NETL - Penn State

University Coalition for Fossil Energy Research

www.energy.psu.edu/ucfer/

UCFER Request for Proposals

UCFER-RFP04-2018

RFP Release Date: December 12, 2018

Submission Deadline:
February 6, 2019 at 5:00 PM Eastern Time

A. Objectives of UCFER

More efficient and cleaner utilization of fossil resources and effective ways to mitigate emissions of carbon dioxide are critically important for sustainable development. As a result, the University Coalition for Fossil Energy Research (UCFER) was established at Penn State by the U.S. Department of Energy's National Technology Laboratory (NETL) through a nationwide open competition in 2015. The objectives of UCFER are to advance basic and applied energy research for more efficient and more environmentally friendly production and utilization of coal, natural gas, and oil including carbon (CO_2) management, and promote multidisciplinary collaboration among the member universities of the Coalition and DOE NETL. Its research will involve the following five core competency areas:

- Geological and Environmental Systems, consisting of research on geomaterials, fluid flow in geologic media, and geospatial and strategic field monitoring.
- Materials Engineering and Manufacturing, consisting of research on the design, development, and deployment of advanced functional and structural materials for use in extreme service environments.
- Energy Conversion Engineering, consisting of the evaluation, integration, control and performance modeling of processes and components for developing innovative energy conversion processes and transformational technologies.
- Systems Engineering and Analysis, consisting of analysis and design of advanced energy systems such as power plants, energy markets, and energy-environment interactions.
- Computational Science and Engineering, consisting of research involving high-performance computing and data analytics that enable the generation of information and insights through the integration of experimental data and engineering analyses.

B. Eligibility

Only researchers employed by member universities of the UCFER are eligible to submit proposals under this solicitation. The current sixteen member universities include the following founding members: Massachusetts Institute of Technology, Penn State, Princeton University, Texas A&M University, the University of Kentucky, the University of Southern California, The University of Tulsa, the University of Wyoming, and Virginia Polytechnic and State University; and the 2017 new members: Carnegie Mellon University, Louisiana State University, The Ohio State University, The University of North Dakota, University of Pittsburgh, The University of Utah, and West Virginia University.

Purchased services, consulting, or subcontracts to non-coalition members shall not be more than 2.5% of the UCFER requested funds. Subcontracts included in your proposal (third party agreements) to coalition members must not exceed 50% of the total requested UCFER funding. No foreign entities including universities may receive UCFER funding.

C. Collaboration Requirements

UCFER represents an innovative and novel approach to engage academic institutions for the purpose of collaboration with NETL R&D. Therefore, collaboration with NETL is mandatory for all UCFER research projects. NETL's research capabilities and expertise are specifically addressed in the attached Research Topic Areas (see Attachment A). Applicants are also encouraged to consider potential collaboration with industry. There should be no costs budgeted for collaboration efforts with NETL. **Any proposal failing to provide written statement of proposed collaboration with NETL will be considered non-responsive and not forwarded for review**.

D. Research Topic Areas

Proposals are being solicited from the UCFER members in the following research areas:

- **Carbon Storage**
- **Coal Beneficiation**
- **Crosscutting Research**
- **Fuel Cell Technology/Natural Gas Conversion to Hydrogen and Solid Carbon Products**

See Attachment A for a description of the research topic areas, objectives, and requirements covered under this solicitation. A description of the core competency areas is provided in Attachment B. Attachment C shows the relationship between a core competency area and research topic areas.

E. Funds Available for This Solicitation

The total amount available for awards under this solicitation is anticipated to be approximately $1,906,000. Estimated funding levels per research area are as follows:

- **Carbon Storage ($480,000)**
- **Coal Beneficiation ($800,000)**
- **Crosscutting ($240,000)**
- **Fuel Cell Technology/Natural Gas Conversion to Hydrogen and Solid Carbon Products ($386,000)**

F. Cost-Share Requirements

Cost-share requirements are based on Technology Readiness Levels (TRLs). TRL definitions are given in Attachment D. Researchers are encouraged to use these TRL definitions in order to evaluate the status of their given technology. "TRL start" is the applicant's evaluation of the technology at onset of the proposed project. "TRL end" would mean the projected end state TRL for their technology. Singular TRL values (no ranges) at both start and end state should be supplied.

There is no minimum cost share requirement for research activities at the basic/fundamental stage. Research at this stage can be classified in the following range of TRLs: 1-2. There is a minimum requirement of 20% cost share for research activities at the applied stage. Research at that stage can be classified in the following range of TRLs: 3-6. Cost share requirements for a proposed project are based on the TRL value at the start state.

When cost share is required, the proposal's cost share must be calculated as a percentage of the total project costs and not a percentage of the funds requested from the UCFER. Cost share, which may be in the form of cash or in-kind contributions, is acceptable as part of the match provided it meets the following criteria:

- Is verifiable, necessary, and reasonable for proper and efficient accomplishment of the project.
- Is incurred within the project performance period. Previously expended research, development, or exploration costs are unallowable.
- Is not included as cost share for any other federal project, is not paid with funds from the federal government, and is otherwise allowable in accordance with applicable federal cost principles and DOE regulations governing cost sharing.
- The value of patents and data contributed to the project is unallowable as cost sharing.

Proposed projects are encouraged to to show TRL advancement on the cover sheet of the proposal specified within a given research topic area. We realize that in some cases significant research findings and results may come from projects that start and end at the same TRL.

G. Subcontract Awards

Subcontracts will be issued from Penn State to the successful applicants through their universities. The duration of the subcontract will vary based on the description of the research topic area guidelines covered under this solicitation in Attachment A. Anticipated start dates of the subcontracts are 45-60 days after Penn State receives all NETL approvals. The start date will

depend on the timing of NETL's administrative review regarding project selection and approval of the Environmental Questionnaires.

If additional documentation/justification is required prior to issuance of a subcontract, a delay in submission could result in a delay in issuance of the subcontract.

H. Submission

The deadline for receipt of proposals is **5:00 p.m. Eastern Time on Wednesday, February 6, 2019**. Proposals received after the deadline will not be accepted. Proposals must be submitted electronically to the web portal: **www.energy.psu.edu/ucfer** to be considered for review and evaluation. Login information has been provided to each member university's Technical Advisory Council (TAC) and Core Competency Advisory Board (CCAB) representatives. Login information can also be obtained by emailing **ucfer-omt@ems.psu.edu**. Applicants are responsible for verifying successful transmission, prior to the application due date and time. Early submissions are encouraged.

As part of the on-line submission process, names and contact information including email for five (5) potential reviewers must be provided on the submittal page. The reviewers may be coalition or non-coalition members with expertise in the research area. Populating this field on the submission page is mandatory or the proposal cannot be submitted. Reviewers who are suggested may or may not be selected for reviewing the proposal; however, this provides the opportunity for broad coverage of expertise in reviewing the proposal. When considering potential reviewers, please make sure that they are neither current nor former collaborators; are neither current nor former associates including advisors, students, or post-doctoral scholars; and are not DOE employees. Also, PIs cannot have any employment arrangements with the reviewer within the last twelve months nor plans for present or future employment.

I. Proposal Format

All proposals must follow the following format. Each page of the proposal should be numbered at the bottom. The font type must be clear and legible, the font must be 12 point, line spacing must be 1.0, margins must be 1 inch (top, bottom, and sides), and the paper size must be 8.5 x 11 inches.

Sections of the Proposal

The proposal must contain the following sections in order. See Attachments E through G for proposal elements.

Checklist — See Attachment E
This is used to ensure that all elements of the proposal have been completed.

Cover Sheet — See Attachment F
Note that the proposal must be signed by an authorized/official university representative.

Table of Contents — One (1) page maximum

Executive Summary (Public Abstract) One (1) page maximum

Provide a one-page summary of the proposed research containing the title of the project and indicating the relevance to the specific research area in the solicitation. It should clearly state the problem, the objectives of the proposed research, idea or concept, the approach, anticipated benefits and impacts, and partner organization(s). This self-contained document should be suitable for use as public abstract. It should be informative to other persons working in the same or related fields and, insofar as possible, understandable to the lay reader. This document must not include any proprietary or sensitive business information as the Coalition and/or DOE may make it available to the public.

Project Description Five (5) page maximum

The main body of the proposal should outline the problem, the proposed approach, the objectives, and plan of work, including the broad design of activities to be undertaken. At a minimum the following should be discussed:

- Statement of the problem.
- Objectives and proposed approach.
- Statement of the work plan.
- Relation of the proposed work to comparable work reported or in progress, including accomplishments of antecedent UCFER projects, if applicable.
- Description of available facilities and major items of equipment available for the work.
- Reference citations: references should be relevant, numbered, cited in the text and listed at the end of the text. The list of numbered references does not count against the page limit.

Project Schedule One (1) page maximum

Include a plan establishing a schedule for accomplishing the work. The plan should include major milestones of the project in bar chart format and should cover the complete period of performance.

Anticipated Results and Impacts One (1) page maximum

Discuss the anticipated benefits and impacts of the research and, if applicable, the viability of the proposed research for commercialization. Describe how the project will advance the basic or applied fossil energy research. Identify any specific groups in the commercial sector that may use the projected results.

Description of the Collaborative Work with NETL Two (2) pages maximum

Under each research topic or subtopic, information is provided about such collaboration opportunities for UCFER researchers as the support NETL can provide, FTE levels of NETL scientists and engineers, and NETL facilities and usage time that will be made available to university coalition researchers.

Proposals are required to describe the nature of the proposed collaborative R&D work with NETL, how and where that work will be conducted, what (if any) NETL facilities, software and equipment will be used, how communications with NETL will be conducted, and the prospects of sustained collaboration in the future. The applicants may propose staff exchanges and sabbatical programs under appropriate arrangements. The applicants may also propose activities

involving jointly advised students, and other research collaborations. Any relevant prior collaboration with NETL shall also be discussed.

The costs for NETL employees (FTEs, etc.) and testing resources are not to be included in proposal budgets. There is no need nor is it encouraged to identify an NETL point of contact in your proposal. No discussion with NETL employees regarding this proposal development effort is needed. If your proposal is selected under the RFP, an NETL employee will be assigned at that time for you to contact.

Description of Equipment (Optional) Two (2) pages maximum

A description of the equipment to be used in the research project can be provided. This must not exceed two pages.

Budget (Refer to Attachment G, Template)

A reasonable budget is an important part of a good proposal. Your budget may request funds under any of the categories listed on Attachment G, as long as the item and amount are considered necessary to perform the work. It is expected that the participants will already have most of the necessary permanent equipment to conduct the research. The majority of the funding is to support research activities. Proposed equipment expenditures are permitted; but their purchase must be justified. Refer to 2 CFR 200.313 for federal regulations regarding equipment. Permanent equipment purchases are discouraged, but will be considered during the proposal evaluation.

Recipients of UCFER funding will be required to provide a presentation on the status of their project at one Annual Technical Review meeting for each year of the project duration. In addition, DOE/NETL strongly recommends that one DOE Program Specific Review meeting per project be attended. The costs for attending the UCFER annual meeting(s) and DOE Program Specific Review meeting are to be included in the travel budget.

Cost-Share Commitments

All cost-share commitments must meet the requirements set forth above and be supported by appropriate documentation. Third parties proposing to provide all or part of the required cost share must include a letter stating their commitment to provide a specific minimum dollar amount of cost-share. The letter should also identify the proposed cost share (e.g., cash, services) to be contributed. Letters must be signed by the person authorized to commit the expenditure of funds and be provided in PDF format. Failure to provide appropriate documentation can result in the proposal being returned without review.

Biographical Sketches Two (2) pages per person maximum

A curriculum vitae of key personnel involved in the project must be provided and should include educational background, professional experience, research interest, honors, professional activities, and ten relevant publications.

Collaborative Documentation

All collaborations with university partners within the UCFER, not included in the budget, should be described with a letter from each collaborator. At a minimum, the letter should describe the collaboration to be provided, resources to be provided, schedule, and budget information.

Other
Letters of support from outside sources are encouraged, but not mandatory. Page limits will be strictly enforced and extra pages will be removed prior to review.

J. Treatment of Proprietary Information

Privileged, confidential, or financial information that the applicant does not want disclosed to the public or used by the federal government for any purpose other than application evaluation, should be specifically identified by page and lines on the proposal cover sheet.

K. Proposal Evaluation/Review Process

All proposals will undergo a preliminary review to ensure that all proposal elements are addressed, and that any potential conflict of interest issues are identified. **Collaboration with NETL is mandatory. Any proposal failing to provide NETL collaboration will be considered non-responsive and not forwarded for review**.

All proposals determined to be responsive to the solicitation will be forwarded for review in accordance with the evaluation criteria set forth in the solicitation and the amount of funding available for the solicitation. It is anticipated that the UCFER Director will notify all applicants around June 2019, by letter, of the final decision regarding their proposals.

L. Evaluation Criteria (Refer to Attachment H)

The proposals will be evaluated per the following 100-point criteria:

- Merit of proposed collaboration with NETL—maximum of 20 points
- Meeting UCFER objectives—maximum of 10 points
- Idea and approach—maximum of 20 points
- Project achievability—maximum of 10 points
- Research impacts—maximum of 20 points
- Qualification of key personnel—maximum of 15 points
- Project management and budget—maximum of 5 points

The proposal evaluation forms are provided in Attachment H for reference. Evaluations will be performed on-line at a secure, members-only, website portal.

M. Environmental Questionnaire

All applicants must prepare Environmental Questionnaire on the NETL form F 451.1-1/3. The Environmental Questionnaire can be found online for downloading at the UCFER member website: www.energy.psu.edu/ucfer/memonly/index.html. The Environmental Questionnaire must be attached at the end of the proposal.

N. Foreign National Documentation

A foreign national is defined as any person who was born outside the jurisdiction of the United States, is a citizen of a foreign country, and has not been naturalized under U.S. law. If applicants propose work with foreign nationals as project team members, they will be required to provide the foreign national information upon selection for award. All successful applicants including foreign nationals as team members, will be required to complete the Foreign National Documentation before they can attend DOE meetings or visit DOE sites. Recipients of subawards under the UCFER will be required to complete Foreign National Documentation, if applicable, to facilitate UCFER responsibilities associated with foreign national access to DOE sites, information, technologies, equipment, programs, or personnel. Any UCFER member failing to comply with the Foreign National requirement will not be eligible to receive DOE funding. Information that will be required includes:

- Completed page 2 of Form 142-1-1A (which can found at www.energy.psu.edu/ucfer/memonly/index.html)
- Colored copy of passport
- Picture visa – from the passport book even if it is expired (color copy)
- LPR card – foreign national may have this instead of a visa (photocopy in color, both front and back)
- EAD card – foreign national may or may not have this (photocopy in color, both front and back of the card
- Other documents that allow foreign national to be in the states, such as I-20, DS-2019, etc.
- Resume (will need this if they are doing an assignment of more than 30 days)

O. Additional Information

Successful project recipients will be required to submit quarterly progress reports and a final technical report. Details on the reporting formats will be provided in the subcontract.

Frequently asked questions (FAQs) from previous solicitation cycles can be found in the 'Member Login' at: www.energy.psu.edu/ucfer/?q=memberonly/FAQs.html. Additional questions should be forwarded to the UCFER Director at ucfer-director@ems.psu.edu.

ATTACHMENT A – RESEARCH TOPIC AREAS

NATIONAL ENERGY TECHNOLOGY LABORATORY

UNIVERSITY COALITION FOR FOSSIL ENERGY RESEARCH (UCFER)



Round 4 Solicitation Research Topics

U.S. DEPARTMENT OF ENERGY | NATIONAL ENERGY TECHNOLOGY LABORATORY

Table 1. Available UCFER funds by Technology Line

NETL Technology Line	Available Research Funds
Carbon Storage	$480,000
Coal Beneficiation	$800,000
Crosscutting Research	$240,000
Fuel Cell Technology	$386,000
TOTAL (Round 4 Solicitation)	**$1,906,000**

Table 2. Overview of UCFER Topics/Subtopics and Award Information for Round 4 Solicitation

UCFER Research Topics by Technology Line	Anticipated Project Period (Months)	Maximum Award Size	Expected Number of Awards	Cost Share Requirement
[O] Carbon Storage				
Subtopic Area O-1: Developing Scale-Up Tools to Extend Laboratory Measurements to the Field	12-24	$240,000-$480,000	0 to 2	TRL 1-2: N/A TRL 3: 20% minimum
[P] Coal Beneficiation				
Subtopic Area P-1: Improved Coal Feedstocks for Power Production and Steel-Making	12	Approx. $300,000	0 to 2	TRL 1-2: N/A TRL 3: 20% minimum
Subtopic Area P-2: Producing High-Value Solid Products from Coal	12	Approx. $300,000	0 to 2	TRL 1-2: N/A TRL 3: 20% minimum
Subtopic Area P-3: American Coal Database	15	Approx. $400,000	0 to 1	TRL 1-2: N/A TRL 3: 20% minimum
Subtopic Area P-4: Coal Products Systems Engineering and Analysis	18	Approx. $300,000	0 to 1	TRL 1-2: N/A TRL 3: 20% minimum
[Q] Crosscutting Research				
Subtopic Area Q-1: Machine Learning for Microstructural Recognition and Reconstruction of Heat-Resistant Alloys	24	Approx. $240,000	0 to 1	TRL 1-2: N/A TRL 3-6: 20% minimum
[R] Fuel Cell Technology/Natural Gas Conversion to Hydrogen and Solid Carbon Products				
Subtopic Area R-1: Novel Reactors for the Co-Production of Hydrogen and Value-Added Solid Carbons	12	Approx. $193,000	0 to 2	TRL 1-2: N/A TRL 3-6: 20% minimum
Subtopic Area R-2: Advanced Catalysts and Catalyst Processing for Producing Hydrogen and Value-Added Solid Carbons	12	Approx. $193,000	0 to 2	TRL 1-2: N/A TRL 3-6: 20% minimum

Table 3. Applicable NETL Core Competencies for each Round 4 Solicitation Research Subtopic

UCFER Research Topics by Technology Line	Geological & Environmental Systems (GES)	Materials Engineering & Manufacturing (MEM)	Energy Conversion Engineering (ECE)	Systems Engineering & Analysis (SEA)	Computational Science & Engineering (CSE)
[O] Carbon Storage					
Subtopic Area O-1: Developing Scale-Up Tools to Extend Laboratory Measurements to the Field	X				
[P] Coal Beneficiation					
Subtopic Area P-1: Improved Coal Feedstocks for Power Production and Steel-Making		X			
Subtopic Area P-2: Producing High-Value Solid Products from Coal		X			
Subtopic Area P-3: American Coal Database					X
Subtopic Area P-4: Coal Products Systems Engineering and Analysis				X	
[Q] Crosscutting Research					
Subtopic Area Q-1: Machine Learning for Microstructural Recognition and Reconstruction of Heat-Resistant Alloys		X			X
[R] Fuel Cell Technology/Natural Gas Conversion to Hydrogen and Solid Carbon Products					
Subtopic Area R-1: Novel Reactors for the Co-Production of Hydrogen and Value-Added Solid Carbons		X			
Subtopic Area R-2: Advanced Catalysts and Catalyst Processing for Producing Hydrogen and Value-Added Solid Carbons		X			

O: CARBON STORAGE

The mission of the Carbon Storage Program at NETL is to develop technologies for commercial readiness by 2030 that ensure safe, secure, efficient, and cost-effective CO_2 injection and containment in storage complexes in diverse geologic settings.

The Carbon Storage Program is addressing significant overarching technical challenges to meet program goals that support the scale-up and widespread deployment of CCS.

These overarching technical challenges include:

- Uncertainty in prediction of plume location, pressure front extent, fluid stabilization, and subsurface integrity (i.e., induced seismicity).
- Inadequate detection/quantification of CO_2 to understand potential risks.
- Lack of understanding of how to optimize CO_2 storage capacity in reservoirs.
- Lack of experience in identifying and characterizing 50+ million metric ton (MMT)-scale storage sites onshore and offshore.
- Untested risk assessment, risk management, and mitigation strategies for 50+ MMT-scale storage sites.
- Lack of cost-effective approaches to permit and otherwise certify 50+ MMT-scale storage sites.

To address these challenges, a technical plan has been created to develop an innovative and integrated approach that tests and validates technologies in a field geo-laboratory setting. The result will be capabilities, which include integrated tools, techniques, and procedures for cost-effective monitoring, verification, and accounting of CO_2 within a storage complex, as well as quantitative capabilities for site- specific risk management. It will also include 50+ MMT-scale storage capacity assessments both onshore and offshore in multiple storage reservoir types (saline formations, oil and natural gas reservoirs, unmineable coal, organic-rich shale, and basalt formations).

Additional information can be found at:

1. National Energy Technology Laboratory, Carbon Storage Program Factsheet link: https://www.netl.doe.gov/File%20Library/Publications/factsheets/Program/program-116.pdf.
2. National Energy Technology Laboratory, Carbon Storage Program Website link: https://www.netl.doe.gov/research/coal/carbon-storage.

Subtopic Area O-1
Developing Scale-Up Tools to Extend Laboratory Measurements to the Field

A vast amount of information from laboratory core floods and field tests has been collected describing the mobility of fluids within reservoir rocks. To distill this raw data into a set of meaningful relationships appropriate for implementation at the reservoir scale, in-depth calculations are typically performed on individual results. The objective of this project is to develop tools, mechanisms, and theories intended to analyze data from experimental core floods to obtain meaningful reservoir properties, scale laboratory measurements to field measurements, and improve predictions of reservoir performance for storage reservoirs.

Collaboration Opportunities with NETL

Geological & Environmental Systems (GES) Core Competency: Up to 0.10 FTE of NETL labor will be available for assisting in integration of data collected through NETL experimentation into a machine learning framework, technique, or algorithm. If needed, lab personnel could assist in designing additional experiments, conducting laboratory tests, acquiring data from experiments, and interpreting data.

Raw data available includes: permeability, relative permeability curves, core composition (XRF), Youngs modulus, Poisson's ratio, bulk modulus, and shear modulus.

Award Information and Funding Amounts

Area of Interest O-1			
Anticipated Project Period	**Maximum Award Size**	**Expected Number of Awards**	**Cost Share Requirement**
12-24 Months	$240,000-$480,000	0 to 2 Awards	TRL 1-2: N/A TRL 3: 20% minimum

P: COAL BENEFICIATION

The Coal Beneficiation Program is focused on enhancing the value of coal as a feedstock and developing new high-value products from coal. Research in this program focuses on developing laboratory and pilot scale technologies for upgrading coal for use in traditional power and heat applications and as a manufacturing feedstock for high value carbon products such as carbon fiber, carbon nanomaterials, battery/electrode materials, carbon materials for 3-D printing applications, carbon-based construction materials, and carbon additives for manufacturing composites. Research in the coal beneficiation program also provides economic analysis of coal markets, technoeconomic studies of coal upgrading technologies, and life cycle studies to evaluate the environmental footprint of beneficiation technologies.

Technology Specific Goals and Priorities

The overarching goals of the program include:

- Improving the efficiency and reliability of power plants by using processing technologies to upgrade and beneficiate coal feedstocks to increase BTU values and remove unwanted impurities
- Creating new physical and chemical processing technologies that beneficiate coal for manufacturing high value carbon materials and products
- Evaluating market opportunities and entry barriers (technical and economic) by assessing how beneficiated coal can be utilized for export markets and as a manufacturing feedstock for high value carbon products

This program can only consider feedstocks that involve domestic coal and/or products derived from domestic coal (e.g. coal fines, coal pitch, coal liquids, char, beneficiated coal). This program cannot consider feedstocks derived from foreign sources.

This program will focus on the carbon components of domestic coal and/or products derived from domestic coal. This program will not consider projects focused on the mineral matter or rare earth elements in these feedstocks.

Challenges

Technical challenges include: 1) developing technologies that improve the quality of coal as a process feedstock (e.g., beneficiation by reducing moisture, increasing heating value, removing contaminants for coal exports and improving domestic power plant performance) 2) developing chemical/physical processes to manufacture nanocarbons for use in both additive and traditional materials manufacturing, 3) evaluating the performance enhancements imparted to materials by the use of coal-based carbon additives and making comparisons with traditional additives, and 4) developing engineering analyses and cost models to characterize which domestic coal reserves are suited for manufacturing applications, the scalability of these manufacturing processes, and how the global markets for coal-based materials will evolve over a five to fifteen-year timeline.

Subtopic Area P-1
Improved Coal Feedstocks for Power Production and Steel-Making

The subtopic on improved coal feedstocks for power production and steel-making focuses on processing coal to improve its BTU value, remove unwanted impurities, modify coal particle size, and adjust the moisture content of coal.

The development of cost-competitive technologies for improving the quality of U.S. coal will increase the marketability of U.S. coal for both domestic and international markets. Research in this area will provide a pathway for commercialization of new or existing coal beneficiation plants that can provide higher value coals for power plants and/or steel making facilities which will improve the operating efficiency of these facilities.

R&D is required on technologies to produce an upgraded coal fuel from run-of-mine coal. R&D to economically upgrade steam coal to metallurgical coal is applicable to this area of interest. While multiple product streams from a coal beneficiation process are desirable, the upgraded solid carbon feedstock must be the primary product from the technology or process. In addition to the primary upgraded solid feedstock, the R&D can also produce (but is not required to) other marketable coal-based byproducts (solid, liquid, or gaseous). These technologies will create cost-competitive, upgraded coal feedstocks for power plants and steel making that increase the value of existing coal assets. Benefits could include lower emissions, improved reliability, reduced capital and operating cost and improved plant efficiency. Potential technology development areas include, but are not limited to, coal dewatering, fine coal cleaning, dry-cleaning processes to upgrade lower-rank coal, chemical treatment and biological processing technologies.

This topic can only consider feedstocks that involve domestic coal and/or products derived from domestic coal (e.g. coal fines, coal pitch, coal liquids, char, beneficiated coal, etc.). This program cannot consider feedstocks derived from foreign sources.

This topic will focus on the carbon components of domestic coal and/or products derived from domestic coal. This program will not consider projects focused on the mineral matter or rare earth elements in these feedstocks.

Collaboration Opportunities with NETL

Materials Engineering & Manufacturing (MEM) Core Competency: Applicants will collaborate with NETL research teams to achieve the research objectives noted above. NETL laboratories and equipment pertinent to research under this topic will be made available for up to 20 working days during the first year. Up to 0.050 FTE of NETL labor could be available for designing the experiments, conducting laboratory tests, modeling reactions, and interpreting data for each project selected.

Award Information and Funding Amounts

Area of Interest P-1			
Anticipated Project Period	**Maximum Award Size**	**Expected Number of Awards**	**Cost Share Requirement**
12 Months	Approx. $300,000	0 to 2 Awards	TRL 1-2: N/A TRL 3: 20% minimum

References

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8. He, X., Zhang, X., Jiao, Y., Zhu, J., Chen, X., Li, C., & Li, H., "Complementary analyses of infrared transmission and diffuse reflection spectra of macerals in low-rank coal and application in triboelectrostatic enrichment of active maceral." *Fuel*, vol. 192, 2017, pp. 93-101. https://www.sciencedirect.com/science/article/pii/S0016236116312303
9. Dyrkacz, G.R., & Bloomquist, C.A.A., "THE EFFICIENT, LARGE SCALE SEPARATION OF COAL MACERALS." Argonne National Laboratory, ACS Energy and Fuels Division, ACS Fuels Volume 33 (3), 1988, pp. 128-135. https://web.anl.gov/PCS/acsfuel/preprint%20archive/Files/33_3_LOS%20ANGELES_09-88_0128.pdf

Subtopic Area P-2
Producing High-Value Solid Products from Coal

This subtopic area focuses on the development of cost competitive technologies for producing solid, high value, carbon products from coal such as carbon fiber, carbon nanomaterials, carbon foams, carbon composites, 3-D printing materials, and/or other solid carbon-based materials that can be used in the production of high-value products to improve the value of U.S. coal and to supplement traditional markets for U.S. coals. The market value of these materials often exceeds the fuel and heat value of coal, which illustrates there are sustainable market forces for manufacturing carbon materials from coal. The results of R&D in this area will provide a pathway for commercialization of new or existing coal beneficiation plants to improve the value chain for coal production.

Proposals are sought that focus on using domestic coal and/or closely related by-products (coal fines, coal pitch, coal char, etc.) as a manufacturing feedstock to produce solid carbon materials and composites. Utilizing coal for producing carbon materials creates new business opportunities by integrating coal into the value-chain of industries that typically do not use coal in their manufacturing processes. Coal-based carbon fiber and carbon fiber-reinforced polymers offer opportunities for producing new forms of lightweight structural materials and composites which have utility in automotive and aerospace applications. Coal-based carbon nanomaterials, such as graphene and carbon quantum dots, offer opportunities to bring down the costs of these materials so they can be used in electronic display screens, pigments/dyes/coatings, enhanced textiles, and structural composites. Inexpensive carbon nanomaterials can also be used in 3-D printing fluids/plastics to enhance the electrical/thermal/optical properties of the final printed material. Coal-based coke, pitch, and carbon nanomaterials can be used to produce electrode materials for a range of applications such as aluminum production, batteries/energy storage, and supercapacitors.

R&D in this area must focus primarily on technologies to produce solid products from coal. The production of liquid precursors that are used to manufacture solid materials will be considered if the research directly illustrates conversion to the solid product (e.g. the production of coal-based monomers with polymerization to a final, characterized, material demonstrated). Projects that focus primarily on the production of gases or liquids will not be considered in this subtopic area. Potential technology focus areas include but are not limited to carbon fibers, carbon nanomaterials, structural materials and composites, and materials for additive manufacturing.

This topic can only consider feedstocks that involve domestic coal and/or products derived from domestic coal (e.g. coal fines, coal pitch, coal liquids, char, beneficiated coal, etc.). This program cannot consider feedstocks derived from foreign sources.

This topic will focus on the carbon components of domestic coal and/or products derived from domestic coal. This program will not consider projects focused on the mineral matter or rare earth elements in these feedstocks.

This topic will give preference to any entity that can demonstrably optimize feedstock and experimental conditions to produce value-added materials like pitch with a capacity of at least 10 gal/batch. Ideally, the laboratory reactor system should include slurry preparation equipment, a reactor system for the coal extraction process, product solids removal and distillation equipment, scrubbing equipment, and required piping and heat exchangers. Such a system can be integrated with the required analytical facilities to produce a small-scale plant and data acquisition system.

Collaboration Opportunities with NETL

Materials Engineering & Manufacturing (MEM) Core Competency: Applicants will collaborate with NETL research teams to achieve the research objectives noted above. NETL laboratories and equipment pertinent to research under this topic will be made available for up to 20 working days during the first year. Up to 0.050 FTE of NETL labor could be available for designing the experiments, conducting laboratory tests, modeling reactions, and interpreting data for each project selected. NETL efforts in this area involve the synthesis of carbon nanomaterials from coal, producing these materials at kilogram scales (or larger), incorporating these materials into composites, and characterizing these composites. NETL laboratories contain specialized synthesis equipment and physical processing equipment (homogenizers, microwave processing, thermal processing, high sheer mixers) for producing 5-10 L batches of graphene fluids, graphene powders, and other related carbon nanomaterials for manufacturing applications.

Award Information and Funding Amounts

Area of Interest P-2			
Anticipated Project Period	**Maximum Award Size**	**Expected Number of Awards**	**Cost Share Requirement**
12 Months	Approx. $300,000	0 to 2 Awards	TRL 1-2: N/A TRL 3: 20% minimum

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Subtopic Area P-3
American Coal Database

Historically, coal has been used in two ways: combustion for power generation and making coke for iron and steel production. Accordingly, coal characterization analyses were performed mainly with these two uses in mind. Many U.S. coals have been collected, preserved in sample banks, characterized, and the data archived. Two examples include the Department of Energy Coal Samples (DECS) bank[1] and the Argonne Premium Coal Sample Bank[2,3], both maintained and curated at the Pennsylvania State University. The sample banks have developed databases of the coal analysis results, which typically include:

- Calorific value[4,5,6] and equilibrium moisture
- Proximate analysis (moisture, volatile matter, fixed carbon, ash)[4,5,6,7]
- Ultimate analysis (carbon, hydrogen, nitrogen, sulfur, and oxygen; first four elements are determined, oxygen is by difference)[6,8]
- Maceral analysis (vitrinite, inertinite, liptinite)[9,10,11]
- Sulfur forms (pyritic S, organic S, sulfate)[12,13,14]
- Mean maximum vitrinite reflectance (VRo)[15,16]
- Ash fusion determination[17]
- Major inorganic and trace elements[18,19]
- Free swelling index[20]
- Hardgrove grindability (HGI)[21]

Other analyses that may have been performed include Gieseler plastometry[22], nuclear magnetic resonance (NMR) analysis[23,24], pyrolysis product analysis[25], and rare earth elements determination[26]. They also often include details on sample history, location, geology, and seam strata information.
These analyses were performed because they were important for discerning the best candidates for combustion or coke making. For example:

- Calorific value is a direct indicator of the energy content of the coal as a fuel.

- In coal-fired boilers, carbon burnout is inversely correlated with the fixed carbon/volatile matter (FC/VM) ratio both of which are reported in the proximate analysis. Also, coals high in inertinite can take longer to burn out than other coals, which is why maceral analysis is important.
- Maceral composition, pyrolysis behavior, and the volatile matter (VM) content will affect the flame stability.
- The ash content and the ash fusion point are indicators of a coal's potential to cause slagging and fouling problems. Another important parameter is the major inorganic elements in the ash, specifically the base-acid ratio (B/A) of the coal ash, which is the ratio of the iron, calcium, magnesium, potassium and sodium oxides to the silicon, aluminum and titanium oxides. Generally, higher B/A ratios indicate that more problems will occur.
- B/A ratio, vitrinite reflectance, and Gieseler plastometry are used to estimate the coke strength and coke reactivity, which are important in steel making processes.
- The Hardgrove Grindability Index (HGI) will indicate how much energy is required to grind the coal.
- The S, N, and VM content (and more recently the trace element content) of the coal are indicators of pollutant emissions.

These tests were developed from decades of testing and experience by combustion engineers and metallurgists, who formed correlations and equations for predicting U.S. coals' behavior in combustion and coke making situations.

Since the establishment of the existing coal sample banks and databases, new analysis techniques have been developed or improved. Some examples include:

- Small angle X-ray scattering for measuring porosity[27]
- Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometry (MS)[28]
- New automated imaging techniques[29] and Advanced Atomic Force Microscopy[30]
- ^{13}C NMR analysis[31]
- Nano IR analysis[32]
- Nano Raman spectral analysis[33]
- In-situ high resolution Scanning Transmission Electron Microscopy (STEM)[34]
- Neutron Spectral Imaging[35]

The utility of these new techniques as predictive tools has yet to be determined; however, as with past techniques, a substantial number of samples need to be analyzed before new correlations can be developed. Some of these techniques have already been used to analyze some coals and the results were reported in the literature but were not added to the databases. Therefore, before performing additional analyses on the coal samples, a survey of the literature should be made to gather existing data from the literature to avoid duplication of efforts. In addition to published literature, there are a variety of other data sources that must be considered, including reactivity data developed by the U.S. Bureau of Mines, and coal data archived by the United States Geological Survey.[36]

More recently, coal is being investigated as a potential feedstock for high-value products, such as carbon nanomaterials, carbon fibers, electrodes, carbon filler materials, and graphene oxide inks for 3-D printing, among others. Many of these high-value products are still in the early development phase and the optimum feedstock coal (and coal characteristics) probably have not yet been identified. To fulfill a wide range of coal data needs, coal databases can be expanded to include analyses results that become available using new characterization techniques.

Finally, computational modeling of coal and coal reactions has grown substantially in the past decade. High-speed computing has gotten to the point that highly complex systems using many variables are being modeled, and modelers are in need of more experimental data than ever before. Some examples of data that may be obtained from existing databases or new characterization techniques and useful for modeling efforts could include:

- Coal char characteristics
- By-product characteristics
- Char oxidation kinetics
- In-situ characterization of coal transformation during heating
- Pyrolysis reactions at various heating rates

This research is to revisit the existing databases so that coal suppliers and users can estimate the impact of coal properties and composition on the performance (e.g. efficiency and reliability) and emissions of power generation facilities. Also, the database may be expanded to satisfy the coal data needs for the present and future coal researchers and consumers of other high-value potential products that can be made from coal.

Objective

NETL is seeking to build a new database of U.S. coals by 1) assessing the data needs of today's coal industry and researchers 2) identifying the data from existing databases and literature sources 3) designing a user-friendly, machine readable, and easily accessible data repository, 4) constructing, populating, and verifying the new database, and 5) documenting the database and assessing next steps and future work.

Description of R&D

Applications are sought to develop a new, readily accessible, machine readable, and easy to use database of U.S. coal information as outlined in the objective above. Applications should address the following set of specific tasks necessary to complete the project, as well as identifying collaboration with NETL, and providing for a stakeholder advisory panel.

1. Workshops to establish data needs and database structure. The application should address the need to run a workshop (or workshops) to determine the user requirements for coal data as well as database accessibility and interaction. The workshop will convene experts from national laboratories, universities, research institutions and industry to discuss coal information needs to support current (e.g., power plants) and potential new (e.g., carbon nanomaterials, carbon fibers, and electrodes) markets that use U.S. coal. This stakeholder input will provide the basis for the design and content of the American Coal Database.

2. Identification of existing data sources. Efforts will include identifying the existing data sets of U.S. coal characteristics, including (but not limited to) those identified in the background section, such that available data can be curated and included in the new database. Researchers need to contact the curators of the existing databases to establish their willingness to participate, to identify the software platform, the data format, and other information identified in the workshop(s). Researchers will also identify literature sources that contain coal analyses that are not currently included in the data sets.

Many of the coals in the current databases came from mines that are now closed. Thus, data for those coals may not be useful to potential users. Proposed work should identify and flag in the database which coals are commercially available. The database should also include seam, longitude, latitude, depth and strata information that may be available for all coal samples for data mining purposes.

3. Design the database. Having collected needs from the users of coal data and identified data sources, the new database will be designed so that it can be easily and freely used by the research community and the industry. The database must be accessible for a variety of uses, including (but not limited to) support queries over the web; provide data to computational chemistry, computational fluid dynamics, and process simulation codes and to software such as Excel and Matlab; and provide interfaces to programming languages such as C/C++, Python, R, and Java. The design must be such that the database can be easily expanded by users after the conclusion of this project. The design will include the form of the data to be generated, including units, significant figures, detection limits, uncertainty, reproducibility, data provenance, and other pertinent information. The platform, format, interfaces, and database management plan must be approved by NETL before the database is developed.

4. Database construction and verification. The database will be built according to the developed design, the identified data sources will be curated, and the database populated. The database, the data therein, and the user interfaces should be rigorously verified using industry standard verification protocols.

5. Reporting. The project should culminate in a final report that includes a detailed description of the database and an evaluation of next steps and future work. As part of the final report, researchers will determine analyses and characterizations that would be needed to fill any data gaps, using both established and emerging techniques. Using the results of coal data and analysis needs from coal users, coal modelers, and coal export markets, researchers will:

- Identify the next logical steps in the comprehensive coal database development;
- Determine new analyses that will need to be performed on the existing coal samples;
- Determine if any new coals should be sampled for addition to the database.

Collaboration Opportunities with NETL

Computational Science & Engineering (CSE) Core Competency: NETL researchers have experience with the usage of computational chemistry, computational fluid dynamic (CFD) and process simulation software. NETL's C3M is a chemistry management software (https://mfix.netl.doe.gov/c3m/) provides direct links between reliable sources of kinetic information (kinetic modeling software, databases, and literature) and commonly used CFD software. Support from NETL researchers equivalent to 0.30 FTEs can be expected to collaborate on the research and support the database development effort, particularly in reviewing the database design and developing an interface to C3M.

Award Information and Funding Amounts

Area of Interest P-3			
Anticipated Project Period	**Maximum Award Size**	**Expected Number of Awards**	**Cost Share Requirement**
15 Months	Approx. $400,000	0 to 1 Award	TRL 1-2: N/A TRL 3: 20% minimum

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Subtopic Area P-4
Coal Products Systems Engineering and Analysis

Development of innovative technologies and processes to produce upgraded coal, as well as high value carbon products from coal is an emerging technology area that will enable improvements to existing markets as well as creation of new products and markets. There is currently not a clear understanding of the resource availability, cost targets or level of cost competitiveness to enter the market to provide the same type of service or function to society.

Objective

The objective of this research area is to identify the processes for transforming coal into upgraded coal and high-value carbon products and to prepare preliminary technoeconomic analyses (TEAs) on these processes to show economic potential.

The information will be used to help determine an economic competitive range needed for emerging technologies to enter the market and establish initial research and development targets or boundaries for early TRL technologies. Systems engineering, and analysis efforts provide critical information to inform decision makers. In addition, a potential benefit of this effort is that increases to domestic coal production and the development of a domestic coal-based carbon product manufacturing industry can provide additional economic benefits, such as jobs, income and tax revenue.

Proposals are sought that prepare preliminary TEAs for processes that can transform a domestic coal into an upgraded coal and/or high-value carbon products and directly address the following questions:

1. What is the current cost of competing production of these processes/products?
2. What is the current cost of production of these processes/products?
3. What are the yields of the product(s)?
4. What are cost targets for these processes/products needed to penetrate the market?
5. What are the advantages/disadvantages of the quality of the end-products using the identified processes as opposed to the current processes/feedstock(s) used in the market today?

Collaboration Opportunities with NETL

Systems Engineering & Analysis (SEA) Core Competency: Applicants will collaborate with NETL to achieve the objectives noted above. Support from NETL researchers equivalent to 0.05 FTEs can be expected provide quantitative and/or statistical analysis of data.

Award Information and Funding Amounts

Area of Interest P-4			
Anticipated Project Period	**Maximum Award Size**	**Expected Number of Awards**	**Cost Share Requirement**
18 Months	Approx. $300,000	0 to 1 Awards	TRL 1-2: N/A TRL 3: 20% minimum

Q: CROSSCUTTING RESEARCH

The Crosscutting Program has a unique ability to identify needs and foster technology development across many applications. The main research topics are Sensors and Controls, High Performance Materials, Simulation-Based Engineering, and Water Management. Research focuses on development of innovative technology, including testing and validation in real-world environments, before it is matured into a more integrated product in other fossil programs.

This topic will be funded by the Simulation-Based Engineering program; therefore, the focus is on computational, modeling, and simulation-based approaches to the research objective–in this case the computational simulation of the microstructure of heat-resistant alloys.

Subtopic Area Q-1
Machine Learning for Microstructural Recognition and Reconstruction of Heat-Resistant Alloys

Affordable, durable, cost effective, heat-resistant alloys necessary for improving the existing fleet of Fossil Energy (FE) power plants, and enabling advanced FE systems, such as advanced ultra-supercritical (A-USC) Rankine cycles, supercritical carbon dioxide (sCO_2) power cycles, etc. Accelerating the development of improved steels, superalloys, and other advanced alloys is of paramount importance in deploying materials solutions to meet the challenges with fossil energy power generation. Data analytics when combined with machine learning and computer vision research provide a powerful method for analyzing disparate information to facilitate alloy development, optimize manufacturing processes and maximize component specific performance. The performance of a component in any energy system is governed by the underlying microstructure and its resistance to change over time. The microstructures of heat-resistant alloys are very complex in nature (e.g., multi-phase, multi-length scale microstructures that evolve continuously with service). The overall aim of this research is to combine data analytics, machine learning, and vision recognition to optimize manufacturing-microstructure-performance in fossil energy systems.

Technology Specific Goals and Priorities

Over the years much information on the mechanical behavior of heat resistant materials has been generated at universities, national laboratories, and industry. Much of this data is only available in abbreviated form for supporting a specific technical point. Recently, it has become apparent that to make significant gains in alloy development, life assessment, and other areas of materials performance, data collection with associated metadata, data organization, and data analysis is needed for broad classes of materials. In pursuing these tasks, it became clear that while much mechanical property information is available, microstructure information is not. The materials used to generate the mechanical properties has also been lost over time, so a better way is needed to develop microstructure information based on metadata available for the alloys within the database. While some information can be developed for current alloys, other microstructure information will have to be constructed computationally based on observation and analysis of current alloys. With the technologies available today it becomes efficient to challenge the problem using a multi-faceted approach: (1 experimental information, derived (chemistry specific) synthetic data, targeted experimentation to fill gaps and explore trends combined with (2 data analytics, machine learning and computer vision research.

Challenges and Objectives

One major challenge will be developing in a systematic manner synthetic phase information and physical constants based on chemistry and proposed operating envelope. From this effort and using other historical data, the second challenge will be constructing a technically accurate representation of material microstructures and key microstructural features from chemistry information, processing information, mechanical data and other associated information that is available for these alloys. From these efforts the third challenge is to develop a methodology whereby data analytics, machine learning and computer vision research can yield representative and technically accurate microstructure information for materials classes at any stage of operation with line of sight relationship with mechanical behavior and other associated alloy class metadata.

Collaboration Opportunities with NETL

Materials Engineering and Manufacturing (MEM) and Computational Science and Engineering (CSE) Core Competencies: Applicants will collaborate with NETL research staff identifying the best route for developing the microstructure datasets and incorporating the datasets into the larger NETL heat resistant alloy database. The data and material (heat-resistant alloy) samples under development may be provided by NETL.

Award Information and Funding Amounts

Area of Interest Q-1			
Anticipated Project Period	**Maximum Award Size**	**Expected Number of Awards**	**Cost Share Requirement**
24 Months	Approx. $240,000	0 to 1 Award	TRL 1-2: N/A TRL 3-6: 20% minimum

References

1. DOE Fossil Energy Crosscutting Research Program Website: https://www.netl.doe.gov/research/coal/crosscutting
2. Aritra Chowdhury, Elizabeth Kautz, Bülent Yener, Daniel Lewis, "Image driven machine learning methods for microstructure recognition" Computational Materials Science, Vol. 123, Oct. 2016, p. 176-187.
3. Brian Decost, Elizabeth Holm, "A computer vision approach for automated analysis and classification of microstructural image data" Computational Materials Science, Vol. 110, Dec. 2015, p. 126-133.
4. Jessica Gola, Dominik Britz, Thorsten Staudt, Marc Winter, Andreas Simon Schneider, Marc Ludovici, Frank Mücklich, "Advanced microstructure classification by data mining methods" Computational Materials Science, Vol 148, June 2018, p. 324-335.

R: FUEL CELL TECHNOLOGY/NATURAL GAS CONVERSION TO HYDROGEN AND SOLID CARBON PRODUCTS

Natural gas can be decomposed to manufacture hydrogen and solid carbon products without producing CO_2. The co-production of hydrogen and carbon products has been shown to improve the overall economics of manufacturing hydrogen for large scale deployment. The co-production of hydrogen and high-value solid carbon materials from natural gas offers opportunities to reduce the costs associated with large-scale hydrogen energy product; create market demand, technologies, and infrastructure to enable hydrogen energy deployment; and utilize domestic natural gas for manufacturing energy and synthetic carbon products.

The Fuel Cell Technology/Natural Gas Conversion to Hydrogen and Solid Carbon Products program aims to develop and enable the deployment of transformational technologies that reduce the cost of hydrogen production and distribution, diversify the feedstock available for economic hydrogen production, enhance the flexibility of the power grid, reduce emissions through novel uses of low-cost hydrogen, generate jobs, and provide global technology leadership for export of next-generation energy solutions. Desired outcomes include: developing a leadership role in the U.S. for hydrogen technologies; using stranded domestic energy resources, such as stranded natural gas reserves for production of hydrogen and novel materials based on solid carbon; diversifying the feedstock utilized for hydrogen production, freeing domestic resources for other applications; and creating novel materials based on solid carbon via processes that generate hydrogen as a co-product.

Currently about 10 million metric tons of hydrogen are produced in the U.S. annually, predominantly through Steam Methane Reforming (SMR) process, which emits approximately 10 kg of CO_2 per kg of produced H_2. In order for natural gas decomposition to compete with this incumbent technology at the same hydrogen production scale, the market should be able to absorb co-produced solid carbon at a scale of tens of millions of metric tons per year. New forms of solid carbon materials that can find applications in high-volume construction and structural materials and be able to compete with present day materials need to be developed.

This program area can only consider projects that utilize natural gas, simulated natural gas, or components of natural gas (e.g. natural gas liquids) to make hydrogen and solid carbon products. Other feedstocks cannot be considered. Other product streams besides solid carbon and hydrogen cannot be considered.

Subtopic Area R-1
Novel Reactors for the Co-Production of Hydrogen and Value-Added Solid Carbons

The thermal decomposition of natural gas is endothermic and requires temperatures of ~1200°C to obtain useful product yields. Catalysts can be used to reduce these process temperatures, but they introduce technical challenges and costs with respect to separating the hydrogen, carbon, and catalyst/support. While traditional thermal reactors, both with and without catalysts, can be used for natural gas decomposition, opportunities exist to develop new reactor and process technologies to

decompose natural gas while maintaining a carbon neutral footprint. New reactor systems and designs can also take advantage of process intensification by combining the reactor and separation units, which can open opportunities for reducing system costs and producing portable, modular, reactor systems.

A range of non-traditional reactor systems have been developed that have properties useful for natural gas decomposition. Concentrated solar power and solar thermal reactors can be utilized to directly heat natural gas feedstocks and initiate decomposition. Catalysts can be utilized in solar reactors to reduce process temperatures, which in turn reduces temperature specifications on the materials used to fabricate the reactors. Plasma- and microwave-based reactors offer opportunities to utilize unique physical processes to drive reactions, such as direct vibrational and electronic excitation of reactants or selective heating of catalyst materials. Molten metal baths and other electrochemical processes also offer unique opportunities for methane decomposition. Catalytic membrane reactors and process intensification approaches show promise for producing an impurity-free stream of hydrogen in systems with smaller physical footprints. Additional research opportunities exist for developing reactor systems that can directly facilitate the separation of carbon products from the catalysts and supports.

Objectives

Research in this subtopic area should focus on the development of unique reactor systems that can decompose natural gas to form hydrogen and solid carbon products while maintaining a CO_2 neutral footprint. Standard catalysts can be incorporated into the reactor/chemical process but the primary objective of work in this subtopic should be the development of novel reactors and their integration into chemical processes. Both hydrogen and solid carbon should be considered as valuable products and means for recovering both of these products should be demonstrated. Specialized research on catalyst development will be considered in **Subtopic Area R-2: Advanced Catalysts and Catalyst Processing for Producing Hydrogen and Value-Added Solid Carbons.**

Research in sub-topic R-1 must focus on how reactors can be used to improve hydrogen and solid carbon production by evaluating:

1) How to optimize reactor design and process conditions for hydrogen production and to also tune the range of low-cost solid carbon products that are made
2) How the reactor/process improves hydrogen/solid carbon production beyond current commercial processes
3) How natural gas composition and impurities impact solid carbon and hydrogen production
4) Methods for recovering the solid carbon and hydrogen from the reactor/process.
5) Analysis of the energy, mass, and solid carbon footprints for the reactor/process.

This subtopic area can only consider projects that utilize natural gas, simulated natural gas, or components of natural gas (e.g., natural gas liquids) to make hydrogen and solid carbon products. Other feedstocks cannot be considered. Other product streams besides solid carbon and hydrogen cannot be considered.

Collaboration Opportunities with NETL

Materials Engineering & Manufacturing (MEM) Core Competency: Applicants will collaborate with NETL research teams to achieve the research objectives noted above. NETL laboratories and equipment pertinent to research under this topic will be made available for up to 20 working days during the first year. Up to 0.050 FTE of NETL labor could be available for designing the experiments, conducting laboratory tests, modeling reactions, and interpreting data for each project selected.

Award Information and Funding Amounts

Area of Interest R-1			
Anticipated Project Period	**Maximum Award Size**	**Expected Number of Awards**	**Cost Share Requirement**
12 Months	Approx. $193,000	0 to 2 Awards	TRL 1-2: N/A TRL 3-6: 20% minimum

References

1. Dagle et. al. U.S. Dept of Energy Report "R&D Opportunities for Development of Natural Gas Conversion Technologies for Co-Production of Hydrogen and Value-Added Solid Carbon Products" ANL-17/11 | PNNL-26726 (2017).
2. Muradov, "Low to near zero CO_2 production of hydrogen from fossil fuels: Status and perspectives", International Journal of Hydrogen Energy 42 (2017) 14508-14088.
3. Abbas et. al. "Hydrogen production by methane decomposition: a review", International Journal of Hydrogen Energy 35 (2010) 1160-1190.
4. Natesakhawat et al. "Improved benzene production from methane dehydroaromatization over Mo/HZSM-5 catalysts via hydrogen-permselective palladium membrane reactors" Catalysis Science and Technology (2015) DOI:10.1039/c5cy00934k.

Subtopic Area R-2
Advanced Catalysts and Catalyst Processing for Producing Hydrogen and Value-added Solid Carbons

The high decomposition temperature for natural gas indicates catalyst materials will be needed to lower process temperatures and enable industrial scale hydrogen and solid carbon production. While catalysts have been evaluated extensively in the literature for this process, research opportunities exist for overcoming catalyst deactivation, improving catalyst regeneration processes–including the separation and recovery of the solid carbon from catalyst, and optimizing the amount/type of low-cost solid carbon produced in order to improve process economics.

A range of traditional metal, metal oxide, and carbon catalysts have been demonstrated in the literature but many of them deactivate because of carbon growth at active sites and the full encapsulation of catalyst particles. Research opportunities exist for modifying catalyst composition, promoters, and physical architectures specifically to overcome this technical barrier. In addition to catalyst parameters, research opportunities exist for regenerating or prolonging the activity of catalysts by adjusting process parameters (temperature, co-feeds, flow rates) or developing new

chemical/physical processing approaches for regenerating catalysts in the hydrogen reactor or in a separate, dedicated, regeneration reactor.

For metal/metal oxide systems, the growth of carbon on the catalyst surface not only deactivates the catalyst but also creates a challenge for separating the high-value solid carbon from the catalyst/support and regenerating the catalyst itself. This separation step is fundamental to a wide range of catalyst systems in the literature. As such, research opportunities exist for separating the catalyst from the carbon. Since this technical challenge is so ubiquitous in the literature, general approaches that can be applied to multiple metal and metal oxide catalysts are desired in this subtopic area.

While the use of catalysts for overcoming kinetic barriers in this process are well established, there are few examples of being able to easily tune to the carbon product through catalyst composition or architecture. For carbon nanotubes, graphene, and other nanostructured carbons, the catalyst composition, structure, and substrate are key parameters that dictate the morphology and quality of the carbon product. Research opportunities exist for developing new catalyst systems where carbon products can easily be tuned to make a range of low-cost, widely applicable carbon materials in the same reactor/chemical process.

Objectives

The overall objective of research in this subtopic is to establish proof-of-concept for new catalyst systems and to obtain data necessary for assessing the scalability and economics of using these catalysts in a hydrogen production facility. Specific objectives include:

- Identification of different solid carbon forms produced by the process.
- Optimization of the metal catalyst composition to obtain the best solid carbon yield.
- Evaluation of methods to recover solid carbon efficiently from the catalyst.
- Optimization of the experimental parameters to obtain the desired solid carbon types.
- Optimizing the amount of hydrogen produced by these catalyst systems.

This subtopic area can only consider projects that utilize natural gas, simulated natural gas, or components of natural gas (e.g. natural gas liquids) to make hydrogen and solid carbon products. Other feedstocks cannot be considered. Other product streams besides solid carbon and hydrogen cannot be considered.

Collaboration Opportunities with NETL

Materials Engineering & Manufacturing (MEM) Core Competency: Applicants will collaborate with NETL research teams to achieve the research objectives noted above. NETL laboratories and equipment pertinent to research under this topic will be made available for up to 20 working days during the first year. Up to 0.050 FTE of NETL labor could be available for designing the experiments, conducting laboratory tests, modeling reactions, and interpreting data for each project selected.

Award Information and Funding Amounts

Area of Interest R-2			
Anticipated Project Period	**Maximum Award Size**	**Expected Number of Awards**	**Cost Share Requirement**
12 Months	Approx. $193,000	0 to 2 Awards	TRL 1-2: N/A TRL 3-6: 20% minimum

References

1. Dagle et. al. U.S. Dept of Energy Report "R&D Opportunities for Development of Natural Gas Conversion Technologies for Co-Production of Hydrogen and Value-Added Solid Carbon Products" ANL-17/11 | PNNL-26726 (2017).
2. Muradov, "Low to near zero CO2 production of hydrogen from fossil fuels: Status and perspectives", International Journal of Hydrogen Energy 42 (2017) 14508-14088.
3. Abbas et. al. "Hydrogen production by methane decomposition: a review", International Journal of Hydrogen Energy 35 (2010) 1160-1190.
4. Siriwardane, R., Tian, H., and Fisher, J., "Production of Pure Hydrogen and Synthesis Gas with Cu-Fe Oxygen Carriers using Combined Processes of Chemical Looping Combustion and Methane Decomposition/Reforming," International Journal of Hydrogen Energy, 40 (2015), 1698-1708.
5. Siriwardane, R., Tian, H., Miller, D., and Richards, G., "Fluidized Bed Testing of Commercially Prepared MgO-Promoted Hematite and CuO–Fe_2O_3 Mixed Metal Oxide Oxygen Carriers for Methane and Coal Chemical Looping Combustion," Applied Energy, 157 (2015), 348-357.
6. U.S. Patent 9,523,499 B1, December 20, 2016, "Regenerable Mixed Copper-Iron-Inert Support Oxygen Carriers for Solid Fuel Chemical Looping Combustion Process".
7. U.S. Patent Application S-135,847 "Production of Pure Hydrogen and Synthesis Gas with Cu-Fe Oxygen Carriers using Chemical Looping Combustion and Methane Decomposition/Reforming".

ATTACHMENT B – NETL CORE COMPETENCY DESCRIPTION

NETL's Research & Innovation Center (RIC) develops, nurtures and exercises the core technical competencies that enable NETL to be an international resource for Fossil Energy Technology Discovery, Development, and Deployment. Through effective leverage of its technical core competencies, and in collaboration with partners from industry, academia, and other government laboratories, the RIC delivers the knowledge and technologies that can enable the affordable, sustainable access and utilization of our abundant, domestic energy resources, by:

- Developing and proving solutions to key barriers to the implementation of emerging energy technologies.
- Exploring and maturing transformational new concepts for next generation energy systems.
- Leveraging core competencies to rapidly respond to issues of National concern.

The RIC is responsible for safe and efficient research operations at its Albany, Morgantown, and Pittsburgh sites; and for implementation of an R&D portfolio that effectively leverages core technical competencies to meet customer needs. Research projects effectively combine science-based simulations with targeted experimental validation from laboratory to demonstration scales, to accelerate the technology development process. Research within the NETL labs typically will focus on technology readiness levels (TRLs) up to level four. Research is coordinated with extramural projects as appropriate to lead to eventual commercial development at higher TRLs. The RIC is also responsible for nurturing the human capital, and designing and implementing the laboratory capabilities, necessary to assure the world-class stature of its technical core competencies.

The core competencies at NETL are developed and maintained within the five divisions of RIC, as described following.

Geological and Environmental Systems (GES)

Leveraging expertise in geomaterials science, fluid flow in geologic media, multi-scale assessments, geospatial data management and analyses, and strategic field monitoring, NETL conducts science and engineering research of natural systems to develop the knowledge and technologies that can enable safe, sustainable production and utilization of domestic energy resources. The competency includes development of numerical modeling with attributes that are unique to subsurface applications. Current NETL subsurface research efforts focus on CO_2 storage, unconventional tight gas resources, hydrates, offshore oil and gas, and geothermal systems. Specific attributes of this research competency include:

Geomaterials science capabilities that are used to characterize natural and man-made materials in the subsurface, and how they change with different in situ conditions, such as pressure, temperature, composition, biological activity, and stress. These capabilities share resources and collaboration with the Materials Science & Engineering focus area.

Combined theory, lab, simulation, and field approaches to measure and predict **fluid flow in geologic media** at all scales, which are focused on the most pressing new problems, including fracture-dominated flow seen in shale gas and oil applications and reduced order modeling required for decision-ready science.

Multiscale assessments to enable accurate analyses of the occurrence and distribution of in situ resources, as well as predictions of the performance of engineered natural systems over a range of time and space scales.

Geospatial data management and analyses that includes a growing suite of knowledge and tools for managing, analyzing, and interpreting data, including big data approaches, needed for multiscale assessments and other energy-related issues.

Development and application of new and innovative **monitoring technologies**, including the development and testing of new protocols and approaches for site characterization and monitoring of engineered natural systems.

Geology and Geospatial Analysis

The Geology and Geospatial Analysis Team characterizes geologic frameworks associated with a variety of energy-related systems supporting environmentally sustainable development. Characterization is robust and includes the analysis of engineered-natural systems in order to assess impacts and risk, and reduce the uncertainty of myriad data sets and modeling results.

The team develops and secures geologic characterization data at a variety of scales, e.g., pore scale to regional scale, employing multiple on-site (e.g., Scanning Electron Microscope) and mobile (e.g., Mobile Sediment Analysis Laboratory) laboratory systems as warranted. Geostatistical approaches are exercised to ensure the fidelity of data sets as is [big] data analytics when complex data sets apply. The team develops subsurface maps and models of earth systems to effectively inform the research program on key issues. Volumes of data are effectively managed and shared with collaborators through NETL's Energy Data eXchange. Both data and predictive outcomes from related modeling activities, e.g., fate and transport, are effectively

communicated to multiple classes of stakeholders through geospatial approaches combined with state-of-the-art visualization methods.

Geochemistry and Water

The Geochemistry and Water Team conducts research to understand the geochemical, microbiological, and physical impacts of energy-related natural resource development and environmental mitigation strategies on natural and engineered geologic systems. In order to do this, the team develops and applies geochemical and biogeochemical testing techniques, and conducts targeted experimentation and modeling of materials behavior in geologic environments. The team conducts field and laboratory studies to determine baseline conditions and assess changes to those conditions. Theoretical and quantitative modeling are used to analyze coupled processes involving fluid flow, temperature flux, chemical and biological reactions. Results demonstrate relationships between system conditions and development of fossil energy resources and carbon storage reservoirs, and enable the improvement of processes for resource recovery and environmental monitoring, protection, and mitigation.

To accomplish those functions, the team draws on research competence in geochemical surface science, mineralogy, metagenomics, isotope analysis, techniques to monitor fluid-rock interactions, reactive transport processes, water quality monitoring and mitigation, and characterization of hydrate-bearing sediments. It develops tools and processes as needed to evaluate biological, chemical, and physical processes in geologic environments. Key facilities are accessible to the team for fluid chemistry analysis, isotope analysis, microbiological DNA sequencing, subsurface process analysis, geomaterials characterization, cement and wellbore integrity investigations, and studies in high-pressure water environments.

Geophysics

The Geophysics Team seeks to better understand underground fluid flow from the pore to reservoir scales. To this end, it conducts world-class research to image fluids and rocks under *in situ* conditions at the micro to macro scales. The team develops and demonstrates predictive capability through coupled geomechanical and fluid-flow models for porous and fractured media at the reservoir scale.

The Geophysics Team performs experiments and develops computer codes for the study of underground fluid flow and deformation of solid materials in an effort to predict the behavior of coupled hydrologic, geomechanical, geophysical, and geothermal processes from the core to the reservoir scale and from short to long time scales. In particular, this Team has expertise and facilities for measurement, imaging, and analysis of fluid and rock properties under in situ conditions, and for measurement of hydrologic properties on permeable and fractured cores under single and multiphase flow situations with varying stress conditions (CT imaging lab; NER-Autolab; Geo/Fluid Lab; and Core Flow Lab). The Team uses its expertise and facilities to develop reduced-order models that simulate the behavior of reservoirs, seals, and other subsurface systems: FRACGEN (reservoir scale fracture generation code) and NFFLOW (discrete fractured reservoir model); NETFLOW (internally developed two-phase pore scale flow code); and NRAP's Integrated Assessment Model, Reservoir Model, and Seal Model. The Team also develops or expands new physics-based techniques of underground investigation, such as underwater laser induced breakdown spectroscopy sensing techniques.

Field Monitoring

The Field Monitoring Team identifies, quantifies, and mitigates potential environmental impacts arising from the development of subsurface energy resources. This Team provides a critical link between NETL's laboratory and computational research competencies, and the regulators and industry that are responsible for the safe, efficient development of subsurface energy resources. This mission is accomplished by 1) working with industry to design and implement field experiments that answer key questions about the safety, efficiency, and environmental performance of emerging energy development methods, 2) developing sentinel technologies that provide early warning of unwanted migration of fluid and gas from the subsurface, and 3) developing methods that identify potential environmental and operational vulnerabilities (legacy wells, faults, sensitive ecosystems, triggered seismicity, etc.) prior to the implementation of energy extraction operations or waste storage/disposal projects.

The Field Monitoring Team conducts airborne, ground-based, and subsurface field investigations using NETL's mobile laboratory facilities, specialized field instruments, contracted airborne and subsurface surveys, and expertise in: 1) monitoring and modeling of air quality, 2) quantification of methane emissions, 3) geophysics (seismic, magnetic, electromagnetic, radiometric, galvanic resistivity, and gravity), 4) spectral imaging and remote sensing (multispectral, hyperspectral, night-time thermal infrared, LiDAR, and differential absorption LiDAR), 5) tracers (gas, liquid, and proppant tracers), 6) measurement of surface and groundwater quality and flow, and 7) geospatial mapping, analysis, and interpretation.

Materials Engineering and Manufacturing (MEM)

NETL's Materials Engineering and Manufacturing Directorate (MEMD) supports NETL's ability to design, develop and deploy advanced materials for use in the extreme service environments and enable advanced energy systems. MEMD provides NETL a deep understanding of materials and their performance at condition, and specializes in the design, development, and deployment of advanced functional and structural materials. MEMD accelerates the development of material solutions through an integrated R&D approach leveraging multi-scale, multi-discipline computational, experimental techniques, and systems analysis; which encompasses the materials development continuum ranging from atomic-level design through translating lab-scale materials concepts to affordable industrial practice, utilizing advanced manufacturing methodologies. MEMD compliments this approach with advanced tools, unique facilities, and broad expertise across a variety of materials classes found in advanced energy systems. MEMD's materials solutions are scaled-up and tested at in-situ conditions for proof of concept in advanced fossil energy systems.

Functional Materials Development

MEMD develops functional materials to enable carbon capture, chemical looping, solid oxide fuel cells (SOFC), C-CBTL, unconventional resource recovery and other advanced energy systems. MEMD specializes in the design, synthesis, fabrication, manufacturing and performance assessment at condition of a wide class of materials (polymers, polymer composites, ionic liquids, functional alloys, ceramics, electro-ceramics, glasses, thin-films, and nano-engineered materials) for advanced energy systems, as follows:

- Solid solvents, sorbents, and membranes (structures and modules) for carbon capture and other gas separation applications.
- Materials for low cost oxygen production for oxy-combustion and gasification systems and durable oxygen carriers for chemical looping systems.
- Sensing materials and devices for harsh environments. Harsh environment sensors are needed for safe carbon storage, unconventional resource recovery and resource/CO_2 transmission, as well as, for improving the efficiency of power generation systems. Research focuses on materials and sensor packages for enhanced detection of environmental conditions (T, pH, composition, etc.) and for enhanced monitoring of component health (corrosion, mechanical strain, etc.) during operation.
- Electro-chemical materials for SOFC and other devices.
- Catalysts for C-CBTL conversion, CO_2 utilization, and other reaction processes.

Structural Materials Development

MEMD develops structural materials to enable unconventional resource recovery, advanced combustion systems, sCO_2 power cycles, advanced turbines, direct power extraction and other advanced energy systems. MEMD specializes in the design, synthesis, fabrication, and manufacturing and performance assessment at condition of heat-resistant alloys, ceramics and refractories as materials of construction and as environmental protection barriers for severe service applications. MEMD focuses on developing cost-effective structural materials that can withstand a combination of mechanical stress, corrosive and erosive environments for upwards of 100,000's hours service life, through improving existing alloys, designing new materials, and

reducing manufacturing cost. MEMD also focuses on a better understanding of the performance (corrosion, wear, hot-corrosion, oxidation, creep and fatigue resistance) to develop materials that resist degradation in severe service environments.

Computational Materials Engineering

MEMD develops multi-scale computational simulations to accelerate the design, development and deployment of new materials and fabrication methods. Simulations are also developed to predict materials (microstructural) stability and functionality under service conditions and times associated with advanced energy systems. MEMD specializes in quantum mechanics, classical mechanics and micro-scale and meso-scale (ab initio, DFT, KMC, MD, CALPHAD, mean field, phase field, finite element analysis, etc.) techniques needed to predict key materials parameters and properties for the functional and structural materials described above. These predictions are used to understand materials behavior and to guide experiments aimed at developing advanced materials.

Materials Characterization

MEMD's ability develop relevant processing-structure-property relationships and to assess materials performance underlies MEMD's ability to develop and deploy advanced functional and structural materials. MEMD specializes in designing laboratory experiments to assess materials performance in simulated service environments. Advanced microstructural characterization and surface analysis techniques are used to interrogate microstructural evolution and response to service conditions, which is critical for developing materials with improved performance characteristics.

Energy Conversion Engineering (ECE)

The ECE consists of both personnel and facilities that specialize in innovative energy conversion processes and transformational technologies for utilization of fossil fuels. Although not limited, focus is predominately on specific devices/processes and their integration into cohesive systems. The Directorate's competency allows for process level R&D, evaluation, integration & control and validation of scalable performance models. This competency is strategically positioned to be complementary with the other core RIC directorates for diligent and successful conceptualization, evaluation, development and demonstration of advanced fossil energy technologies. Some of the more specific aspects this directorate encompass are as follows.

Thermal Sciences

This aspect of the Energy Conversion Engineering competency represents the underlying expertise associated with a significant percentage of the applied problems in energy conversion engineering. Carbon management goals for Fossil Energy systems will require significant improvement in cycle efficiencies. This requirement will drive power generation systems to higher temperatures and pressures than used today. NETL facilities provide a unique test platform combining intermediate scale, high pressure, optical accessibility for model validation and advanced simulation capabilities for development and testing of new power generation system concepts. To address these issues, NETL utilizes expertise in fluid mechanics, aerodynamics, reacting flow, gas dynamics, sprays and multi-phase flow, thermal radiation, acoustics, and heat and mass transfer. NETL operates unique facilities that can provide fundamental data on many of these topics; the data is used for numeric model development, and applied to devices of interest in energy conversion. Example facilities include: ambient and high-pressure combustion labs, with laser diagnostics, turbine heat transfer research, oxy-fuel combustion facilities, magnetohydrodynamics (MHD) flow facility, chemical looping reactors and both high temperature and low temperature multi-phase solids flow facilities with diagnostics.

Innovative Energy and Water Processes

This team will employ a range of scientific and engineering principles, tools and methods that will allow us to successfully develop a variety of new transformational energy conversion systems, both in fossil energy as well as fossil-renewable hybrid systems. Some of the present technologies being applied toward improving energy conversion systems are: plasma generation for direct energy extraction using MHD principles (plant efficiency improvements); photons and phonons in new diagnostics and sensors (for new high temperature/pressure operation and longer lifetimes; cyber-physical methods to help advance coupled energy conversion systems for improved exergy utilization (i.e., hybridization of fossil energy as well as renewable energy components with examples being fuel-cell and gas turbine hybrids, and gas turbine and geothermal energy); chemical and physical methods in the transport of important fossil energy materials (e.g., water purification of produced brines). The team will leverage the capabilities in all other RIC teams toward achieving these advanced high efficiency fossil energy conversion technologies.

Reaction Engineering

The principal focus and strength of the Reaction Engineering group is on innovation in chemical reaction processes with bench-scale reactor research, evaluation and development. A significant portion of the science is based on conversion of various fossil and renewable fuels into synthesis gas, chemicals and other fuels along with separation and clean-up processes. Both catalytic and non-catalytic expertise exists, however, the group is building a significant capability of alternative nontraditional catalytic conversion based on microwave, radio frequency (RF) and plasma. Close interaction with the RIC Materials Directorate is maintained to conduct the necessary fundamental through applied science activities to evaluate and develop these technologies.

Multiphase Flow Science

This aspect of the Energy Conversion Engineering competency represents reactor performance modeling expertise associated with the various energy conversion concepts being pursued in the Directorate and across the RIC. With a current specialty focus on multi-phase gas/solid reactions systems. This team/capability has experienced personnel and equipment/facilities to develop and conduct detailed, scalable, high-speed computational fluid-dynamic (CFD) modeling of multi-phase reactions. Central to NETL's multiphase flow science team is the laboratory's suite of multiphase computational fluid dynamics (CFD) code, called Multiphase Flow with Interphase eXchanges (MFIX). MFIX has been developed specifically for modeling reacting multiphase systems. This open-source suite of software tools has over three decades of development history and more than 3,500 registered users worldwide. This software has become the standard test bed for comparing, implementing, and evaluating multiphase flow constitutive models and has been applied to an extremely diverse range of applications involving multiphase flows. Central to the development, testing, validation, and application of the models within MFIX is NETL's supercomputer "Joule". Joule brings 503 TFlops of floating point operational power to the RIC. With over 24,000 computational cores dedicated to fossil energy R&D, Joule allows researchers across the RIC to advance the state-of-the-art in computational multiphase flow science. The multiphase flow science team research and development combines development and application of multiphase computational fluid dynamic models with small-scale, well-resolved experiments to develop accurate models and to provide validated computational tools.

Systems Engineering and Analysis (SEA)

The Systems Engineering and Analysis Directorate supports NETL's Mission through 1) analysis of its existing research portfolio and potential of new technology ideas, 2) identification of new innovative energy concepts, and 3) analysis of interactions between energy systems at plant, regional, national and global scales. It conceives, plans, manages, and conducts research in the areas of energy process analysis, process systems engineering research, energy systems analysis, and energy markets analysis. The Directorate's activities range from analysis of single energy processes (such as a power plant integrated with carbon capture and compression) to interacting energy systems (such as the grid and the environment) to modeling and analysis of economy-wide markets. In addition, this Directorate conducts research focused on the development and utilization of advanced models coupled with optimization and uncertainty quantification to support decision-making and process innovation.

Energy Process Analysis

The Energy Process Analysis Team (EPAT) develops and utilizes models and simulations to guide and support NETL's existing research portfolio, provide insight on the potential of new technology ideas, identify new energy concepts, and analyze interactions between energy systems at the plant scale. The team conceives, plans, manages, and conducts plant- and plant subsystem-level performance and cost model development and analysis, including those incorporating novel energy conversion and/or environmental control technologies. The team develops and maintains standards, tools, and databases to support the efficient, timely execution of high quality analyses, including those carried out by external entities. These analyses may be for specific or multiple technologies (e.g., NETL Baseline Studies), and apply to technologies spanning the technology readiness spectrum, from new concepts to commercial technologies. Analyses inform existing and future intramural and extramural R&D, as well as serve as a basis for the evaluation of external techno-economic analyses, technology maturation plans, technology readiness assessments, etc. These analyses support strategic planning, portfolio analysis, and program evaluation efforts. The team utilizes an up-to-date suite of commercial process simulation tools and maintains extensive capital cost estimation capabilities.

Process Systems Engineering Research

The Process Systems Engineering (PSE) Research Team is concerned with the discovery, design and operation of energy systems, including generation and distribution, in the context of many conflicting goals. Research in PSE develops systematic decision-making techniques for maximizing profits, minimizing costs, and meeting environmental and technical constraints. PSE involves the development and utilization of advanced models coupled with optimization and uncertainty quantification to support decision-making. This includes capabilities such as techno-economic analyses based on fundamental models and rigorously optimized processes (complementing the type of analyses performed by Energy Process Analysis), screening new concepts and materials in the context of complete processes, identification of new process concepts, simultaneous product and process design (i.e., determining the best material and process for a given application), evaluation of operability and flexibility, and process integration. In addition, this team will develop and apply next generation computational tools and rigorous models to enable process synthesis, design, optimization, process intensification, and uncertainty quantification. These tools will be applied to identify and develop new, innovative energy

systems, which are capable of meeting environmental and economic objectives. Scope of these systems range from process to region to global. This team will also apply advanced models to help develop and scale up innovative processes in cooperation with industry partners.

Energy Systems Analysis

The Energy Systems Analysis Team (ESAT) core activity areas include sustainable energy analysis, resource assessment, and energy security and assurance analysis. The team looks across broad areas of inquiry in support of NETL's enduring missions of effective resource development and environmental sustainability. The team develops methodologies, and deploys tools and models furthering analysis in these areas. Core analysis functions and activities involve Sustainable Energy Analysis and Energy Security and Assurance. Sustainable Energy Analysis includes multiple aspects of Life Cycle Analysis. In addition, this team conducts resource assessments and analyses of the availability of domestic resources such as fossil fuels, water, and rare earth elements as well as of the CO_2 storage potential and costs of various geologic formations. Energy Security and Assurance includes activities related to Energy Security Assessments (such as supply-side pathways to enhance security), Infrastructure and Reliability Assessments (such as electricity system dispatch, pipeline networks, and electricity system resilience) and Emerging Energy Concepts that are focused on the identification and evaluation of novel energy concepts, such as integration of renewable energy technologies with fossil energy platforms.

Energy Markets Analysis

The Energy Markets Analysis Team (EMAT) develops and utilizes economic modeling and analysis techniques to investigate regional, national and/or international impacts of state of the art and transformational energy technologies under a wide spectrum of possible future scenarios. A variety of complex energy models are leveraged to support NETL's current research portfolio and programs, identify new program opportunities, perform novel analyses, and provide rapid response analysis support for NETL, DOE, and the National Laboratory Complex. The EMAT assesses current and projected trends in sectors directly and indirectly related to both the domestic and international energy economy. These include regulatory and legislative actions, energy supply and demand, technology cost and availability, financial markets, resource constraints (such as water availability), and other relevant areas. This information is used to construct alternative future scenarios, which are then represented in a variety of models to assess existing and potential impact of NETL R&D activities to the energy-economy and the environment. Integrated assessment models, such as the National Energy Modeling System (NEMS), are used to evaluate the role of NETL's technology portfolio under a myriad of possible future conditions, as well as determine secondary impacts – such as water consumption – of competing scenarios. Such analyses identify potential market opportunities, inform the development of program goals and targets, estimate level of market deployment, and estimate direct and indirect impacts to the energy-economy and environment.

Computational Science and Engineering (CSE)

In support of the DOE and NETL missions, the capabilities in high-performance computing and data analytics maintained by this directorate enable the generation of information and understanding beyond the reach of experiments alone, through the integration of experimental information with computational sciences and engineering across time and length scales.

Hardware and Network

The core computing resource for Computational Sciences & Engineering is named "Joule", a 503-TFLOP supercomputer. Joule is composed of 1512 nodes, each containing 16 Intel Sandy Bridge cores, 32 or 64 GBs of RAM, 2TB of RAID1 local scratch space, and a QDR InfiniBand network connection. The InfiniBand network provides full bisection bandwidth to all nodes via a full fat tree topology. In total, the supercomputer provides 25,192 cores, 76 TBs of memory, 9 PBs of local scratch storage, and 1 PB of permanent storage. Please visit http://hpc.netl.doe.gov for more information.

A small development cluster using Intel Knights Corner MIC processors is also available for software optimization and testing. The planned successor to Joule will leverage a combination of new Intel Broadwell CPUs and Intel Knights Landing MIC processors and will provide up to 5 PFLOPs of performance.

HPC resources are accessed via a custom login client that provides both text-based and persistent GUI sessions, file transfer, and collaborative desktop sharing. It is useable from any network inside or outside NETL without restriction. The system is connected to 3ROX's High-Speed Optical Network (HSON), as well as NETL core network.

Data Analysis and Visualization

This competency includes development of data science, data analytics, data architecture and complex data visualization methodologies and tools, with attributes that are unique to fossil energy applications. It represents NETL's emerging expertise in data-intensive, domain-guided statistical design for optimal manufacturing, computational process and materials engineering, with uncertainty quantification to support decision-making, and additional scientific insight into complex, noisy, high-dimensional, and high-volume data sets from experiments and simulations. The Data Analysis and Visualization Team develops and utilizes unique capabilities in parallel and distributed computing, not only SQL databases, data ingestion, integration and preprocessing (cleaning, parsing, organizing according to the tidy/structured data principles, managing, maintaining, and validating), machine learning, artificial intelligence, fast and scalable exploratory data analysis, statistical inference, feature discovery, mathematical and semi-supervised generalized higher-order system equation modeling to identify relationships and latent variables, advanced expert systems, and knowledge-based technologies.

The team is equipped to construct and explore databases with a variety of languages including R, Python, C/C++, CUDA, MATLAB, Java, VisIt, ParaView, Blender, Ensight, Tecplot, FFmpeg, and Chimera. Several purpose-built visualization systems are also available. These contain 256 GBs of RAM and four Nvidia GPUs, as well as local RAID6 storage. These systems are specifically designed to allow visualization and exploration of large datasets and are accessible using the same remote access client as used for Joule, access. The visualization systems are also

available as large-memory nodes for offline data analysis. The uncertainty quantification analysis software PSUADE is available on Joule. PSUADE, which is free software from Lawrence Livermore National Laboratory allows the user to assess uncertainties due to variabilities in model input parameters, boundary conditions, missing physics and model implementation in numerical simulations and data-driven phenomenological models.

Software & Automation

Several commercial and open-source CFD and Multiphysics software packages available, including Ansys, FLUENT, OpenFOAM, COMSOL, NETL's MFiX Suite (http://mfix.netl.doe.gov), and Barracuda. Many computational chemistry simulation codes are also available, including VASP and Gaussian. Available visualization tools include Paraview, Ensight, Visit, and TecPlot.

A full suite of Intel and GNU development tools are available for users developing or porting code. Source code management is provided by an NETL hosted GitLab site, which supports multilevel user permissions, code reviews, issue tracking, and wiki capabilities. A continuous integration (CI) server, Jeknins, offers regression testing for improved software quality assurance. Allinea DDT is available for interactive debugging of serial and MPI based C, C++, and Fortran programs. Software performance analysis tools include Intel VTune and Allinea MAP.

Informational Access & Infrastructure

Many details about Joule and the other computational resources are available at http://hpc.netl.doe.gov.

ATTACHMENT C – CORE COMPETENCY TABLE

UCFER Research Topics by Technology Line	Geological & Environmental Systems (GES)	Materials Engineering & Manufacturing (MEM)	Energy Conversion Engineering (ECE)	Systems Engineering & Analysis (SEA)	Computational Science & Engineering (CSE)
[O] Carbon Storage					
Subtopic Are O-1: Developing Scale-Up Tools to Extend Laboratory Measurements to the Field	X				
[P] Coal Beneficiation					
Subtopic Area P-1: Improved Coal Feedstocks for Power Production and Steel-Making		X			
Subtopic Area P-2: Producing High-Value Solid Products from Coal		X			
Subtopic Area P-3: American Coal Database					X
Subtopic Area P-4: Coal Products Systems Engineering and Analysis				X	
[Q] Crosscutting Research					
Subtopic Area Q-1: Machine Learning for Microstructural Recognition and Reconstruction of Heat-Resistant Alloys		X			X
[R] Fuel Cell Technology/Natural Gas Conversion to Hydrogen and Solid Carbon Products					
Subtopic Area R-1: Novel Reactors for the Co-Production of Hydrogen and Value-Added Solid Carbons		X			
Subtopic Area R-2: Advanced Catalysts and Catalyst Processing for Producing Hydrogen and Value-Added Solid Carbons		X			

ATTACHMENT D – NETL TECHNOLOGY READINESS LEVELS

TRL	Definition	Description
1	Basic principles observed and reported	Core Technology Identified. Scientific research and/or principles exist and have been assessed. Translation into a new idea, concept, and/or application has begun.
2	Technology concept and/or application formulated	Invention Initiated. Analysis has been conducted on the core technology for practical use. Detailed analysis to support the assumptions has been initiated. Initial performance attributes have been established.
3	Analytical and experimental critical function and/or characteristic proof-of-concept validated	Proof-of-Concept Validated. Performance requirements that can be tested in the laboratory environment have been analytically and physically validated. The core technology should not fundamentally change beyond this point. Performance attributes have been updated and initial performance requirements have been established.
4	Basic technology components integrated and validated in a laboratory environment	Technology Validated in a Laboratory Environment. The basic technology components have been integrated to the extent practical (a relatively low-fidelity integration) to establish that key pieces will work together, and validated in a laboratory environment. Performance attributes and requirements have been updated.
5	Basic technology components integrated and validated in a relevant environment	Technology Validated in a Relevant Environment. Basic technology component configurations have been validated in a relevant environment. Component integration is similar to the final application in many respects. Data sufficient to support planning and design of the next TRL test phase have been obtained. Performance attributes and requirements have been updated.
6	Prototype validated in a relevant environment	Prototype Validated in Relevant Environment. A prototype has been validated in a relevant environment. Component integration is similar to the final application in most respects and input and output parameters resemble the target commercial application to the extent practical. Data sufficient to support planning and design of the next TRL test phase have been obtained. Performance attributes and requirements have been updated.
7	System prototype validated in an operational system	System Prototype Validated in Operational Environment. A high-fidelity prototype, which addresses all scaling issues practical at pre-demonstration scale, has been built and tested in an operational environment. All necessary development work has been completed to support actual technology testing. Performance attributes and requirements have been updated.
8	Actual technology successfully commissioned in an operational system	Actual Technology Commissioned. The actual technology has been successfully commissioned for its target commercial application, at full commercial scale. In almost all cases, this TRL represents the end of true system development.
9	Actual technology operated over the full range of expected operational conditions	Commercially Operated. The actual technology has been successfully operated long-term and has been demonstrated in an operational system, including (as applicable) shutdowns, startups, system upsets, weather ranges, and turndown conditions. Technology risk has been reduced so that it is similar to the risk of a commercial technology if used in another identical plant.

Glossary of Terms

Actual Technology: The final product of technology development that is of sufficient size, performance, and reliability—ready for use at the target commercial application. The technology is at Technology Readiness Levels (TRLs) 8–9.

Basic Technological Components Integrated: A test apparatus that ranges from (1) the largest, most integrated and/or most realistic technology model that can reasonably be tested in a laboratory environment, to (2) the lowest-cost technology model that can be used to obtain useful data in a relevant environment.

Commissioning/Commission: The actual system has become operational at target commercial conditions and is ready for commercial operations.

Concept and/or Application: The initial idea for a new technology or a new application for an existing technology. The technology is at TRLs 1–3.

Core Technology: The idea, new concept, and/or new application that started the research and development (R&D) effort. Examples include: (1) a new membrane material, sorbent, or solvent; (2) new software code; (3) a new turbine component; (4) the use of a commercial sensor technology in more durable housing; or (5) the use of a commercial enhanced oil recovery technology to store CO_2. Typically this is a project's intellectual property.

Fidelity: The extent to which a technology resembles its intended use in the target commercial application.

Integrated: The functional state of a system resulting from the process of bringing together one or more technologies or subsystems and ensuring that each function together as a system.

Laboratory Environment: An environment isolated from the commercial environment in which lower-cost testing is performed to obtain high-quality, fundamental data at earlier TRLs. For software development, this a small-scale, simplified domain for a software mockup.

Operational System: The environment in which the technology will be tested as part of the target commercial application.

Performance Attributes: All aspects of the technology (flux, life, durability, cost, etc.) that must be tested to ensure the technology will work at the target commercial application, including all needed support systems. It is likely that the performance attributes list will increase as the technology matures. Performance attributes must be updated as new information is received and formally reviewed at each TRL transition.

Performance Requirements: Criteria that must be met for each performance attribute before the actual system can be used at its target commercial application. These will be determined through consideration of technology test data, funding program goals, systems analysis, etc. Performance requirements may change over time, and it is unlikely that all of them will be known at a low TRL.

Program: The funding program. The program goals will be used to judge project value and, in concert with systems analysis, will support acceptable performance requirements for the project. The funding program will also determine whether the system will be tested under one or several sets of target commercial applications.

Project: The funding mechanism for technology development, which often spans only part of the technology development arc. Some projects may contain aspects that lack dependence; these may have different TRL scores, but this must be fully justified.

Proof-of-Concept: Reasonable conclusions drawn through the use of low-fidelity experimentation and analysis to validate that the new idea—and resulting new component and/or application—has the potential to lead to the creation of an actual system.

Prototype: A test apparatus necessary to thoroughly test the technology, integrated and realistic as much as practical, in the applicable TRL test environment.

Relevant Environment: More realistic than a laboratory environment, but less costly to create and maintain than an operational environment. This is a relatively flexible term that must be consistently defined by each program (e.g., in software development, this would be "beta testing").

Target Commercial Application: This refers to one specific use for the actual system, at full commercial scale, which supports the goals of the funding program. A project may include more than one set of target commercial applications. Examples are:

1. Technologies that reduce the cost of gasification may be useful for both liquid fuels and power production.
2. Technologies that may be useful to monitor CO_2 storage in more than one type of storage site.

Technology: This includes R&D work on all technology aspects, both within and external to any given project, that must be done for the project's core technology to translate into an actual system. It is likely that what comprises the technology will increase as the TRL score increases. This includes concepts and/or applications (TRLs 1–3), components and/or systems (TRLs 4–5), prototype in a relevant environment (TRL 6), high-fidelity prototype in an operational environment (TRL 7), and the actual technology (TRLs 8–9).

Technology Aspects: Different R&D efforts, both within and external to any given project. Examples include material development, process development, process simulation, contaminant removal/control, and thermal management.

Validated: The proving of all known performance requirements that can reasonably be tested using the test apparatus of the applicable TRL.

ATTACHMENT E - CHECKLIST

PI: _____

Affiliation: _____

Project Title: _____

To assure your application is complete, we have provided the following checklist. Please ensure you include/comply with the following items. You may be ineligible for award if all requirements of this RFP are not met on the proposal due date.

☐	Cover page completed and signed by PI and authorized representative.	
☐	Table of Contents	One (1) page maximum
☐	Executive Summary (public abstract)	One (1) page maximum
☐	Project Description	Five (5) pages maximum
☐	Project Schedule	One (1) page maximum
☐	Anticipated Results	One (1) page maximum
☐	Budget with appropriate justification	
☐	Cost-Share Commitments/ Letters of Commitment (?)	
☐	Biographical Sketches	Two (2) pages per person maximum
☐	Environmental Questionnaire	
☐	Collaboration with NETL	Two (2) pages maximum
☐	Collaboration with industry?	
☐	Letters of Support, required for proposals with cost share	

Clear Page

ATTACHMENT F - COVER SHEET

Proposal Submitted to: UCFER Operations Management Team
Via www.energy.psu.edu/ucfer
EMS Energy Institute
The Pennsylvania State University
C-211 Coal Utilization Laboratory
University Park, PA 16802-2323

Date of Submission: _____

Title of Proposal: _____

Area of Interest (See Attachment A) Pick from dropdown

Subtopic Area, if any (See Attachment A) Pick from dropdown

TRL at start (See Attachment D): _____ TRL at end: _____

Total Project Costs (TPC): $ _____

Requested UCFER Funding: $ and (% of TPC) _____

Cost Share Commitments: Cash $ and (% of TPC)_____
In-Kind $ and (% of TPC)_____

Project Duration (total months): _____

Institution Name: _____

Principal Investigator:_____

Phone: _____ Fax: _____ Email: _____

Address: _____

_____

_____

Other Participants: _____

Collaboration with NETL? ◯ Yes ◯ No

Collaboration with industry? ◯ Yes ◯ No

Does the proposed project work involve foreign national? ◯ Yes ◯ No

PROPRIETARY INFORMATION: Does this proposal contain Proprietary or Confidential Information?

◯ NO ◯ YES (if yes, complete paragraph on next page)

Clear Page

Notice of Restrictions on Disclosure and Use of Data

The data contained on pages _____ of this proposal are submitted in confidence and contain privileged or confidential commercial and/or financial information. Such data may be used or disclosed only for evaluation purposes. If funded, the Government would have the right or use or disclose data from this project to the extent provided the DOE/PSU Cooperative Agreement. This restriction does not limit the Government's right to use or disclose data obtained without restrictions from any source, including the proposer.

Proposal Submitted by:	Proposal Approved by:
_____	_____
Signature of PI	Name and Title of Authorized Representative

ATTACHMENT G - BUDGET

Name of PI: _____

	REQUESTED UCFER	COST-SHARE
Salaries and Wages Identify all personnel in the proposal. Include title and percent of effort NOTE: The use of undergraduate and graduate students is encouraged, when appropriate. The basis for proposed percent of effort or labor hours should be identified (historical hours, engineering estimates).	$_____	$_____
Fringe Benefits	$_____	$_____
Materials and Supplies List types required and estimated costs. NOTE: State whether amounts proposed are based on catalog prices or other cost estimating.	$_____	$_____
Equipment Items exceeding $5,000 and having a 2-year life are defined as permanent equipment. List item and dollar amount with justification and/or provide a quotation.	$_____	$_____
Travel (*See Note 5) State the type and extent of travel and its relation to the project.	$_____	$_____
Publication/Information Dissemination Estimate costs of documenting, preparing, publishing and sharing research findings.	$_____	$_____
Joint Collaboration with Other University or Industrial Partner As a subcontractor.		
_____	$_____	$_____
_____	$_____	$_____
_____	$_____	$_____
Other Direct Costs _____ Itemize and justify. (**See note below) _____	$_____	$_____
_____	$_____	$_____
_____	$_____	$_____
Facilities and Administration (F&A) Specify current rate(s) and base. Note: A copy of the negotiated agreement should be included with the proposal. If none exists, a disclosure of the contents of the rate should be made.	$_____	$_____
TOTALS	$ 0.00	$ 0.00

**__Attach additional pages of justification as necessary.__

Clear Page

***NOTES:**

1) Purchased Services, consulting or subcontracts proposed to non-coalition members shall not be more than 2.5% of the UCFER requested funds.

2) Subcontracts included in your proposal (third party agreements) to current coalition members must not exceed 50% of the total requested UCFER funding. Budgets and work statements from each proposed subcontractor must be included with your proposal.

3) Foreign entities including universities cannot receive UCFER funding.

4) Fees or profits will not be paid on any award resulting from this solicitation. Nor can fee or profit be considered as cost-sharing.

5) Recipients of UCFER funding will be required to provide a presentation on the status of their project at one Annual Technical Review meeting for each year of the project duration. In addition, DOE/NETL strongly recommends that one DOE Program Specific Review meeting per project be attended. The costs for attending the UCFER annual meeting(s) and DOE Program Specific Review meeting are to be included in the travel budget.

ATTACHMENT H – PROPOSAL EVALUATION CRITERIA

UCFER PROPOSAL RATING DESCRIPTION
(To be used on the following tabulation worksheet, which will be online for reviewers)

Proposal Title:

1. **NETL Collaboration – Proposal demonstrates clearly the level of collaboration anticipated with NETL:**
   1. Not adequate
   2. Somewhat adequate
   3. Adequate
   4. Very adequate
   5. Exceptionally adequate

2. **Meeting UCFER Objectives – The goals or objectives of the proposed project with respect to consistency with UCFER goals are:**
   1. Not adequate
   2. Somewhat adequate
   3. Adequate
   4. Very adequate
   5. Exceptionally adequate

3. **Idea and Approach – The scientific and/or technical merits and originality of the proposed idea or concept and approach to specifically address the problem relevant to an Area of Interest (and Subtopic Area, if any) are likely be:**
   1. Extremely small
   2. Small
   3. Significant
   4. Very significant
   5. Extremely significant

4. **Project Achievability – With the approach suggested and time and budget available, the objectives of the proposed research are:**
   1. Not achievable
   2. Possibly achievable
   3. Likely achievable
   4. Most likely achievable
   5. Definitely achievable

5. **Research Impacts – The impact of the proposed research, if successful, on the fossil energy science and technology development will be:**
   1. Very low
   2. Low
   3. Average
   4. High
   5. Very high

6. **Qualification of Key Personnel – principal investigator's and senior investigator's experiences and accomplishments related to the proposed research is:**
   1. Very limited
   2. Limited
   3. Adequate
   4. Good
   5. Exceptional

7. **Project Management & Budget – The project management plan, including a well-defined milestone chart and schedule, and the budget value relative to the outlined work are:**
   1. Very inadequate
   2. Inadequate
   3. Adequate
   4. Very good
   5. Exceptionally good

UCFER Proposal Score Tabulation

Project Name/PI

Relative Weighting x Evaluator Rating = Project Score

Criteria	Relative Weighting	Rating (Out of 5)	Project Score
Merit of Collaboration with NETL	4		
Meeting UCFER Objectives	2		
Idea and Approach	4		
Project Achievability	2		
Research Impacts	4		
Qualification of Key Personnel	3		
Project Management & Budget	1		
		Total (Maximum=100)	

Illustrative Example

Relative Weighting x Evaluator Rating = Project Score

Criteria	Relative Weighting	Rating (Out of 5)	Project Score
Merit of Collaboration with NETL	4	3	12
Meeting UCFER Objectives	2	3	6
Idea and Approach	4	3	12
Project Achievability	2	3	6
Research Impacts	4	3	12
Qualification of Key Personnel	3	4	12
Project Management & Budget	1	4	4
		Total (Maximum=100)	64