and increase carbon capture by 13% over conventional pressure-swing adsorption technology. Hydrogen-separation membranes also have other potential applications, such as in dehydrogenation reactions for producing olefins, hydrogen production from natural gas, decomposition of ammonia from gasifier product gas, and separation of H_2S from gasifier product gas and tail gas from petrochemical processing.

Primary Project Goal:

The goal of this project is to develop dense hydrogen transport membranes that non-galvanically (i.e., without electrodes or external power circuits) separate pure hydrogen from coal gasifier-produced product streams at commercially significant fluxes under industrially relevant operating conditions.

Objectives:

The project objective is to develop dense ceramic and cermet 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, CO, CO_2, CH_4, H_2S, mercury, halides, and other impurities. Hydrogen-separation membranes can be classified into five broad categories: porous (microporous and nanoporous), 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. Palladium metallic membranes give high hydrogen flux, but they suffer from hydrogen embrittlement, CO and H_2S poisoning, and catastrophic failure due to phase changes. Dense ceramic and cermet membranes are being developed 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; the ability to supply CO_2 stream at coal-gasifier pressures (an important aspect for CO_2 sequestration efforts); and tolerance of steam, CO, CO_2, CH_4, and H_2S.

Membrane development at Argonne focused initially on beryllium cerium yttrium oxide ($BaCe_{0.8}Y_{0.2}O_{3-\delta}$ [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 non-galvanic hydrogen flux. To increase the electronic conductivity, and thereby increase the hydrogen flux, various cermet membranes were developed in which 40–50 vol% of a metal (or alloy) is dispersed in a ceramic matrix. In these 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 an additional transport path for hydrogen. A ~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 (~100 $ft^3/hr/ft^2$) 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 is studying their stability in simulated syngas mixtures typical of a gasifier stream. Preliminary data on stability in mixed streams has been collected, and long-term experiments are planned. In order to meet/exceed the flux target (listed in *Hydrogen from Coal Multi-Year RD&D Plan*), the project team is modifying the microstructure and surface exchange activity of HTMs and fabricating thinner membranes on porous support structures. In real-world applications, it is expected that thin film HTMs on porous supports will be used in either shell-and-tube or stacked flat-plate geometries (similar to geometries currently used in solid oxide fuel cells and OTMs). The project is measuring the flux at 450°C–900°C and up to ~300 psig to evaluate the membrane performance under real-world conditions in a coal plant. In order to evaluate the durability, fracture toughness of the cermet membranes has been measured in the temperature range 25°C–1200°C. Measured mechanical properties will be used in a life-time analysis model to predict mean time to failure (Weibull analysis). The project team will develop methods to form gastight seals between the membranes and metal/alloys to form manifolds for testing membrane performance. Combining water gas shift and hydrogen separation steps in a single membrane reactor would allow process intensification and increase efficiency; therefore, water-gas shift activity of HTMs will be investigated. Using the 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).

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

12: DE-FC26-07NT43027

Project Number DE-FC26-07NT43027	**Project Title** Investigation of Hydrogen-Fueled Internal Combustion Engine Durability			
Contacts DOE/NETL Project Mgr.	**Name** Robie Lewis	**Organization** Fuels Division	**Email** Robie.Lewis@NETL.DOE.gov	
Principal Investigator	Garrett Paul Beauregard	Electric Transportation Engineering Corporation	gbeauregard@etecevs.com	
Partners	Roush Industries Sacré-Davey Innovations Argonne National Laboratory			
Stage of Development				
__Fundamental	__Applied	__ Proof of Concept	_X_ Prototype Testing	__ Demonstration

Technical Background:

It is of great importance to NETL to gain a better understanding of the durability of hydrogen-fueled internal combustion engines (HICEs) and whether or not they are able to meet the long-term needs of vehicle operators. This project seeks to answer this question using accelerated aging of a HICE in an engine dynamometer laboratory along with field testing of the eight HICE vehicles operating in the Integrated Waste Hydrogen Utilization Project.

The laboratory investigation is designed to collect data from a hydrogen-fueled engine operating on an engine dynamometer at high loads (alternating between maximum power and maximum torque) for a total of 1,000 hours. The 1,000-hour durability test is based on the 300-hour automotive industry standard for rapidly accumulating the equivalent of 100,000 miles of service on an engine. Operating at maximum torque and power places maximum stress on the engine, including reciprocating components, lubricating oil, the fuel delivery system, and the ignition system. The 1,000-hour engine durability test provides data describing the engine's ability to survive long periods of operation at high stress levels. This data also provides an indication of the engine’s expected durability through 100,000 miles of operation, something that is not easily achieved through on-road driving in a short period of time.

The field investigation is designed to collect data from real-world HICE operation in diverse fleets, providing a direct measurement for the DOE focus area of hydrogen-fueled engine durability in a vehicle application. By observing and documenting actual vehicle operation over a three-year period, the proposed project will be uniquely able to provide data regarding the durability of HICEs and their ability to meet the long-term needs of vehicle operators. By performing specific analyses and inspections during the field-test period, the proposed project will be able to document any changes in performance or engine condition, leading to a determination of failure modes should they occur. The final engine teardown inspection and analysis provides the ability to document engine condition and the effects of hydrogen use after significant real-world use.

Relationship to Program:

This project will support important hydrogen engine advances within the hydrogen utilization pathway focus of the Hydrogen and Clean Fuels Program. This project provided data from laboratory testing of a HICE engine operated on an engine dynamometer with varying loads for a period of 1,000 hours, including 300 hours of operation alternating between maximum torque and maximum power. The project also provides data to determine the durability of hydrogen-fueled engines through a fleet of eight HICE-powered pickup trucks operating on public roadways for a period of three years. This project will provide data from a teardown analysis of these engines, including material analyses for certain engine components.

Primary Project Goal:

The primary goal of this project is to comprehensively determine long-term HICE durability issues and provide recommendations for the reduction of risk associated with these durability issues.

Objectives:

The objective of this project is to determine the durability issues associated with the use of hydrogen fuel in an internal combustion engine. A HICE jointly developed by Roush Industries and Electric Transportation Engineering Corporation will be used as the basis for the proposed program of work. Engine durability will be determined through accelerated aging in an engine dynamometer laboratory and through field testing in diverse fleets.

13: DE-FC26-06NT42759

Project Number DE-FC26-06NT42759	**Project Title** Development of a Hydrogasification Process for Co-Production of Substitute Natural Gas (SNG) and Electric Power from Western Coals			
Contacts DOE/NETL Project Mgr.	**Name** C. Elaine Everitt	**Organization** Fuels Division	**Email** Elaine.Everitt@netl.doe.gov	
Principal Investigator	Raymond S. Hobbs	Arizona Public Service	raymond.hobbs@aps.com	
Partners	Billiton New Mexico Company Electric Transportation Engineering Company Boeing WorleyParsons Air Products and Chemicals			
Stage of Development				
__ Fundamental	__ Applied	X Proof of Concept	__Prototype Testing	__ Demonstration

Technical Background:

The Advanced Hydrogasification Process (AHP) is being developed to utilize the United States' abundant western coal supply to address concerns of diminishing domestic oil and natural gas resources as energy providers, while also incorporating a renewable energy source and reducing greenhouse gas emissions. Arizona Public Service (APS) is the prime recipient for this cooperative project to develop the AHP with DOE.

Like many utilities, APS is required to produce a significant percentage of its electricity from renewable sources (currently 15% by 2025). As these resources are not dispatchable, these goals are at odds with the need to maintain a highly reliable electric grid. Carbon dioxide (CO_2) emission mitigation regulations appear to be a certainty, while new electric production capacity must be built. The need for the AHP is further supported by two inevitabilities: (1) without a viable CO_2 strategy, the future use of coal to produce electricity faces regulatory and legal challenges, and (2) electric utility renewable energy portfolio requirements will increase over time, making a dispatchable renewable fuel more valuable.

APS currently operates 4,000 megawatts (MW) of natural gas generation. This is a preferred means of generation, as it utilizes fuel defined by the State of California as a "clean fuel." Furthermore, natural gas plants have a capital cost that is low compared to other generation alternatives; are simple to operate; are highly efficient (60%); and can be located near load centers, reducing transmission line requirements. However, like many utilities, APS is facing serious financial difficulty due to the volatile price of natural gas these plants use, creating significant rate increases and economic instability for our customers.

There is a real need for an alternative means of electric generation that utilizes renewable energy sources yet is dispatchable to support a reliable grid. The AHP project is designed to investigate one possible generation alternative.

Hydrogasification research was initiated by DOE during the 1970s. The Gas Research Institute, now the Gas Technology Institute (GTI), had aggressively pursued research based on hydrogasification much earlier, providing a more efficient process to produce synthetic natural gas (SNG) than the traditional partial oxidation process followed by methanation. In 1982, DOE research stopped when the price of natural gas fell. Osaka Gas and Electric, together with British Gas, resumed research in 1992. The Japanese government joined the effort, and that program was renamed ARCH (Advanced Rapid Coal Hydrogasification). The ARCH research program terminated when the price of natural gas fell again, and the DOE Energy Information Administration forecasted a favorable economic future and reserves future for natural gas.

The AHP utilizes coal as a source for carbon, as well as hydrogen produced from renewable resources, in a process (hydrogasification) that produces SNG with low greenhouse gas (CO_2) emissions.

Hydrogen can be produced from many sources. In the AHP, large-scale electrolysis produces hydrogen and oxygen at a commercial efficiency of 75% higher heating value (HHV). Through incremental use of renewable energy (such as wind power), this hydrogen can be produced without CO_2 emissions. Grid energy (from baseload nuclear or coal generation) can also be used incrementally to firm the hydrogen supply and increase load factor during non-peak periods. In this manner, off-peak and seasonal renewable energy can be stored indefinitely in the existing infrastructure and used in a wide array of applications, including electric production. Hydrogen (produced using renewable energy) that is converted to natural gas (a desirable fuel for power generation or industrial use) via coal hydrogasification and stored and distributed using the existing gas pipeline infrastructure provides a strategy toward sustainability.

The APS AHP process is an integrated five-step systems process: (1) hydrogen production using incremental renewable energy to minimize CO_2 emissions, (2) SNG production by hydrogasification of coal, (3) oxycombustion of coal/char to produce electricity, (4) carbon recycling of CO_2 emissions through biological processes, and (5) biofuels production by reutilization of carbon. The combination of these steps creates an integrated process that delivers energy and fuel in a long-term, sustainable process.

The AHP project is being conducted over three phases.

In **Phase I**, thermogravimetric analysis tests were run, a chemical process model was created, and preliminary engineering and economic studies were performed. Considerable effort was also expended in reviewing DOE’s prior hydrogasification research efforts from the 1960s through 2002 (i.e., the Japanese and British Gas ARCH project).

Project accomplishments from Phase I include the following: In Phase I of the project, the AHP chemical process model was developed by Nexant using AspenPlus. The AHP chemical process model used a feed rate of 1,000 tons per day (tpd) of western coal (New Mexico, Fruitland Formation). Product gas from the hydrogasifier, at 60% carbon conversion, was predicted at a nominal 56.9% hydrogen (H_2), 21.6% methane (CH_4), 3.5% carbon monoxide (CO), and 0.86% CO_2 (percent by volume). After gas cleaning and separation, the pipeline-injected SNG composition was CH_4 (97.2% by volume) and H_2 (0.44% by volume). Nexant calculated the system efficiency at 64% including water electrolysis (75%). BHP Billiton Coal Company chose New Mexico subbituminous coal from the Fruitland formation. This decision was based upon the one-billion-ton reserve availability BHP Billiton has under lease, and their willingness to host both the engineering-scale plant (Phase III) and a potential future commercial plant. Air Products performed the hydrogen supply studies based upon the New Mexico location.

The hydrogasifier configuration and resulting carbon conversion efficiency was a key decision point, along with the requirement that downstream product gas treatment use existing commercial technology. An entrained flow aerosol hydrogasification reactor using 200-mesh pulverized coal was chosen for the AHP. This decision was facilitated by the success of research conducted by Rockwell and the Advanced Research Cooperation in Environmental Health research programs, which both achieved favorable results using a similar technique. In this configuration, hot hydrogen is injected into a dispersed coal flow, rapidly heating the coal, thereby facilitating maximum disruption of the coal particle during the formation of CH_4. The reaction time for this process was estimated to be a few seconds. The reactor operating temperature was established at 1,600ºF–1,800ºF to maximize the formation of CH_4 and minimize the formation of CO, CO_2, and tars. Reactor operating pressure was established at 1,000 pounds per square inch (psi), as high operating pressure is thermodynamically preferred for CH_4 formation.

In addition to production of SNG, the scope of this project required that electricity be coproduced. This is achieved using unreacted char from the hydrogasifier. Literature data indicated that a carbon conversion efficiency of 50% was achieved during previous research. Under the AHP project, testing was also conducted by GTI using a laboratory-scale high pressure thermogravimetric analysis on a New Mexico Fruitland Formation coal sample provided by project partner BHP Billiton. Results from the GTI tests demonstrated that about 90% carbon conversion was achieved when the test reached equilibrium. In the AHP chemical process model, unreacted char from the hydrogasifier is fed to an oxyburner to create steam for electric production, eliminating any issues with entrained hydrogen in the char from the hydrogasifier and producing pure CO_2 for process use or sequestration. An alternative to this step is to produce syngas with the char. However, the NETL research program in utility boiler oxyburners is complimentary to burning the char, and this approach was well received by APS executive management based on its practicality. The oxygen required by the oxyburner will be available as a byproduct from hydrogen production through electrolysis.

Air Products performed hydrogen supply studies upon the proposed New Mexico location for the engineering-scale and commercial facilities. This study considered the production of hydrogen by electrolysis using a combination of wind and grid energy. It examined alternatives that included the following: (1) electrolysis at the wind farm site with a hydrogen pipeline transporting the hydrogen to the mine-mouth site hydrogasification facility, and (2) the transmission of wind-generated electricity from the wind farm to the electrolyzers at the mine-mouth hydrogasification facility. For the AHP, the later approach was selected.

WorleyParsons created a preliminary engineering plant design and construction cost estimate for a commercial-scale facility from the AHP Nexant 1,000 tpd dried coal chemical process model. The WorleyParsons design used three hydrogasifier trains of the AHP chemical process model to produce 118.4 million standard cubic feet per day (MMscfd) of SNG, 131.4 MW of net electric power for resale, 20.5 tpd of sulfur for resale, and 217 gallons per minute (gpm) of excess condensate water. The plant was based upon the physical conditions in the Farmington, NM area, including easy access to natural gas transmission pipelines and adequate water resources. The plant design required 3,235 tpd of local coal, 286 MMscfd of hydrogen, 48 MMscfd of oxygen, and 1,748 gpm of water. The plant site occupied approximately 70 acres. SNG was injected into the local El Paso Gas pipeline at 985 pounds per square inch gauge (psig) with a heating value greater than 967 British thermal units per standard cubic feet cubic meter (Btu/scf).

The construction cost for the commercial-scale facility was estimated by WorleyParsons to be $691 million (in 2007 dollars). Operation and maintenance costs were estimated to be $45 million per year (with $11.2 million in fixed operating costs, $6 million in material costs, $4.7 million in chemical costs, $21.7 million in coal costs, and $1 million in ash disposal costs). The cost of hydrogen is significant to these calculations, and it is estimated in two components: equipment and energy. In support of the WorleyParsons cost estimate, Stat Oil estimated that the cost of their 2 MW electrolyzer in volumes of 1 gigawatt (GW) would be $500 per kilowatt (kW). GE Global Research estimated that their electrolyzer would cost $400/kW in large volume (52 kilowatt-hours [kWh] are required to produce 1 kilogram [kg] of hydrogen at 75% efficiency [HHV]). WorleyParsons utilized an electrolyzer cost of $500/kW. Energy costs vary substantially based upon the season, time of day, internal vs. external use, and internal vs. external production. On the APS electric system, the lowest-cost energy is the marginal cost of nuclear energy ($7 per megawatt-hour [MWh]); marginal energy from coal cost is $23/MWh, and wind energy cost is variable at $40–$80/MWh. However, 50% of the annual time electricity can be purchased on the Palo Verde bus for an average of $30/MWh (2006 study using a cap of $40/MWh), due to system demand. WorleyParsons utilized an energy cost of $25/MWh for their hydrogen production costs.

Based on the process feasibility determination made in Phase I and the favorable economics estimated by WorleyParsons, a decision was made to proceed with Phase II work to validate process assumptions and refine cost estimates.

The AHP project is currently in **Phase II**. In this phase, hydrogasification kinetics will be created with a bench-scale kinetics reactor (BSRx). Test results will then be used to update both the process model and the preliminary engineering and economics study. Also in Phase II, flue gas containing CO_2 will be injected into a scalable algae farm, and a biofuel sample (i.e., JP8 military aviation fuel) will be produced using algae grown in the bioreactor/farm. The algae farm will operate for one year while integrated with an APS power plant.

Phase II has several key activities, relating to both the SNG and the algae.

With respect to the **SNG**, Phase II includes work to accomplish the following:

- Design a BSRx to validate reaction kinetic assumptions
- Engineer and construct the BSRx and supporting systems
- Create a computational fluid dynamics (CFD) model for the hydrogasifier design
- Conduct tests, using Fruitland Formation coal supplied by BHP BIlliton, with the BSRx to determine reaction kinetics and optimum operating envelope
- Produce the kinetics equations for hydrogasification
- Validate the CFD model using test results from the BSRx to further predict BSRx behavior for untested conditions
- Update the chemical process model using developed kinetics
- Modify preliminary engineering and cost studies based upon test results

The BSRx has been engineered and constructed. It meets American Society of Mechanical Engineers certification under Section VIII with a rating of 1,050 psi at 1900ºF. The reactor can feed pulverized coal at rates up to 15 lb/hr. The hydrogen injection temperature can be varied up to 1,600ºF. The reactor has no ceramic lining. The hydrogen preheater is made of Inconel 625, and the reactor is made of Inconel 617. The BSRx assembly, which includes a coal feeding system and ash collection pots, is a 42 ft vertical design. The hydrogasification reaction zone has a 1.75-inch internal diameter and is 13 ft long. The CFD modeling has been completed by NETL to assist with reactor head assembly design and the hydrogen nozzles. The BSRx is being installed at an APS facility, immediately adjacent to the APS hydrogen fueling station, which has been in operation for 7 years, producing more than 12,000 kg of hydrogen at 6,000 psi. Its control room has been installed, including gas chromatography and mass spectrometry systems. Gas control and electric systems will be installed and connected to the BSRx over the next several weeks. Preoperational testing and commissioning will then be conducted, with first coal tests occurring in the 2nd quarter of 2009.

With respect to the **algae**, Phase II includes work to accomplish the following:

- Create a process to extract lipids from selected algal species
- Create biofuel from lipids extracted from algae grown in power plant emissions
- Design and build a scaleable algae farm to capture CO_2
- Demonstrate 90% carbon capture with algae
- Demonstrate that selected species of algae will not aggregate heavy metals to hazardous levels

There are three general types of algae culture systems today: (1) raceway, (2) tubular bioreactor, and (3) pond. Raceways are commercial systems used to grow a single species, and they are considered to be the lowest-cost farm systems, producing algae for about $5,000/ton (dry) at growth rates up to about 20 g/m^2 per day. Raceways are open systems, and as a result they are subject to many predation problems, evaporation losses, and low CO_2 capture efficiency. The largest raceway system is about 50 acres. Tubular bioreactors are closed and typically small-diameter glass tubes. These bioreactors are expensive to build and operate, but they are completely automatic, growing very high quality products, and they have very high CO_2 capture efficiencies. These systems are effective for the production of pharmaceuticals, human food products, chemicals, etc. Production costs are about $10,000/ton (dry). The largest tubular bioreactor system, in Germany, is about 3 acres. Ponds are used in fisheries applications and grow algae as needed for the primary business, and they generally yield low growth (5 g/m^2 per day) of many species of algae. All of these types of commercial algae farms typically purchase CO_2 at a cost of about $500/ton.

APS began its evaluation of algae as a CO_2 recycling option in early 2005, before initiation of the DOE-funded activity, when a Massachusetts Institute of Technology (MIT) research and development (R&D) project began injecting flue gas from the campus utility boiler into a series of algae-filled tubes. Shortly thereafter, APS contracted with the newly formed GreenFuel Technologies to perform a demonstration of CO_2 recycling from algae in Arizona at the Red Hawk Power Plant. A tubular system (called GEN3), similar to that developed in the MIT R&D project, was built and operation was initiated at Red Hawk in August 2005. GEN3 was operated continuously with flue gas until November 2006. The GEN3 system was expensive, energy intensive, and maintenance intensive; but it grew algae at a high rate (57 g/m^2 per day). Additionally, GreenFuel's GEN3 design could not be scaled for utility use. GreenFuel subsequently constructed a new prototype system (called GEN5 or vertical thin film [VTF]), in an attempt to address some of the limitations of the GEN3 system, and placed it into operation in April 2007. The GEN5 system was a 1,000 m^2 system, and while it initially grew algae as designed, it failed by June 2007 due to challenges in maintaining the correct culture conditions for the algae. The GEN5 system was then reduced to 100 m^2 and operated for three weeks. After the three-week operational period, GreenFuel ended its GEN5 system operation in August 2007. It was estimated that several million dollars were spent in developing and demonstrating the GEN5 system.

GreenFuel claimed very high growth rates with the GEN5 system, but experienced severe problems in continuous operation. GreenFuel then developed a horizontal thin film system, which was low cost and low growth rate (20 grams/m^2 per day), but never deployed this system at APS. Meanwhile, during the contractual period between APS and GreenFuel, GreenFuel engaged Inventure to develop a proprietary process to produce biodiesel from algal lipids and ethanol from the remaining biomass. Inventure produced a product that met the ASTM International requirements for biodiesel and ethanol. Further algae testing occurred when APS hired GreenFuel to perform "adaptation studies" of several candidate algae at its 2000 MW Four Corners Power Plant in Farmington, NM. After three months of studies using the water and flue gas at Four Corners, GreenFuel provided an Adaptation Report in December 2007, showing that several algal species had flourished in the Four Corners environment.

GreenFuel's R&D is proprietary, and APS was under a nondisclosure agreement for all of the algal research hosted at its facilities. Algal companies and research programs have sprung up across the United States, numbering in the hundreds by December 2008. Confidentiality is a common trait among these companies and programs, making open discussions very difficult. However, the experience gained by APS from the work it partially funded with GreenFuel allowed it to add a carbon capture component to the SNG work underway in cooperation with DOE. Under the current Phase II project scope, a scalable algae system will demonstrate CO_2 capture at a natural gas power plant using algae. The algae will be fed flue gas from the plant using a stack slipstream. The demonstration system will contain at least 120,000 liters of algae culture in a bioreactor (closed system). APS will measure the reduction in CO_2 between the gas stream entering and leaving the bioreactor.

This project will construct a demonstration system using 6 m and 10 m bioreactors. The bioreactors have a unique design and address the issues of volumetric efficiency, CO_2 transport, oxygen management, light management, and thermal management. The target cost on the bioreactor is \$10/m^2. The 6 m bioreactor contains about 15,000 liters of algae culture, while the 10 m system contains 40,000 liters. The target growth rate in the bioreactors will be an annual average of 25 g/m^2 per day. A prototype 6 m bioreactor is undergoing evaluation at the APS test site. The target production cost of the demonstration will be \$1,000/ton (dried algae) at a CO_2 reduction rate of 72 tons/acre per year. The bioreactor is only one system in the farm. The APS farm will comprise several bioreactors, a harvest system, a flue gas/CO_2 management system, a water management system, a nursery, and product packaging. The prototype harvest system has been built. A key point of the demonstration will be the continuous operation of the farm for one year. In addition to demonstrating CO_2 capture, the bioreactors must be robust, maintainable, and low cost.

The demonstration system will be developed using two algal test areas. The APS test site is located in downtown Phoenix. Facilities at the test site include the laboratory, algal nursery, 70 ft diameter thermal pond, 180 L bag farm with supporting infrastructure, and bioreactor fabrication area. During the first quarter of 2009, nannochloropsis algae will be grown in the nursery and bag farm for inoculation into the prototype 6 m bioreactor. The 6 m bioreactor will undergo performance testing. The prototype harvesting system will be evaluated with the inoculated bioreactor. The second test site is located at the APS 1,000 MW Red Hawk power plant, 55 miles west of Phoenix and adjacent to the APS 4,000 MW Palo Verde Nuclear Generating Station. This will be the site of the operational demonstration system. During the 4th quarter of 2008, a 12.5 kilovolt (kV) feeder was installed to provide power for the demonstration operation and a 300 ft stack slipstream has been installed at the demonstration site. A PBR-4000G tubular bioreactor has been received from Germany and will be installed in the modified 150 ft greenhouse serving as the inoculant reactor. An advanced CO_2 separation membrane system has been received from Membrane Technology Research and will be installed in the flue gas/CO_2 management area. This advanced membrane is anticipated to increase the CO_2 in a product stream from about 4% at the stack to about 36%. Construction at Red Hawk will continue until full system operation begins during the 3rd quarter of 2009.

APS will produce a small sample of military fuel from algae grown in power plant emissions during this phase. Oils or lipids are produced within several algal species. The amount of lipid can vary within a species based upon environmental conditions. Algal lipids for biofuel production, such as for biodiesel, are much discussed. About 32,000 L of algal culture were grown from April through August 2008 at the APS test site for laboratory lipid extraction studies, from which about 320 kg of algal paste was sent to six separate laboratories. Extraction analysis from nannochloropsis, chlorella, and selensatrum have proven challenging, with lower than expected neutral lipid content. No attempt has been made to maximize lipid production by stressing the algae. Lipid analysis showed a majority of carbon-16 and carbon-18 chains distribution. Additional extraction evaluations are underway. One gallon of algal oil is currently being extracted and will be sent to ConocoPhillips for research work in producing biofuel.

A CFD model of the bioreactor is currently being developed in collaboration with NETL. This model will include bioreactor flow dynamics, heat transfer, and photosynthesis-driven algal growth. The CFD model results will assist in future improvement of the bioreactor. Actual bioreactor performance results will be applied to the CFD model. This approach will provide an effective modeling tool for bioreactor engineering.

Phase III of the project will encompass the engineering, construction, and operation of an engineering scale hydrogasification reactor and necessary appurtenances.

Relationship to Program:

This project will support important coal-to-syngas gasification advances within the alternate hydrogen production pathway focus area of the Hydrogen and Clean Fuels Program. This project was selected from among applications received in response to a DOE-NETL Funding Opportunity Announcement entitled “Co-Production Advanced Technology / Process Concepts,” which was co-sponsored by the Hydrogen and Clean Fuels Program.

Gasification-based technology is the only environmentally friendly technology that provides the flexibility to coproduce H_2, SNG, and premium hydrocarbon liquids including transportation fuels, and electric power in desired combinations from coal and other carbonaceous feedstocks. Rising costs and limited supply of crude oil and natural gas provide a strong incentive for the development of coal gasification–based coproduction processes. This project addresses the coproduction of SNG and electricity from coal. SNG is a hydrogen carrier, is easily stored, is a fuel source for existing natural gas combined cycle power production and is easily transported via an existing nationwide natural gas pipeline network. The efficient production of SNG from coal offers supply and price stability, as well as an existing transportation infrastructure, to an electric power generation infrastructure that has grown highly dependent on natural gas.

The technical advantages of AHP with the potential to benefit the Hydrogen and Clean Fuels Program include the following:

- AHP can gasify high-moisture and high-ash-content subbituminous and lignite coals without the severe energy penalties associated with other gasification technologies.
- The hydrogasification reactor operates at a lower temperature than partial oxidation reactors, which is expected to alleviate slag-handling and refractory maintenance problems.
- The hydrogasification reactor produces a higher fraction of CH_4 than partial-oxidation reactors, thereby reducing the "lift" required by methanation.
- AHP allows for the introduction of renewable hydrogen into the process, providing a renewable energy addition to electric utility generation portfolios, thus reducing CO_2 production.
- Hydrogen production from wind energy allows for the transfer of energy through wind, without the penalties of time of day and the wind’s intermittent nature.
- Assessments show that the process will be more efficient than alternatives because of lower reaction temperatures and higher CH_4 production in the initial reaction.
- Water consumption for the process will be lower than with other gasification technologies because of reduced water requirements for slag handling.
- While there are clearly several areas of risk and uncertainty that require tests and development, the AHP uses a large portion of commercially available components, which are expected to speed its commercial application.
- AHP facilities could be built using a modular concept that may be expanded over time, or they may be built in combination with existing or future coal-combustion facilities.

The technical advantages of CO_2 capture from the flue gas process with the potential to benefit the Hydrogen and Clean Fuels Program include the following:

- Biological capture, as proposed by the APS team, provides for a closed system that is capable of assuring low CO_2 releases to the atmosphere.
- The proposed method of capture is designed to work at a power plant site.
- The proposed design offers flexibility to fit a wide variety of power plant sites.
- Work on harvesting provides a means to monetize the biological product on a large scale.

- The design will be far less expensive to fabricate and operate than other known designs.
- The carbon emissions from power plants are captured and reutilized (e.g., as a biomass product or as algal-based biofuel).

Primary Project Goal:

The primary goal of this project is to prove the commercial viability of hydrogasification production of SNG and algal CO_2 recycling. To fulfill this goal, this project seeks to demonstrate the following:

- Production of CH_4 from western coal with hydrogasification
- Recycling of power plant CO_2 emissions into algal biomass with a scalable system
- Creation of biofuel from power plant CO_2 emissions

Objectives:

The objective of the project is to develop and demonstrate a coal hydrogasification–based process for producing SNG from coal at an engineering scale. Results of the R&D project will be utilized to develop a process design for commercial-scale coproduction of SNG and electricity with near-zero emissions meeting the following performance targets:

- Overall process efficiency greater than 50%
- SNG production cost below market
- Capture and sequestration of CO_2 equivalent to 90% of emissions from power production
- Water usage at least 50% below that of a comparable gasification or synthesis gas methanation process plant
- Ability to use low-rank western coals
- Potential to incorporate an algae process for CO_2 recycling

The AHP project will conduct R&D for a coal hydrogasification-based process for the coproduction of SNG and electricity with near-zero emissions, in a phased approach to facilitate evaluation of the APS concept process.

14: DE-FC26-03NT41874

Project Number DE-FC26-03NT41874	**Project Title** An Industrial Based Consortium to Develop Premium Carbon Products from Coal			
Contacts DOE/NETL Project Mgr.	**Name** John Stipanovich	**Organization** Fuels Division	**Email** stipanov@netl.doe.gov	
Principal Investigator	Bruce G. Miller	Pennsylvania State University - OSP	bgm3@psu.edu	
Partners	West Virginia University There have been 61 members as part of the second contract, and they are listed below. Members that have received subawards are identified with the number of subawards they received listed after their name. Note that many projects have had industrial partners as subcontractors that are not noted here: Air Products and Chemicals Inc.; Alcoa (Alcoa Primary Metals; Alcoa/Alcoa Technical Center; Composite Structures, Division of Alcoa Composites); Applied Sciences Inc.-1; Asbury Graphite Mills, Inc.; Carbon Sales, Inc.; Carbone of America; Caterpillar Inc.; Charah Environmental Inc.; CII Carbon LLC; City of Redlands; Coal Tech Petrographic Associates, Inc.; Detroit Edison; Electric Power Research Institute's Upgraded Coal Interest Group (UCIG); Engineering Performance Solutions LLC; Entelechy; F.B. Leopold Company, Inc.; Fiber Materials Inc.; Fisher Mining Co.; Graf Tech International Ltd./ UCAR Carbon Co. Inc.-5; Graphite Metallizing Corp.; Graphite Sales, Inc.; Greater Cincinnati Water Works; HYCET, LLC; Inorganic Specialist, Inc.-2; Jeddo Coal Co.; Koppers Industries, Inc.; Morgan AM&T Pure Carbon; Neenah Foundry; NewCarbon, Inc./ NewCarbon, LLC; NORIT Americas Inc.; Pennsylvania State University-23; Pittsburgh Mineral & Environmental Technology, Inc.; Premium Anthracite Wales LTD; Premium Carbon Products, LLC-3; PrepTech, Inc.; Pure Carbon Company; Reading Anthracite Company; Reilly Industries, Inc.; Rio Tinto Aluminum; RJ Lee Group, Inc.; Rohm & Haas Co.; Sasol; Sasol Carbo-Tar; Schunk Kohlenstofftechenik GMBH - Research and Development; SGL Carbon, LLC; Sorbent Technologies Corp.; Southern Company Services Inc.; Southern Illinois University; Thai Carbon & Graphite Co., Ltd.; The F.B. Leopold Company, Inc.; U. S. Steel Corp.; University of Florida-2; University of Kentucky, Center for Applied Energy Research-6; University of North Dakota Energy and Environmental Research Center; US Filter Environmental Services; US Filter Westates; US Filter Westates Carbon, A Siemens Business; Weaver Industries, Inc.; West Materials Inc.; West Virginia University-8; Western Kentucky University			
Stage of Development				
__ Fundamental R&D	X Applied R&D	__ Proof of Concept	__ Prototype Testing	__ Demonstration

Technical Background:

Since 1998, Pennsylvania State University (PSU) has been successfully operating the Consortium for Premium Carbon Products from Coal (CPCPC), which serves as a vehicle for industry-driven research on the promotion, development, and transfer of innovative technology on premium carbon products from coal to the U.S. carbon and coal industries. The CPCPC is an initiative led by PSU, who is responsible for consortium management; its co-charter member, West Virginia University (WVU), along with NETL, provide the base funding for the program. CPCPC began in 1998 under DOE Cooperative Agreement No. DE-FC26-98FT40350. This agreement ended November 2004, but CPCPC activity has continued under the present cooperative agreement, No. DE-FC26-03NT41874, which started October 1, 2003.

Relationship to Program:

This project will support important advances within the polygeneration focus area of the Hydrogen and Clean Fuels Program. Polygeneration will enhance a coal facility's profitability by producing a variety of high-value, coal-derived chemicals and/or carbon materials that can be incorporated into the central or alternate pathway for hydrogen production. Furthermore, CPCPC benefits the coal and carbon industries by providing alternate uses for coal and coal by-products and by developing new materials to market.

Primary Project Goal:

The primary goal of the CPCPC is to promote the use of secure, domestic coal resources to produce environmentally benign, high-value carbon products, such as carbon fibers, activated carbons, binder pitches, cokes for baked anodes and graphite, carbon foams, and carbon nanotubes.

Although coal is the largest domestic fossil fuel hydrocarbon resource in the United States, estimated to last over 200 years at the present consumption rate, most of the premium carbon products developed and manufactured in the United States are derived mainly from petroleum, creating a dependence on foreign imports to manufacture essential carbon products for the domestic market. To ensure sustainable development of carbon products, the inherent potential of the great abundance of coal in the United States must be applied to produce and supply environmentally benign and affordable premium carbon products for the general public.

Since 1998, the CPCPC has striven to promote the recognition of coal as a valuable resource for producing premium carbon products. Multiple successful products and processes have been funded so far, including low-cost carbon fibers from coal for lighter vehicles, large-scale production of inexpensive activated carbon for water and air treatment, high-quality binder pitches and cokes from coal, nanoporous carbon derived from coal tar pitch for ultracapacitor applications, a reactive milling process to produce novel hydrogen storage materials and nanocarbons, an asymmetrical electrochemical capacitor derived from coal, and an all-coal anode. Throughout its continuation, the industrially driven consortium will remain committed to further promote projects that use coal to ensure the sustainable development of the U.S. carbon industry.

Objectives:

The objective of this project is to continue the successful operation of the CPCPC. The CPCPC has experienced tremendous success with its organizational structure that includes PSU and WVU as charter members, numerous industrial affiliate members, and strategic university affiliate members together with NETL, forming a vibrant and creative team for innovative research in the area of transforming coal to carbon products. The key aspect of CPCPC is its industry-led council that selects proposals submitted by CPCPC members to ensure that CPCPC target areas have strong industrial support.

15: DE-FC26-05NT42439

Project Number DE-FC26-05NT42439	**Project Title** Development of Nanocrystalline Doped Ceramic Enabled Fiber Sensors for High Temperature In-Situ Monitoring of Fossil Fuel Gases			
Contacts DOE/NETL Project Mgr.	**Name** Susan Maley	**Organization** Gasification Division	**Email** susan.maley@netl.doe.gov	
Principal Investigator	Hai Xiao	New Mexico Institute of Mining and Technology	xiaoha@mst.edu	
Partners	Junhang Dong, University of Cincinnati Jerry Lin, Arizona State University			
Stage of Development				
_X_ Fundamental	__ Applied	__ Proof of Concept	__ Prototype Testing	__ Demonstration

Technical Background:

Inexpensive and reliable in situ gas sensors are a highly desired item for advanced process control and life-cycle management in advanced power and fuel systems. These systems, which are under development by NETL, are exposed to harsh conditions, requiring constant monitoring to assist in attaining and maintaining high system efficiency and environmental performance. Generally, the measurements of interest within these conditions are temperature, pressure, and gas species (typically hydrogen gas [H_2], carbon monoxide [CO], carbon dioxide [CO_2], hydrogen sulfide [H_2S], oxygen gas [O_2], and other trace species and/or contaminants). Continuous in situ monitoring of gas constituents in hot zones enables the proper mixing of fuels, ensures appropriate heat content, and allows predictive control of conversion processes. Unfortunately, current gas-sensing technology is incapable of operating directly in the harsh environment of power and fuel systems with high temperatures, high pressures, the presence of particulates, and a corrosive atmosphere.

The lack of suitable instrumentation and sensors for harsh environments is a primary driver for NETL's research and development (R&D) in the area of sensors. Sensor R&D includes fundamental technology development through applied engineering and prototype demonstration. Fundamental work includes the exploration of new sensor materials, novel approaches to sensing, and innovative device designs that offer functionality in harsh high-temperature environments.

Optical-fiber sensors are very attractive for applications in harsh environments. These sensors are made of doped, fused silica materials and have the proven advantages of being small, lightweight, immune to electromagnetic interference, resistant to chemical corrosion, highly sensitive, capable of remote operation, and robust in hostile environments. A promising strategy under investigation to construct optical-fiber gas sensors is to coat gas-sensitive optical materials directly onto structured fiber devices, causing gas molecules to selectively interact with coated functional material, changing its optical properties. The resulting changes are converted and amplified by the fiber device to produce an optical signal indicating the amount of target gas molecules existing in the environment. Successful development of such fiber-optic gas sensors requires highly integrated multidisciplinary efforts in the areas of materials, chemistry, sensor devices, and instrumentation.

Among the many types of fiber devices, long-period fiber grating (LPFG)—an optical resonance device with sensitivity to the refractive index of the surrounding environment—has been extensively investigated for chemical sensing. A LPFG sensor has the unique advantages of high sensitivity, immunity to optical power loss variation, and the ability to multiplex many sensors to share the same signal processing unit. In addition, LPFGs made by CO_2 laser irradiation and electric arc modification have successfully survived temperatures up to 800°C.

Doped ceramic materials (i.e., solid oxide materials) have been widely studied for high-temperature membrane, catalysis, and sorption separation applications. Many of these doped ceramics can selectively interact with the gases commonly found in fossil energy systems at high temperatures through such processes as adsorption of gas molecules on the surface or grain boundary (chemisorption), gas dissolution into the crystal structure (physisorption), and involvement in defect reactions. These interactions cause changes in material surface properties, crystal lattice parameters and density, electron states, defect population, and band gap energy, which in turn alter the refractive index. As a result, different optical gas sensors may be constructed to detect gas-induced change in the refractive index of coated nanocrystalline ceramic film.

This project works to develop a new type of optical fiber-based gas sensor for in situ monitoring of fossil fuel gases under harsh conditions in fossil energy systems. The new sensor has three integrated functional components: a structured optical fiber device for generation, amplification, and transmission of optical signals; a doped nanocrystalline ceramic thin film coated on the surface of the fiber device for selectively reacting with specific gas species, causing signature changes of the optical signal; and a microporous overcoat for protecting the sensor material. The proposed research has focused primarily on fundamental issues in the development of gas-selective doped ceramic materials, the synthesis of nanocrystalline ceramic film coatings with desirable microstructures, the design of special optical fiber devices, and the determination of the selectivity, sensitivity, reversibility, and stability of materials and devices in simulated industrial environments.

The project involves interdisciplinary efforts on the part of three professors with complementing experience in relevant technical areas: Dr. Jerry Y.S. Lin, professor of chemical and material engineering at Arizona State University, is in charge of selecting and improving doped ceramic materials with desirable chemical and optical properties; Dr. Junhang Dong, associate professor of chemical engineering at the University of Cincinnati, focuses on the synthesis and characterization of nanocrystalline thin films on structured optical fibers and the development of effective protection for the sensor in harsh conditions; and Dr. Hai Xiao, principal investigator of the project and associate professor of electrical engineering at the Missouri University of Science and Technology, works on developing and characterizing various fiber sensor structures based on the properties of the new materials.

Upon successful demonstration of the feasibility of making operable sensor devices using doped ceramics and optical fibers, the longer range goal is to utilize these devices for in situ monitoring of the composition of common syngas out of a gasifier (H_2, CO). The measurement data can be used for control and optimization of the gasification processes. In addition, these sensors may be used for monitoring the quality of gaseous fuels in other processes.

Relationship to Program:

This project will support in situ hydrogen production advances within the central hydrogen production pathway focus area of the Hydrogen and Clean Fuels Program. This project aims to develop a new type of doped nanocrystalline ceramic-coated optical-fiber sensor for in situ monitoring of syngas compositions at high temperatures. If successful, the developed technology may be used to improve the efficiency and reliability of gasifiers by providing the long-desired capability of in situ monitoring of syngas composition, enhancing the operation of fuels.

Fundamental research involved in this project also provides a number of technical breakthroughs that may benefit the technical community:

1. Identification of a valid approach for developing gas sensors for applications in harsh environments by physical and functional integration of optical-fiber devices and gas-sensitive optical thin-film materials.
2. The successful development of robust, miniaturized fiber sensor platforms with proven feasibility for high-temperature gas sensing may be useful for sensing applications in other harsh environments.
3. The interdisciplinary approach utilized to functionally integrate nanomaterials with microdevices may prove to be exemplary of the techniques for harvesting the unique properties of nanomaterials (i.e., doped nanocrystalline ceramic materials) for practical sensing applications.

Primary Project Goal:

The primary goals of this multidisciplinary research program are to develop a novel sensor construct using doped nanocrystalline ceramic-coated optical-fiber sensors and to demonstrate the feasibility of in situ monitoring of syngas compositions at high temperatures (500°C) through laboratory testing.

Objectives:

The specific technical objectives of this project include the following:

- Identify single-phase or heterophase doped ceramic sensor materials with desirable chemical, structural, and optical properties for the detection of common syngas components including H_2, CO, CO_2, and H_2S.
- Synthesize nanocrystalline ceramic films and protective silicalite layers on structured optical fibers.
- Design and fabricate structured fiber devices for enhanced sensor performance (for H_2 and CO only).
- Test the developed sensors in simulated laboratory environments (for H_2 and CO only).

16: DE-FC26-03NT41873

Project Number DE-FC26-03NT41873	**Project Title** Development of Continuous Solvent Extraction Processes for Coal-Derived Carbon Products			
Contacts DOE/NETL Project Mgr.	**Name** John Stipanovich	**Organization** Fuels Division	**Email** stipanov@netl.doe.gov	
Principal Investigator	Elliot B. Kennel	West Virginia University	Elliot.Kennel@mail.wvu.edu	
Partners	GrafTech International Ltd., Parma OH, Peter Stansberry. Koppers Inc., Harmarville PA, Robert Wombles. Quantex Energy Inc, Gilbert Chalifoux.			
Stage of Development				
__ Fundamental	X Applied	__ Proof of Concept	__ Prototype Testing	__ Demonstration

Technical Background:

Coal is converted to value-added products through a mild direct-liquefaction process. A mild direct-liquefaction process is one in which thermal pyrolysis and depolymerization, rather than hydrogenation, are the predominant processes. Using this process, just enough hydrogen is added to create a liquefied coal, rather than a fully upgraded light crude, which is produced through conventional direct liquefaction. The resulting product is a thick slurry from which mineral matter and fixed carbon are removed via centrifugation to produce a heavy, synthetic (ash-free) crude.

This heavy crude can be processed to create value-added carbon products including needle coke, anode-grade coke, binder pitch, carbon foam, carbon fibers, and others. Batch operation is costly, causing continuous processes at lower temperature, pressure, and residence time to be sought.

The ash-containing residue is not a waste product, but rather can be blended with gasifier fuels (subbituminous coal, lignite, or fuel coke) and used to produce power or additional hydrogen. The goal is to have near-zero-waste products, as is the case for many petroleum refineries.

Hydrogen can be used to upgrade and purify (desulfurize) heavy feedstocks via conventional techniques. Hence, the desire to produce an enhanced yield of light products could be accommodated through the use of hydrogen generated via coal gasification and reforming, or through other means. The strategy in this project has been to emphasize the liquefaction process rather than the upgrading process, because the latter is well established in the petroleum refining and upgrading industry.

This project strongly synergizes DOE efforts to produce low-cost hydrogen by whatever means. The existence of plentiful hydrogen, as well as a mild liquefaction capability, provides a method to produce crude hydrocarbons using domestic feedstocks.

Relationship to Program:

This project will support important liquid fuels advances within the alternate hydrogen production pathway focus area of the Hydrogen and Clean Fuels

Program. It also complements FutureGen and other gasification systems by producing gasification feedstocks and utilizing hydrogen.

This project seeks to develop domestic supplies for commodity products supporting heavy industry. Specifically, binder pitch, anode coke, impregnation pitch, and other heavy hydrocarbon products support the metals smelting industry, including both Hall-Heroult electrochemical systems and arc furnaces for steel smelting. In addition, the heavy liquid hydrocarbons can be upgraded to produce a synthetic crude to replace imported petroleum crude. This process is better suited for heavy hydrocarbon products (e.g., pitches, cokes, and fuel oil) rather than light hydrocarbon products (e.g., methane, gasoline, and diesel).

Primary Project Goal:

The primary project goal is to demonstrate continuous processes for coproduction of synthetic heavy crude from coal, from which pitches, cokes, and other carbon products can then be produced via conventional refining technology.

Objectives:

Phase I

Task 1.0 Development of a Continuous Process

The purpose of this task is to convert the West Virginia University solvent extraction pilot plant from its existing batch system configuration to a continuous process configuration. The product will be a synthetic pitch (Synpitch) containing solvent-extracted hydrocarbons, using commodity solvents rather than specialty chemical solvents. Therefore, the overall cost of the final product can be lower than the cost of conventional coal tar pitch. The following steps are required for continuous production:

a. Adding a coal feeder and a liquid dispensing pump and ultrasonic mixer at the inlet of the continuous stirred tank reactor. Raw coal or mildly hydrogenated coal can be used as a solid feedstock.
b. Adding a wiped film evaporator at the final stage of the pilot plant to fractionate 1-Methyl-2-pyrrolidinone (NMP) or other excess solvents with low boiling points.
c. Adding a rotary kiln-type furnace for recovery and drying of the solid byproduct. Note that final drying is not required for Synpitch itself.

Finally, a combination of feedstocks, including solvents, should be selected such that the output from the system matches the desired final product (Synpitch) as closely as possible. The product will be recovered using liquid fractionation, which is easier than solid separation and drying.

Task 2.0 Carbon Product Manufacture

This task seeks to demonstrate the suitability of Synpitches for use in fabricating pitches and cokes for various uses.

Subtask 2.1. Production Definition

With the aid of subcontractors Koppers Industries and GrafTech Inc., specifications will be developed for the Synpitches produced by the solvent extraction process to make products that include the following:

a. Isotropic binder pitch (for graphite electrodes used in steelmaking furnaces)
b. Isotropic coke (for specialty or nuclear-grade graphite fabrication)
c. Anisotropic coke (for anodes used in aluminum production furnaces)
d. Highly anisotropic needle coke (for graphite electrodes used for steel production)
e. Spinnable pitches (for fiber production, both isotropic and anisotropic)
f. Pitch precursors (for carbon foams)

Specifications for Synpitch products will include required composition, impurity content, quinoline-insoluble content, toluene-insoluble content, melting point, molecular weight, aromatic content, etc. In turn, formulations will be developed for Synpitches that can meet those specifications. Hydrogen donor solvents and catalysts will be considered as the means to accomplish a mild hydrogenation of Synpitch with moderate temperature and pressure.

Binder pitch is the Synpitch product that is most likely to result in a significant market share in a large market. Specifically, this project will target binder pitch used for electrodes in steelmaking. Binder pitches can also be used for fabricating carbon composites and for other applications as well. West Virginia University has provided GrafTech Inc. with blends of Synpitch to be used as a binder pitch. GrafTech Inc. has fabricated electrode samples, which will be used for a standard suite of tests including density, compressive strength and modulus, electrical resistivity, coefficient of thermal expansion, air permeability, air reactivity, x-ray diffraction, ash content, and impurity content. These tests will be used as a means of evaluating the binder pitch. GrafTech Inc. will identify the most promising combinations in terms of cost and performance. These materials will be considered for a large-scale demonstration in Phase II of this effort.

Subtask 2.3 Foam and Fiber Synthesis

Low-cost Synpitches have been developed as precursors for carbon foams and carbon fibers. West Virginia University has previously shown that Synpitches produce isotropic fibers with increased strength. Improvements are also expected in anisotropic fibers and mesophase fibers produced from Synpitches. West Virginia University will spin pitch fibers and measure their strength, modulus, electrical resistivity (which can be used to infer thermal conductivity), and coefficient of thermal expansion.

Trials will be carried out for carbon foams as well. West Virginia University foaming protocols have resulted in a very high crush energy (joules/kg) as compared to conventional materials.

PHASE II

Task 3.0 Binder Pitch Demonstration in Production Electrodes

After electrode performance has been shown to be acceptable in Phase I Task 2, synthetic binder pitch will be fabricated and blended with Koppers binder pitch to be used in a trial production of electrodes at GrafTech Inc. Normally a trial of this magnitude would require about 15 tons of binder pitch. Thus, a blend containing 10% Synpitch requires 1.5 tons of Synpitch.

The graphite electrodes were used in the production of steel at a fully commercial plant. The performance of the electrodes will be noted and compared to state-of-the-art electrodes. Both the useful lifetime of the electrodes, as well as characteristics of the steel product will be evaluated according to standard acceptance testing protocols. Standard GrafTech Inc. methodologies for estimating costs will be used to determine the life-cycle costs of electrodes fabricated using Synpitch.

Task 4.0 Composite Synthesis

Synpitches will be developed to produce anisotropic coke, which will be used to produce anodes for use in the aluminum industry.

PHASE III

Task 5.0 Continuous Coke Production

Anisotropic coke has been extruded from relatively low hydrogen-content Synpitch. The Synpitch must have a high content of dissolved coal so that it does not form a low-viscosity liquid as it is heated through the devolatization stage. Synpitch-derived needle coke produced from this process will be supplied to GrafTech Inc. along with synthetic binder pitch developed in Task 3.0. Electrodes will be manufactured and evaluated as before.

Task 6.0 Novel Feedstocks

This task develops new feedstocks that result from processes such as hydrogenation, solvent extraction, liquefaction, and gasification. These processes do not require petroleum derivatives or coke-oven products. In addition, solvent extraction can be highly compatible with coproduction plants via gasification and/or liquefaction processes. Other commodity hydrocarbon liquids will be evaluated for their usefulness as coal solvents. Products fabricated in Phase I and Phase II will be repeated using these feedstocks. The ability of these processes to enhance power plant fuel cycles will be specifically evaluated.

17: DE-FC26-06NT42804

Project Number DE-FC26-06NT42804	**Project Title** Long-Term Environmental and Economic Impacts of Coal Liquefaction in China			
Contacts DOE/NETL Project Mgr.	**Name** John Stipanovich	**Organization** Fuels Division	**Email** stipanov@netl.doe.gov	
Principal Investigator	Jerald J. Fletcher	West Virginia University	jfletch@wvu.edu	
Partners	Richard Bajura, Director, National Research Center for Coal and Energy, West Virginia University (Co-Principal Investigator) Qingyun Sun, Research Assistant Professor and Associate Director, U.S.-China Energy Center, West Virginia University (Co-Principal Investigator) Timothy R. Carr, Dept. of Geology and Geography, West Virginia University Samuel J. Friedmann, Energy & Environmental Directorate, Lawrence Livermore National Laboratory NETL and Fossil Energy HQ staff, U.S. Department of Energy Xiangkun Ren, Vice President, China Shenhua Coal Liquefaction Co. Ltd.			
Stage of Development				
__ Fundamental R&D	__ Applied R&D	__ Proof of Concept	__ Prototype Testing	X Demonstration

Technical Background:

This project developed from a meeting on July 21, 2002 between Yuzhuo Zhang (then President of the China Shenhua Coal Liquefaction Company Ltd. [CSCLCL]) and 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 of 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 and presented a seminar on the current CSCLCL plans and the potential for future cooperation. During his visit, Dr. Zhang met with a variety of researchers and administrators from both WVU and NETL. Given the influence that NETL had on the development of many of the 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 WVU with initial support for collaborative activities with CSCLCL beginning September 1, 2003 through the Coal to Chemicals (CTC) support contract.

Discussions with Shenhua representatives continued. Based on mutual WVU and CSCLCL interests, a memorandum of understanding (MOU) was signed in December 2003 to promote joint research on the economic and environmental impacts of coal liquefaction in China and to 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 State of America and the Ministry of Science and Technology (MOST) of the People's Republic of China (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 the operation of such a facility could have on the region.

The project is very much in line with the Hydrogen and Clean Fuels Program 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 Development and Reform Commission (NDRC) of the People's Republic of China, which 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.

Relationship to Program:

This project will support important advances within the alternate hydrogen production pathway focus area of the Hydrogen and Clean Fuels Program by supporting joint research and development at the international level and optimizing fuel availability through direct coal liquefaction processes. Additionally, the process used in this project seeks to reduce carbon dioxide (CO_2) emissions while providing increased energy security through alternative fuels.

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 and the NDRC 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 related activities.

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.

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

The primary long-term benefits to China are related to potentially better environmental quality if the project identifies environmental issues that were not expected or not previously addressed. Successful implementation of a carbon storage project for the direct coal liquefaction (DCL) plant has implications for carbon management for clean coal projects not only in China, but throughout the world.

Primary Project Goal:

The primary project goal is to better understand the development and implementation of DCL and related clean coal technologies in the People's

Republic of China through joint research efforts with the China Shenhua Coal Liquefaction Co. Ltd.

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.

Within the context of this overall objective, there are three specific research efforts and a communication and collaboration activity. The first research effort is to describe and quantify the environmental impacts expected from the world's first commercial DCL plant now under development in Inner Mongolia. The second research effort is to describe and quantify the economic impacts that the DCL plant will have on the local region. The third research effort is to develop an understanding of the processes considered and selected for alternative clean coal utilization activities in China. The communication and collaboration activity will directly support DOE/Fossil Energy activities under Annex II of the US-China Fossil Energy Protocol. The third research effort supports the first two research efforts as well as communication and collaboration activities.

APPENDIX F: LIST OF ACRONYMS AND ABBREVIATIONS

Acronym/ Abbreviation	**Definition**
μm	micrometer
Å	angstrom
Ag	silver
AHP	Advanced Hydrogasification Process
Al_2O_3	aluminum oxide
APS	Arizona Public Service
Ar	argon
ARCH	Advanced Rapid Coal Hydrogasification
As	arsenic
ASME	American Society of Mechanical Engineers
Au	gold
Ba	barium
BCY	$BaCe_{0.8}Y_{0.2}O_{3-\delta}$
Be	beryllium
BPD	barrels per day
BSG	bench-scale gasifier
BSRx	bench -scale kinetics reactor
BTL	biomass to liquids
BTRD	Board on Research and Technology Development
Btu/scf	British thermal units per standard cubic feet cubic meter
Ca	calcium
CAER	Center for Applied Energy Research
CBTL	coal and biomass to liquids
CCC	Copyright Clearance Center
Cd	cadmium
CEM	continuous emissions monitors
cermet	ceramic-metal composite
CFB	circulating fluidized bed
CFD	computational fluid dynamics
CFFS	Consortium for Fossil Fuel Science
CH_4	methane

Acronym/ Abbreviation	**Definition**
Cl	chlorine
Co	cobalt
CO	carbon monoxide
CO_2	carbon dioxide
COS	carbonyl sulfide
CPCPC	Consortium for Premium Carbon Products from Coal
Cr	chromium
CRTD	Center for Research and Technology Development
CSCLCL	China Shenhua Coal Liquefaction Company Ltd
CSTR	continuous stirred tank reactor
CTC	Coal to Chemicals
CTL	coal-to-liquid
Cu	copper
DCL	direct coal liquefaction
DFT	density functional theory
DMF	dimethylfuran
DOE	U.S. Department of Energy
EF	entrained flow
EFR	entrained flow reactor
EMR	electron magnetic resonance
EPRI	Electric Power Research Institute
EXAFS	extended x-ray absorption fine structure
fcc	face-centric cubic
Fe	iron
FE	Office of Fossil Energy
Fe_2O_3	iron(III) oxide, ferric oxide
Fe_3O_4	magnetite
Fe_5C_2	iron carbide
FeCo alloy	ferrocobalt alloy
FEG	field emission gun
FeO	ferrous oxide, iron(II) oxide
F-T	Fischer-Tropsch
FTE	full-time equivalent

Acronym/ Abbreviation	**Definition**
FTIR	Fourier transform infrared
gal	gallon
GC	gas chromatograph
GC-MS	gas chromatography – mass spectrometry
GHG	greenhouse gas
gpm	gallons per minute
GTC	Gasification Technologies Council
GTI	Gas Technology Institute
GTL	gas-to-liquids
GW	gigawatt
H	hydrogen atom/element
H_2	hydrogen gas
H_2O	water
H_2S	hydrogen sulfide
HCCI	homogenous charge compression ignition
HCN	hydrogen cyanide
Hg	mercury
HHV	higher heating value
HICE	Hydrogen-fueled internal combustion engine
HRTEM	high-resolution transmission electron microscopy
HTF	horizontal thin film
HTM	hydrogen transport membrane
IC	internal combustion
ICP-AES	inductively coupled plasma atomic emission spectroscopy
ICP-MS	inductively coupled plasma mass spectrometry
ICRC	Integrated Concepts & Research Corporation
IFAC	International Federation of Automatic Control
IGCC	integrated gasification combined cycle
INL	Idaho National Laboratory
K	potassium
K&C	Knowledge & Community
KBR	Kellogg Brown & Root
keV	kiloelectronvolt

Acronym/ Abbreviation	**Definition**
kg	kilogram
kV	kilovolt
kW	kilowatt
kWh	kilowatt-hour
LEIS	low-energy ion-scattering spectroscopy
LPFG	long-period fiber grating
Mg	magnesium
MIT	Massachusetts Institute of Technology
mm	millimeter
MMscfd	million standard cubic feet per day
Mn	manganese
Mo	molybdenum
MOST	Ministry of Science and Technology
MOU	memorandum of understanding
MW	megawatt
MWh	Megawatt-hour
N	nitrogen
Na	sodium
NDRC	National Development and Reform Commission
NETL	National Energy Technology Laboratory
NEXAFS	near-edge x-ray absorption fine structure
NH_3	ammonia
Ni	nickel
nm	nanometer
NMP	1-Methyl-2-pyrrolidinone
NMR	nuclear magnetic resonance
NO_x	nitrogen oxides
O	oxygen atom/element
OCC	Office of Clean Coal
OMB	Office of Management and Budget
ORD	Office of Research and Development
OSAP	Office of Systems Analysis and Planning
OTM	oxygen transport membrane

Acronym/ Abbreviation	**Definition**
P	phosphorus
Pb	lead
PBE	Perdew, Burke, and Ernzerhof
Pd	palladium
Pd_4S	palladium sulfide
PI	principal investigator
ppb	parts per billion
ppm	parts per million
psi	pounds per square inch
psig	pounds per square inch gauge
PSU	Pennsylvania State University
Pt	platinum
R&D	research and development
RD&D	research, demonstration, and development
S	sulfur
Sb	antimony
SCF	supercritical fluid
SCNT	stacked-cone carbon nanotubes
SCW	supercritical water
SEM	scanning electron microscope
Si	silicon
SNG	substitute/synthetic natural gas
STEM	scanning transmission electron microscopy
STM	scanning tunneling microscopy
STP	standard temperature and pressure
syngas	coal-derived synthesis gas
TEM	transmission electron microscope
TMS	Technology & Management Services, Inc.
tpd	tons per day
UOP	Universal Oil Products
UV-vis	ultraviolet-visible
V	vanadium
vol%	volume percent

Acronym/ Abbreviation	**Definition**
VTF	vertical thin film
VWN	Vosko-Wilk-Nusair
WGS	water-gas shift
wt%	weight percent
WVU	West Virginia University
XAFS	x-ray absorption fine structure
XPS	x-ray photoelectron spectroscopy
XRD	x-ray diffraction
Y_2O_3	yttrium oxide
Zn	zinc
ZrO_2	zirconium dioxide