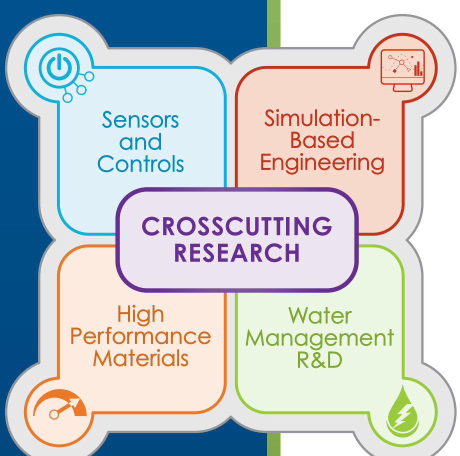
NATIONAL ENERGY TECHNOLOGY LABORATORY

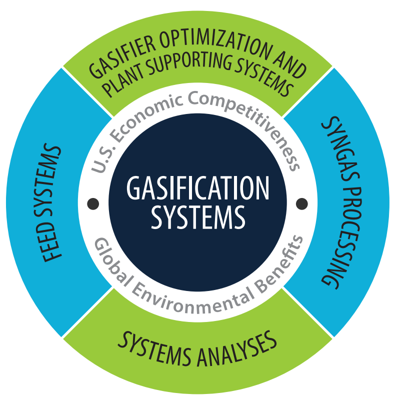
2017 Project Review Meeting

for Crosscutting Research, Gasification Systems, and Rare Earth Elements Research Portfolios

ABSTRACT BOOK

MARCH 20 – 23, 2017
Omni William Penn Hotel, Pittsburgh, PA





REE
RARE EARTH ELEMENTS
FROM COAL AND COAL BY-PRODUCTS

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

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REVIEW MEETING CHAIRS

Patricia Rawls
Maria Reidpath
Mary Anne Alvin
David Lyons
Robert Romanosky
U.S. Department of Energy
National Energy Technology Laboratory

Meeting Coordinators

Karen Lockhart
SSC-Deltha, LLC

Dale Cunningham
Sextant Technical Services

Conference Project Abstracts	https://goo.gl/Qnp6O7
Crosscutting Research Portfolio Handbooks	https://goo.gl/BZLY7Q
Rare Earth Elements Portfolio Handbooks	https://goo.gl/lWjspr

MONDAY, MARCH 20 TRACK A – WILLIAM PENN BALLROOM

7:30 a.m. REGISTRATION AND CONTINENTAL BREAKFAST

8:30 a.m. **Plenary Session**

- **Welcome and Opening Remarks**
  Dr. Grace Bochenek, Director, National Energy Technology Laboratory, U.S. DOE
- **Office of Fossil Energy Update**
  Mr. Douglas Hollett, Acting Assistant Secretary for Fossil Energy, U.S. DOE
- **Crosscutting Research Program Overview**
  Dr. Robert Romanosky, Acting Technology Manager, Crosscutting Research, NETL, U.S. DOE
- **Gasification Systems Program Overview**
  Mr. K. David Lyons, Acting Technology Manager, Gasification Systems, NETL, U.S. DOE
- **Crosscutting Activities in Systems Engineering and Analysis**
  Mr. Travis Shultz, Supervisor, Energy Process Analysis Team, NETL, U.S. DOE

10:00 a.m. **MORNING BREAK**

TRACK A CROSSCUTTING RESEARCH

10:30 a.m. **SESSION 1 – WIRELESS SENSORS**
Moderator – *Robert Fryer*, National Energy Technology Laboratory

- **Wireless 3D Nanorod Composite Arrays-Based High-Temp Surface Acoustic Wave Sensors for Selective Gas Detection Through Machine Learning Algorithms**, Dongwook Kwak, University of Connecticut
- **Metal Oxide/Nitride Heterostructured Nanowire Arrays for Ultra-Sensitive and Selective Multi-Mode High Temperature Gas Detection**, Bo Zhang, University of Connecticut

11:30 a.m. **LUNCH (ON YOUR OWN)**

1:00 p.m. **SESSION 2 – WIRELESS SENSORS**
Moderator – *Sydni Credle*, National Energy Technology Laboratory

- **High Temperature Integrated Gas and Temperature Wireless Microwave Acoustic Sensor System for Fossil Energy Applications**, *Mauricio Pereira da Cunha*, University of Maine
- **Low-Cost Efficient and Durable High Temperature Wireless Sensors by Direct Write Additive Manufacturing for Application in Fossil Energy Systems**, *Md. Taibur Rahman*, Washington State University
- **Novel Temperature Sensors and Wireless Telemetry for Active Condition Monitoring of Advanced Gas Turbines**, *Anand Kulkarni*, Siemens Corporation

2:30 p.m. **WORKING BREAK**
Moderator – *Jason Hissam*, National Energy Technology Laboratory

- **MFIX-DEM PHI: Perf and Capability Improvements Towards Industrial Grade Open-Source DEM Framework with Integrated Uncertainty Quantification**, *Manogna Adepu*, Arizona State University

3:00 p.m. **SESSION 3 – SENSORS**
Moderator – *Otis Mills*, National Energy Technology Laboratory

- **Distributed Wireless Antenna Sensors for Boiler Condition Monitoring**,
  Haiying Huang, University of Texas at Arlington
- **Investigation of "Smart Parts" with Embedded Sensors for Energy System Applications**,
  Yirong Lin, University of Texas at El Paso
- **Metal Three Dimensional (3D) Printing of Low-Nitrous Oxide (NOX) Fuel Injectors with Integrated Temperature Sensors**, *Philip Morton*, University of Texas at El Paso
- **Additive Manufacture of Smart Parts with Embedded Sensors for In-Situ Monitoring in Advanced Energy Systems**,
  Hai Xiao, University of Missouri System

MONDAY, MARCH 20 TRACK B – THREE RIVERS ROOM

7:30 a.m. REGISTRATION AND CONTINENTAL BREAKFAST

8:30 a.m.

Plenary Session

- **Welcome and Opening Remarks**
  Dr. Grace Bochenek, Director, National Energy Technology Laboratory, U.S. DOE
- **Office of Fossil Energy Update**
  Mr. Douglas Hollett, Acting Assistant Secretary for Fossil Energy, U.S. DOE
- **Crosscutting Research Program Overview**
  Dr. Robert Romanosky, Acting Technology Manager, Crosscutting Research, NETL, U.S. DOE
- **Gasification Systems Program Overview**
  Mr. K. David Lyons, Acting Technology Manager, Gasification Systems, NETL, U.S. DOE
- **Crosscutting Activities in Systems Engineering and Analysis**
  Mr. Travis Shultz, Supervisor, Energy Process Analysis Team, NETL, U.S. DOE

TRACK B CROSSCUTTING RESEARCH

10:30 a.m. **SESSION 1 – STRUCTURAL MATERIALS**
Moderator – *Charles Miller*, National Energy Technology Laboratory

- **Predicting the Oxidation/Corrosion Performance of Structural Alloys in Supercritical CO2**,
  John Shingledecker, Electric Power Research Institute Inc.
- **Alloy Performance in sCO2 Environments: Effects of sCO2 Exposure**,
  Omer Dogan, NETL – Research and Innovation Center

11:30 a.m. **LUNCH (ON YOUR OWN)**

1:00 p.m. **SESSION 2 – FUNCTIONAL MATERIALS**
Moderator – *Barbara Carney*, National Energy Technology Laboratory

- **Developing Novel Multifunctional Materials for High-Efficiency Electrical Energy Storage**,
  Feng Yuan Zhang, University of Tennessee
- **Vertically-Aligned Carbon-Nanotubes Embedded in Ceramic Matrices for Hot Electrode Applications**,
  Yongfeng Lu, University of Nebraska - Lincoln
- **Novel Silica Nanostructured Platforms with Engineered Surface Functionality and Spherical Morphology for Low-Cost High-Efficiency Carbon Capture**, *Nicholas Pizzi*, Delaware State University

2:30 p.m. **AFTERNOON BREAK**

3:00 p.m. **SESSION 3 – FUNCTIONAL MATERIALS**
Moderator – *Anthony Zinn*, National Energy Technology Laboratory

- **Engineering Accessible Adsorption Sites in Metal Organic Frameworks for CO_2 Capture**,
  Saki Golafale, Clark Atlanta University
- **Post Combustion Carbon Capture Using Polyethylenimine (PEI) Functionalized Titanate Nanotubes**,
  Melisa Stewart, Prairie View A&M University
- **Serration Behavior of High-Entropy Alloys**,
  Karin Dahmen, University of Illinois
- **Reduced Cost Bond Layers for Multi-Layer Thermal/Environmental Barrier Coatings**,
  Jeffrey Fergus, Auburn University

MONDAY, MARCH 20 TRACK C – RIVERBOAT ROOM

7:30 a.m. REGISTRATION AND CONTINENTAL BREAKFAST

8:30 a.m.

Plenary Session

- **Dr. Grace Bochenek**, Director, National Energy Technology Laboratory, U.S. DOE
- **Mr. Douglas Hollett**, Acting Assistant Secretary for Fossil Energy, U.S. DOE
- **Dr. Robert Romanosky**, Acting Technology Manager, Crosscutting Research, NETL, U.S. DOE
- **Mr. K. David Lyons**, Acting Technology Manager, Gasification Systems, NETL, U.S. DOE
- **Mr. Travis Shultz**, Supervisor, Energy Process Analysis Team, NETL, U.S. DOE

TRACK C GASIFICATION SYSTEMS

10:30 a.m. **SESSION 1 – NOVEL TECHNOLOGIES**
Moderator – *Steven Markovich*, National Energy Technology Laboratory

- **Dry Solids Pump Feed Technology Program**,
Tim Saunders, Gas Technology Institute.
- **Integrated WGS/Precombustion Carbon Capture Process**,
Gokhan Alptekin, TDA Research

11:30 a.m. **LUNCH (ON YOUR OWN)**

1:00 p.m. **SESSION 2 – ADVANCEMENTS IN AIR SEPARATION**
Moderator – *Seth Lawson*, National Energy Technology Laboratory

- **OTM-Enhanced Coal Syngas for Carbon Capture Power Systems and Fuel Synthesis Applications**,
Juan Li, Praxair, Inc.
- **Low Cost Air Separation Process for Gasification Applications**,
Gokhan Alptekin, TDA Research
- **Development of Two-Phase Dense Fluid Expander for Advanced Cryogenic Air Separation and Low-Grade Heat Recovery**,
Scott Marchessault, Air Products and Chemicals, Inc.

2:30 p.m. **AFTERNOON BREAK**

3:00 p.m. **SESSION 3 – CHEMICAL LOOPING FOR COAL GASIFICATION**
Moderator – *Steven Markovich*, National Energy Technology Laboratory

- **Chemical Looping Coal Gasification SubPilot Unit Demonstration and Economic Assessment for IGCC Applications / Pilot Scale Operation and Testing of Syngas Chemical Looping for Hydrogen Production**, *Andrew Tong*, Ohio State U.
- **Warm Syngas Cleanup Operational Testing at Tampa Electric Company's Polk 1 IGCC Site**,
Raghubir Gupta, Research Triangle Institute
- **Application of Chemical Looping with Spouting Fluidized Bed for Hydrogen Rich Syngas Production from Catalytic Coal Gasification**, *Kunlei Liu*, University of Kentucky

4:30 p.m. **15-MINUTE BREAK**

4:45 p.m. **PANEL SESSION – ADVANCED REACTION**
Moderator – *James Fisher*, National Energy Technology Laboratory

- **Advanced Reaction Systems FWP Overview and Path to Development**,
James C. Fisher II, NETL – Research and Innovation Center
- **Microbial Enhanced Coalbed Systems**,
Djuna Gulliver, NETL – Research and Innovation Center
- **Reaction Intensification: Testing Systems and Enabling Materials**,
Jonathan Lekse, NETL – Research and Innovation Center
- **Virtual Reactor Design, Validation, and Optimization through CFD Modeling**,
Dirk Van Essendelft, NETL – Research and Innovation Center

TUESDAY, MARCH 21 TRACK A – WILLIAM PENN BALLROOM

7:30 a.m. REGISTRATION AND CONTINENTAL BREAKFAST

8:30 a.m.

Plenary Session

- **Overview of Advanced Fossil Technology Systems**
  Mr. Angelos Kokkinos, Director AFETS, U.S. DOE
- **Overview of Energy Advanced Energy Systems**
  Mr. Regis Conrad, Director Advanced Energy Systems, U.S. DOE
- **University Coalition for Fossil Energy Research**
  Dr. Chunshan Song, Director, Energy Institute, Pennsylvania State University
- **Technology Maturation in Power Generation**
  Mr. Thomas Alley, Jr., VP Generation, Electric Power Research Institute

10:00 a.m. **MORNING BREAK**

TRACK A CROSSCUTTING RESEARCH

10:30 a.m. **SESSION 4 – SENSORS**
Moderator – *Karol Schrems*, National Energy Technology Laboratory

- **Advanced Ceramic Materials and Packaging Technologies for Realizing Sensors Operable in Advanced Energy Generation Systems**, *Jason Fish*, Sporian Microsystems Inc.
- **High-Temperature Sapphire Pressure Sensors for Harsh Environments**,
  Alexandra Garraud, University of Florida

11:30 a.m. **LUNCH (ON YOUR OWN)**

1:00 p.m. **SESSION 5 – ADVANCED PROCESS CONTROLS**
Moderator – *Jessica Mullen*, National Energy Technology Laboratory

- **Advanced Control Architecture and Sensor Information Development for Process Automation, Optimization, and Imaging of Chemical Looping Systems**, *Andrew Tong*, Ohio State University
- **Development of Integrated Biomimetic Framework with Intelligent Monitoring, Cognition and Decision Capabilities for Control of Advanced Energy Plants**, *Debangsu Bhattacharyya*, West Virginia University Research Corporation
- **Sensors and Controls (Engineering of Complex Systems)**,
  Zachary Reinhart, Ames National Laboratory

2:30 p.m. **AFTERNOON BREAK**

3:00 p.m. **SESSION 6 – SENSORS**
Moderator – *Robert Fryer*, National Energy Technology Laboratory

- **Passive Wireless Sensors Fabricated by Direct-Writing for Temperature and Health Monitoring of Energy Systems in Harsh-Environments**, *Nandhini Ranganathan & Michael Comparetto* (Student Researchers), West Virginia University
- **Smart Refractory Sensor Systems for Wireless Monitoring of Temperature, Health and Degradation of Slagging Gasifiers**,
  Edward Sabolsky, West Virginia University Research Corporation
- **Scenario Simulations of Potential Cost Savings from R&D in Sensors and Controls for Coal-Fired Power Plants**,
  Chris Nichols, NETL – Research and Innovation Center

4:30 P.M. TO 6:00 P.M. **POSTER SESSION**

TUESDAY, MARCH 21 TRACK B – THREE RIVERS ROOM

7:30 a.m. REGISTRATION AND CONTINENTAL BREAKFAST

8:30 a.m.

Plenary Session

- **Overview of Advanced Fossil Technology Systems**
  Mr. Angelos Kokkinos, Director AFETS, U.S. DOE
- **Overview of Energy Advanced Energy Systems**
  Mr. Regis Conrad, Director Advanced Energy Systems, U.S. DOE
- **University Coalition for Fossil Energy Research**
  Dr. Chunshan Song, Director, Energy Institute, Pennsylvania State University
- **Technology Maturation in Power Generation**
  Mr. Thomas Alley, Jr., VP Generation, Electric Power Research Institute

10:00 a.m. **MORNING BREAK**

TRACK B CROSSCUTTING RESEARCH

10:30 a.m. **SESSION 4 – COMPUTATIONAL MATERIALS**
Moderator – *Rick Dunst*, National Energy Technology Laboratory

- **New Mechanistic Models of Long Term Evolution of Microstructure and Mechanical Props of Nickel Based Alloys**, *Alex Greaney*, Oregon State University
- **Computational Design and Perf Prediction of Creep-Resistant Ferritic Superalloys**, *Peter Liaw*, University of Tennessee

11:30 a.m. **LUNCH (ON YOUR OWN)**

1:00 p.m. **SESSION 5 – COMPUTATIONAL MATERIALS**
Moderator – *Karol Schrems*, National Energy Technology Laboratory

- **Computational Design and Discovery of Ni-Based Alloys and Coatings: Thermodynamic Approaches Validated by Experiments**, *Zi-Kui Liu*, Pennsylvania State University
- **Use of Data Analytics in Advanced Alloy Development: Trends and Modeling**, V*yacheslav (Slava) Romanov*, NETL – Research and Innovation Center
- **Oxidation and Microstructural Evolution: Computational Investigations & Model Development**, *Youhai Wen*, NETL – Research and Innovation Center

2:30 p.m. **AFTERNOON BREAK**

3:00 p.m. **SESSION 6 – ADVANCED MATERIALS AND IDAES**
Moderator – *Jason Hissam*, National Energy Technology Laboratory

- **Rational Design of Mixed-Metal Oxides for Chemical Looping Combustion of Coal Via Computational Experimental Studies**, *Fanxing Li*, North Carolina State University
- **Update on Techno-Economic Viability of A-USC Systems**, *Travis Shultz*, NETL – Research and Innovation Center
- **Institute for the Design of Advanced Energy Systems (IDAES)**, *Anthony Burgard*, NETL – Research and Innovation Center

4:30 P.M. TO 6:00 P.M. **POSTER SESSION**

TUESDAY, MARCH 21 TRACK C – RIVERBOAT ROOM

7:30 a.m. REGISTRATION AND CONTINENTAL BREAKFAST

8:30 a.m.

Plenary Session

- **Overview of Advanced Fossil Technology Systems**
  Mr. Angelos Kokkinos, Director AFETS, U.S. DOE
- **Overview of Energy Advanced Energy Systems**
  Mr. Regis Conrad, Director Advanced Energy Systems, U.S. DOE
- **University Coalition for Fossil Energy Research**
  Dr. Chunshan Song, Director, Energy Institute, Pennsylvania State University
- **Technology Maturation in Power Generation**
  Mr. Thomas Alley, Jr., VP Generation, Electric Power Research Institute

10:00 a.m. **MORNING BREAK**

TRACK C MODULAR GASIFICATION-BASED ENERGY SYSTEMS WORKSHOP

10:30 a.m. **SESSION 4 – PANEL SESSION**
Moderator – *Dave Lyons*, Acting Gasification Technology Manager, National Energy Technology Laboratory

Panel Members:

- **Dr. Geo Richards**, Senior Fellow, NETL
- **Dr. Raghubir Gupta**, VP, RTI
- **Mr. Sean Kelly**, Director, OTM Systems, Praxair
- **Dr. Charles Freeman**, Energy & Environment Directorate, PNNL

11:30 a.m. **LUNCH (ON YOUR OWN)**

1:00 p.m. **SESSION 5 – FACILITATED BREAKOUT SESSIONS**

PARTICIPANTS BREAK INTO SMALL FOCUS GROUPS

2:30 p.m. **AFTERNOON BREAK**

3:00 p.m. **SESSION 6 – REPORTING OUT SESSION**
Moderator – *Dave Lyons*, Acting Gasification Technology Manager, National Energy Technology Laboratory

- **Breakout Session Leads Report on Discussions**
- **Final Remarks**
- **Adjourn (4:00 PM)**

4:30 P.M. TO 6:00 P.M. **POSTER SESSION**

WEDNESDAY, MARCH 22 TRACK A – WILLIAM PENN BALLROOM

TRACK A CROSSCUTTING RESEARCH

7:00 a.m. REGISTRATION AND CONTINENTAL BREAKFAST

8:00 a.m. **SESSION 7 – SIMULATION-BASED ENGINEERING**
Moderator – *Omer Bakshi*, National Energy Technology Laboratory

- **Evaluation and Demonstration of Commercialization Potential of Carbon Capture Simulation Initiative Tools within GProms, Advanced Simulation Platform**, *Adekola Lawal*, Process Systems Enterprise
- **The SMARTER Project (Science of Multicomponent Alloys: Roadmap for Theoretical and Experimental Research)**, *Matthew Kramer*, Ames National Laboratory
- **Development of Reduced Order Model for Reacting Gas-Solids Flow Using Proper Orthogonal Decomposition**, *Janhavi Chitale*, Florida International University
- **Advancement of CFD-based Tools for Design and Optimization of Energy Devices**, *Jeff Dietiker*, NETL – Research and Innovation Center

10:00 a.m. **MORNING BREAK**

10:30 a.m. **SESSION 8 – SIMULATION-BASED ENGINEERING**
Moderator – *Otis Mills*, National Energy Technology Laboratory

- **High Fidelity Computational Model for Fluidized Bed**, *Vinod Kumar*, University of Texas at El Paso
- **Kinetic Theory Modeling of Turbulent Multiphase Flow**, *Bo Kong*, Ames National Laboratory

11:30 a.m. **LUNCH (ON YOUR OWN)**

1:00 p.m. **SESSION 9 – OPTICAL SENSORS**
Moderator – *Jessica Mullen*, National Energy Technology Laboratory

- **Distributed Fiber Sensing Systems for 3D Combustion Temperature Field Monitoring in Coal-Fired Boilers Using Optically Generated Acoustic Waves**, *Xingwei Wang*, University of Massachusetts – Lowell
- **Robust Metal-Ceramic Coaxial Cable Sensors for Distributed Temp Monitoring in Harsh Environments of Fossil Energy Power Systems**, *Adam Trontz* (Student Researcher) & *Shixuan Zeng* (Student Researcher), University of Cincinnati
- **Reduced Mode Sapphire Optical Fiber and Sensing System**, *Dan Homa*, Virginia Polytechnic Institute and State University

2:30 p.m. **AFTERNOON BREAK**

3:00 p.m. **SESSION 10 – SENSORS & CONTROLS**
Moderator – *Sydni Credle*, National Energy Technology Laboratory

- **Optical Fiber Based Sensors for Future Fossil Energy Applications**, *Paul Ohodnicki*, NETL – Research and Innovation Center
- **Adaptive Electrical Capacitance Volume Tomography for Real-Time Measurement of Solids Circulation Rate at High Temperatures**, *Qussai Marashdeh*, Tech4Imaging
- **Sensors and Controls – Merged Environment for Simulation and Analysis IMESA**, *Paolo Pezzini*, Ames National Laboratory
- **Evolving Robust and Reconfigurable Multi-Objective Controllers for Advanced Power Systems**, *Shauharda Khadka*, Oregon State University

WEDNESDAY, MARCH 22 TRACK B – THREE RIVERS ROOM

TRACK B CROSSCUTTING RESEARCH

7:00 a.m. REGISTRATION AND CONTINENTAL BREAKFAST

8:00 a.m. **SESSION 7 – COMPUTATIONAL MATERIALS**
Moderator – *Vito Cedro*, National Energy Technology Laboratory

- **Physics-based Creep Simulation of Thick Section Welds in High Temperature and Pressure Applications**, *Thomas M. Lillo*, INL – Idaho National Laboratory
- **Advanced Alloy Design Concepts for High Temperature Fossil Energy Applications**, *Yukinori Yamamoto*, ORNL – Oak Ridge National Laboratory
- **Weldability of Creep Resistant Alloys for Advanced Power Plants**, *Xinghua Yu*, ORNL – Oak Ridge National Laboratory
- **Computational System Dynamics (Computational Design of Multiscale Systems)**, *Richard LeSar*, Ames National Laboratory

10:00 a.m. **MORNING BREAK**

10:30 a.m. **SESSION 8 – STRUCTURAL MATERIALS**
Moderator – *Anthony Zinn*, National Energy Technology Laboratory

- **Gas Turbine Materials Life Assessment and Non-Destructive Evaluation**, *Jiangang Sun*, ANL – Argonne National Laboratory
- **Development of Nondestructive Evaluation (NDE) Methods for Structural and Functional Materials**, *Jiangang Sun*, ANL – Argonne National Laboratory

11:30 a.m. **LUNCH (ON YOUR OWN)**

1:00 p.m. **SESSION 9 – ADVANCED MANUFACTURING**
Moderator – *Omer Bakshi*, National Energy Technology Laboratory

- **Ceramic High Temperature Thermoelectric Heat Exchanger and Heat Recuperators in the Power Generation Systems**, *Xueyan Song*, West Virginia University Research Corporation
- **Additive Manufacturing of Fuel Injectors**, *Mahdi Jamshidinia*, Edison Welding Institute, Inc.
- **High Temperature Ceramic Heat Exchanger for Solid Oxide Fuel Cell**, *Jose Luis Cordova*, Mohawk Innovative Technology, Inc.

2:30 p.m. **AFTERNOON BREAK**

3:00 p.m. **SESSION 10 – STRUCTURAL MATERIALS AND WATER TREATMENT & REUSE**
Moderator – *Barbara Carney*, National Energy Technology Laboratory

- **Micro Channel Heat Exchangers based on Alloy 230: Exposure Characteristics and Mechanical Behavior**, *Omer Dogan*, NETL – Research and Innovation Center
- **Creep-Fatigue-Oxidation Interactions: Predicting Alloy Lifetimes under Fossil Energy Service Conditions**, *Sebastien Dryepondt*, ORNL – Oak Ridge National Laboratory
- **Optimization of Advanced Steels for Cyclic Operation Through an Integration of Material Testing, Modeling and Novel Component Test Validation**, *John Siefert*, Electric Power Research Institute Inc.
- **Exploring Energy-Water Issues in the United States**, *Vince Tidwell*, SNL – Sandia National Laboratories

WEDNESDAY, MARCH 22 TRACK C – RIVERBOAT ROOM

TRACK C RARE EARTH ELEMENTS

7:00 a.m. REGISTRATION AND CONTINENTAL BREAKFAST

8:00 a.m. Plenary Session
Mr. Angelos Kokkinos, Director AFETS, U.S. DOE
Ms. Mary Anne Alvin, Technology Manager, Rare Earth Elements, NETL, U.S. DOE
Dr. Alex King, Ames National Laboratory, U.S. Department of Energy
Mr. Morgan Summers, Systems Engineering and Analysis, NETL, U.S. DOE

10:00 a.m. **MORNING BREAK AND INVITED POSTERS (UNIVERSITY OF KENTUCKY AND TETRATECH INC.)**

10:30 a.m. **SESSION 8 – RARE EARTH ELEMENTS**
Moderator – *Rick Dunst*, National Energy Technology Laboratory

- **Pilot-scale Testing of an Integrated Circuit for the Extraction of Rare Earth Minerals and Elements from Coal and Coal Byproducts Using Advanced Separation Technologies**, *Rick Honaker*, University of Kentucky
- **High Yield and Economical Production of Rare Earth Elements from Coal Ash**, *Dorin Preda*, Physical Sciences Inc.

11:30 a.m. **LUNCH (ON YOUR OWN)**

1:00 p.m. **SESSION 9 – RARE EARTH ELEMENTS**
Moderator – Charles Miller, National Energy Technology Laboratory

- **Plasma ARC Gasification Based Rare Earth Element Recovery from Coal Fly Ash**, *Ken Jeffers*, Southern Research Institute
- **Economically Viable and Environmentally Benign High Performance Technology to Recover REE from Coal by-products**, *Gary Carlson*, Tusaar, Inc
- **Overview and Accomplishments of R&ICs Rare Earth Elements from Coal and Coal By-Products**, *Evan Granite*, NETL – Research and Innovation Center

2:30 p.m. **AFTERNOON BREAK AND INVITED POSTERS (WEST VIRGINIA UNIVERSITY AND XLIGHT CORPORATION)**

3:00 p.m. **SESSION 10 – RARE EARTH ELEMENTS**
Moderator – *Anthony Zinn*, National Energy Technology Laboratory

- **Novel Membrane and Electrodeposition-based Separation and Recovery of Rare Earth Elements from Coal Combustion Residues**, *Heileen Hsu-Kim*, Duke University
- **Recovery of Rare Earth Elements (REEs) from Coal with a Closed Loop Leaching Process**, *Rick Peterson*, Battelle Memorial Institute
- **Recovery of Rare Earth Elements (REEs) from Coal Mine Drainage**, *Paul Ziemkiewicz*, WV Water Research Institute
- **A Pollution-Prevention and Economically Viable Technology for Separation of Rare Earth Elements from Powder River Basin (PRB) Coal Ashes**, *Maohong Fan*, University of Wyoming

5:00 p.m. **15-MINUTE BREAK**

5:15 p.m. **SESSION 10A – RARE EARTH ELEMENTS**
Moderator – *Anthony Zinn*, National Energy Technology Laboratory Rare Earth Elements Charles Miller

- **Bench-Scale Technology to Economically Separate, Extract and Concentrate Mixed REEs from Coal and Coal Byproducts including Aqueous Effluents**, *Steven Benson*, University of North Dakota
- **Development of a Novel CFD Model for Large-Scale REE Extraction Process**, *Sofiane Benyahia*, NETL – Research and Innovation Center
- **Evidence of Mobilization of REE: Geological Aspects of REE Formation in the United States**, *Tracy Bank*, AECOM

THURSDAY, MARCH 23 TRACK A – WILLIAM PENN BALLROOM

TRACK A CROSSCUTTING RESEARCH

7:30 a.m. REGISTRATION AND CONTINENTAL BREAKFAST

8:30 a.m. **SESSION 11 – WATER TREATMENT & REUSE**
Moderator – *Barbara Carney*, National Energy Technology Laboratory

- **Advanced Integrated Technologies for Treatment and Reutilization of Impaired Water in Fossil Fuel-Based Power Plant Systems**, *Jason Trembly*, Ohio University
- **Model-Based Extracted Water Desalination System for Carbon Sequestration**, *Rachel Gettings*, GE Global Research
- **Dewatering of High Salinity Brines**, *Jason Arena*, NETL – Research and Innovation Center

10:00 a.m. **MORNING BREAK**

10:30 a.m. **SESSION 12 – WATER TREATMENT & REUSE**
Moderator – *Jessica Mullen*, National Energy Technology Laboratory

- **Low-Energy Water Recovery from Subsurface Brines**, *Young Chul Choi*, Research Triangle Institute
- **Advanced Thermally Robust Membranes for High Salinity Produced Brine Treatment**, *Rajinder Singh*, LANL – Los Alamos National Laboratory

11:30 a.m. **LUNCH (ON YOUR OWN)**

1:00 p.m. **SESSION 13 – WATER TREATMENT & REUSE**
Moderator – *Maria Reidpath*, National Energy Technology Laboratory

- **Fouling-Resistant Membranes for Treating Concentrated Brines for Water Reuse in Advanced Energy Systems**, *Zachary Hendren*, Research Triangle Institute
- **Development of Membrane Distillation Technology Utilizing Waste Heat for Treatment of High Salinity Wastewaters**, *Omkar Lokare*, University of Pittsburgh
- **Treatment of Produced Water from Carbon Sequestration Sites for Water Reuse, Mineral Recovery and Carbon Utilization**, *Jay Renew*, Southern Research Institute

2:30 p.m. **AFTERNOON BREAK**

3:00 p.m. **SESSION 14 – WATER TREATMENT & REUSE**
Moderator – *Omer Bakshi*, National Energy Technology Laboratory

- **Integrated Sensors for Water Quality**, *Laurel Frediani*, Sporian Microsystems Inc.
- **Wireless Networked Sensors in Water for Heavy Metal Detection**, *Hang Ruan*, Nanosonic Inc.
- **Evaluating the Techno-Economic Feasibility of Forward Osmosis Processes Utilizing Low Grade Heat**, *Daniel Gingerich*, Carnegie Mellon University
- **An Integrated Supercritical System for Efficient Produced Water Treatment and Power Generation**, *Seyed Dastgheib*, University of Illinois

THURSDAY, MARCH 23 TRACK B – THREE RIVERS ROOM

TRACK B **CROSSCUTTING RESEARCH**

7:30 a.m. REGISTRATION AND CONTINENTAL BREAKFAST

8:30 a.m. **SESSION 11 – AUSC MATERIALS**
Moderator – *Vito Cedro*, National Energy Technology Laboratory

- **Advanced Ultra-Supercritical Component Testing**,
  Horst Hack, Energy Industries of Ohio Inc.
- **Properties of Advanced Ni-Based Alloys for A-USC Steam Turbines**,
  Phil Maziasz, ORNL – Oak Ridge National Laboratory
- **Materials Qualification and Deployment for High Efficiency Coal Fired Boilers**,
  Bruce Pint, ORNL – Oak Ridge National Laboratory

10:00 a.m. **MORNING BREAK**

10:30 a.m. **SESSION 12 – AUSC MATERIALS**
Moderator – *Rick Dunst*, National Energy Technology Laboratory

- **Advanced Ultrasupercritical Materials Thick-Walled Cycling Header Development for Comtest-AUSC**,
  Buchi Ganta, Alstom Power, Inc
- **Corrosion Issues in Advanced Coal Fired Boilers**,
  Bruce Pint, ORNL – Oak Ridge National Laboratory

11:30 a.m. **LUNCH (ON YOUR OWN)**

1:00 p.m. **SESSION 13 – ADVANCED MANUFACTURING**
Moderator – *Vito Cedro*, National Energy Technology Laboratory

- **Low Cost Fabrication of ODS Materials**,
  Glenn Grant, PNNL – Pacific Northwest National Laboratory
- **Microstructure and Properties of Ni-based Components fabricated by Additive Manufacturing**,
  Sebastien Dryepondt, ORNL – Oak Ridge National Laboratory
- **Solid State Joining of Creep Enhanced Ferritic Steels**,
  Glenn Grant, PNNL – Pacific Northwest National Laboratory

2:30 p.m. **AFTERNOON BREAK**

3:00 p.m. **SESSION 14 – STRUCTURAL MATERIALS**
Moderator – *Karol Schrems*, National Energy Technology Laboratory

- **Advanced Materials Issues in Supercritical Carbon Dioxide**,
  Bruce Pint, ORNL – Oak Ridge National Laboratory
- **Status of NETL Superalloy Development: Melt Processing & Heat Treatment**,
  Paul Jablonski, NETL – Research and Innovation Center
- **Heat Resistant 9 Cr Steels: Creep Analysis Comparisons**,
  Jeff Hawk, NETL – Research and Innovation Center
- **Concentrated Solid Solution Alloys: Computational Modeling and Experimental Validation**,
  Michael Gao, AECOM

THURSDAY, MARCH 23 TRACK C – RIVERBOAT ROOM

TRACK C **CROSSCUTTING RESEARCH**

7:30 a.m. REGISTRATION AND CONTINENTAL BREAKFAST

8:30 a.m. **SESSION 11 – DIRECT POWER EXTRACTION**
Moderator – *Jason Hissam*, National Energy Technology Laboratory

- **Analysis, Simulation, and Experimental Validation for MHD Energy Conversion**, *Rigel Woodside*, NETL – Research and Innovation Center
- **Effect of Potassium Carbonate on Electrodes in a High-Velocity Oxy-Fuel Combustion Flame**, *Peter Hsieh*, NETL – Research and Innovation Center
- **Combustion Synthesis of Boride-Based Electrode Materials for Magneto Hydrodynamic (MHD) Direct Power Extraction**, *Sergio Cordova*, University of Texas at El Paso

10:00 a.m. **MORNING BREAK**

10:30 a.m. **SESSION 12 – DIRECT POWER EXTRACTION**
Moderator – *Maria Reidpath*, National Energy Technology Laboratory

- **High Temp High Velocity Direct Power Extraction Using an Open Cycle Oxy Combustion System**, *Norman Love*, University of Texas at El Paso
- **Novel High Temperature Carbide and Boride Ceramics for Direct Power Extraction Electrode Applications**, *Andres Behrens* (Student), Florida International University

11:30 a.m. **LUNCH (ON YOUR OWN)**

1:00 p.m. **SESSION 13 – DIRECT POWER EXTRACTION**
Moderator – *Otis Mills*, National Energy Technology Laboratory

- **Precursor-Derived Nanostructured Silicon Carbide Based Materials for Magnetohydrodynamic Electrode Applications**, *Fumio Ohuchi*, University of Washington
- **Boride Based Electrode Materials with Enhanced Stability under Extreme Conditions for MHD Direct Power Extraction**, *Indrajit Charit*, Regents of the University of Idaho

2:30 p.m. **AFTERNOON BREAK**

3:00 p.m. **SESSION 14 – MFIX**
Moderator – *Jason Hissam*, National Energy Technology Laboratory

- **Use of an Accurate DNS Method to Derive, Validate and Supply Constitutive Equations for the MFIX Code**, *Yifei Duan*, University of Texas at San Antonio
- **Interfacing MFIX with PETSC and HYPRE Linear Solver Libraries**, *Gautham Krishnamoorthy*, University of North Dakota
- **MFIX-DEM Enhancement for Industry-Relevant Flows**, *William Fullmer*, University of Colorado

2017 COMBINED REVIEW MEETING POSTER PRESENTATIONS
Sternwheeler Room

1 **Investigation of High Temperature Silica Based Fiber Optic Materials**, *Dan Homa*, Virginia Polytechnic Institute and State University

2 **Raman Spectroscopy for the On-Line Analysis of Oxidation States of Oxygen Carrier Particles**, *Hergen Eilers*, Washington State University

3 **Engineering Metal Oxide Nanomaterials for Fiber Optical Sensor Platforms**, *Peng Chen*, University of Pittsburgh

4 **A Guideline for the Assessment of Uniaxial Creep and Creep-Fatigue Data and Models**, *Jack Chessa*, University of Texas at El Paso

5 **Enabling Technologies for Surface Acoustic Wave (SAW) Sensors in Harsh Environments**, *Robert Fryer*, NETL - Research and Innovation Center

6 **Development of Control Strategies for the Dynamic Operation of a 10MWe Supercritical CO2 Recompression Brayton Cycle**, *Eric Liese*, NETL - Research and Innovation Center

7 **Advanced Sensors and Controls FWP, Diagnostics and Sensor Applications in R&IC Research**, *Ben Chorpening*, NETL - Research and Innovation Center

8 **NETL Insights Into Hybrid Power Systems: Opportunities and Overcoming Challenges**, *Lawrence Shadle*, NETL - Research and Innovation Center

9 **R&IC-SEA Water Management Research**, *Erik Shuster*, NETL - Research and Innovation Center

10 **Continuous Water Quality Sensing for Flue Gas Desulfurization Wastewater**, *Lee Moradi*, University of Alabama At Birmingham

11 **Developing Cost Effective Biological Removal Technology for Selenium Nitrate from Flue Gas Desulfurization (FGD) Wastewater from an Existing Power Generating Facility**, *Sanjaya*, West Virginia State University

12 **The Fundamental Creep Behavior Model of GR.91 Alloy by Integrated Computational Materials Engineering (ICME) Approach**, *Yu Zhong*, Florida International University

13 **Development of a Physically-Based Creep Model Incorporating ETA Phase Evolution for Nickel-Base Superalloys**, *Walter Milligan*, Michigan Technological University

14 **Improved Models of Long Term Creep Behavior of High Performance Structural Alloys for Existing and Advanced Technologies Fossil Energy Power Plants**, *Jiaodong Gong*, QuesTek Innovations LLC

15 **Additive Manufacturing of Energy Harvesting Material System for Active Wireless Microelectromechanical Systems (MEMS) Sensors**, *Ryan Wicker*, University of Texas at El Paso

2017 COMBINED REVIEW MEETING POSTER PRESENTATIONS, Cont.
Sternwheeler Room

16 **ICME for Creep of NI-Base Superalloys in Advanced Ultra-Supercritical Steam Turbines**, *Stephen Niezgoda*, Ohio State University

17 **Optical and Thermodynamic Properties of Pure- and La-doped $SrTiO_3$**, *Yuhua Duan*, NETL - Research and Innovation Center

18 **Band-gap opening properties of graphene binding with low-concentration**, *Yuhua Duan*, NETL - Research and Innovation Center

19 **Intermediate Temperature Nano-Structured Ceramic Hollow Fiber Membranes for Oxygen Separation**, *Chris Xue*, University of South Carolina

20 **Advancing Coal Catalytic Gasification to Promote Optimum Syngas Production**, *Francine Battaglia*, Virginia Polytechnic Institute and State University

21 **Production of High-Purity O_2 via Membrane Contactor with Oxygen Carrier Solutions**, *Shinguang Li*, Gas Technology Institute

22 **Catalytic PRB Coal/CO_2 Gasification for Fuels and Chemicals with Two Different Types of Syngas and Negative or Low CO_2 Emissions**, *Maohong Fan*, University of Wyoming

23 **Increasing the Rate and Extent of Microbial Coal to Methane Conversion through Optimization of Microbial Activity, Thermodynamics, and Reactive Transport**, *Matthew Fields*, Montana State University

24 **Optimization, Scaleup, and Design of Coal-Dependent Methanogenesis in Preparation for In-Situ Field Demonstration**, *Matthew Fields*, Montana State University

25 **Ceramic Proppant Design for In-Situ Microbially Enhanced Methane Recovery**, *Taylor Sparks*, University of Utah

26 **Optimized Microbial Conversion of Bituminous Coal to Methane for In-Situ and Ex-Situ Applications**, *Yanna Liang*, Southern Illinois University

27 **Wave Liquefaction: a REMS Approach to Manufacture Fuels, Chemicals, and Materials from Coal**, *George Skoptsov*, H Quest

28 **Small-scale pilot plant for the gasification of coal and coal/biomass blends and conversion of derived syngas to liquid fuels via Fischer-Tropsch synthesis**, *Kunlei Liu*, University of Kentucky Research Foundation

29 **Design and Fabrication of Novel Mixed Ion-Electron Conducting Membranes for Oxygen Separation**, *Balakrishnan Nair*, HiFunda LLC

03-20-2017 – 1030A

FE0026219 – WIRELESS 3D NANOROD COMPOSITE ARRAYS BASED HIGH TEMPERATURE SURFACE-ACOUSTIC-WAVE SENSORS FOR SELECTIVE GAS DETECTION THROUGH MACHINE LEARNING ALGORITHMS

ORGANIZATION: University of Connecticut **PRINCIPAL INVESTIGATOR**: Yu Lei
TEAM MEMBERS: Pu-Xian Gao, Sanguthevar Rajasekaran
PRESENTER: Dongwook Kwak (Student Researcher)

ABSTRACT

In situ, real-time monitoring the composition of combustion gases usually requires sensors to be operative at high temperature environment. Up to date, commercially available sensor technology for such harsh environment is extremely limited due to the high requirements for sensing materials and sensor performance. Therefore, there is an urgent need to advance high temperature stable sensing materials and develop novel high temperature sensing strategy to realize fast, sensitive, selective, rugged, and cost-effective high-temperature gas sensors for power and fuel systems. The project objective is to combine the concept of high-temperature stable passive wireless SAW sensor arrays with novel high-temperature stable perovskite coated three-dimensional (3D) metal oxide nanorod composites as well as machine learning algorithms to achieve highly selective and wireless detection of gas species in high-temperature mixed gas environment. This work will advance the fundamental understanding of gas-responsive high temperature sensing materials and machine-learning based high temperature wireless SAW gas detection with high sensitivity, enhanced selectivity and high temperature stability in general and, if successful, might have an enormous impact on in-situ, real-time, wireless harsh environment sensing and detection technology, thus could bring a potential leap in various combustion monitoring and control devices development.

03-20-2017 – 1100A

FE0011577 – OXIDE BASED HETEROSTRUCTURED NANOWIRE ARRAYS FOR ULTRA-SENSITIVE AND SELECTIVE MULTI-MODE HIGH TEMPERATURE GAS DETECTION

ORGANIZATION: University of Connecticut **PRINCIPAL INVESTIGATOR**: Pu-Xian Gao
TEAM MEMBERS: Bo Zhang, Hui-Jan Lin, Can Cui, Yu Lei
PRESENTER: Bo Zhang (Student Researcher)

ABSTRACT

Using vapor phase and solution phase deposition methods, heterostructured nanowire arrays have been successfully fabricated composed of metal oxide nanowire cores and nanoparticle decorations of perovskite, metal oxide and noble metal nanoparticles on ceramic planar substrates. Various electron microscopy and spectroscopy techniques have been utilized to investigate the physico-chemical characteristics of heterostructured nanowires. Multi-mode gas sensing platform has been achieved at high temperature to include photocurrent, electrical resistance and electrochemical impedance modes. Depending on the selections of comprising materials, dimensions and post-treatment processes, trace amount decoration of perovskite and noble metal nanoshells may enable formations of catalytic filters, sensitizers and hetero-junctions that can drastically enhance nanosensor performance in both oxidative and reductive gas atmospheres and improve the detection limit to ppb level. Specifically the progress on the materials-synergy effect in Ga_2O_3/(La, Sr)FeO_3 and ZnO-Au-Fe_2O_3 core-shell nanowire array sensors are updated and discussed toward CO and NO_2 sensing. Toward mixture gas conditions, the multi-mode metal oxide based nanowire array sensors may allow selective and sensitive detection of multiple species in a single-device platform.

03-20-2017 – 1300A

FE0026217 – INTEGRATED HARSH ENVIRONMENT GAS / TEMPERATURE WIRELESS MICROWAVE ACOUSTIC SENSOR SYSTEM FOR FOSSIL ENERGY APPLICATIONS

ORGANIZATION: University of Maine **PRINCIPAL INVESTIGATOR**: Mauricio Pereira da Cunha
TEAM MEMBERS: Robert Lad (Co-PI), Paul Ohodnicki
PRESENTER: Mauricio Pereira da Cunha

ABSTRACT

The overall goals of this project are to develop and demonstrate the performance of an integrated gas / temperature microwave acoustic sensor capable of passive operation (no batteries) over the range 350°C to 1000°C in harsh environments relevant to fossil energy technology, with specific applications to coal gasifiers, combustion turbines, solid oxide fuel cells, and advanced boiler systems.

The wireless sensor system is based upon a surface acoustic wave (SAW) sensor platform that is configured using a high temperature piezoelectric crystal (langasite) with electrodes capable of stable operation in high-temperature harsh-environment conditions, and sensitive doped films to detect H_2, O_2, and NO_x gases, and to also monitor the gas temperature in the harsh environment.

The project outcomes will significantly advance the capabilities of harsh environment sensor technology to benefit the needs of fossil energy power plants. Acquiring temperature and gas composition data from wireless sensors at diverse harsh environment locations in power plants will aid in increasing fuel burning efficiency, reducing gaseous emissions, and reducing maintenance costs through condition-based monitoring.

03-20-2017 – 1330A

FE0026170 – LOW-COST, EFFICIENT AND DURABLE HIGH TEMPERATURE WIRELESS SENSORS BY DIRECT WRITE ADDITIVE MANUFACTURING FOR APPLICATION IN FOSSIL ENERGY SYSTEMS

ORGANIZATION: Washington State University **PRINCIPAL INVESTIGATOR**: Rahul Panat
TEAM MEMBERS: Md. Taibur Rahman (WSU), Russell Moser (WSU), Juan Gomez (UT, El Paso), P. Dubey (UT, El Paso), C. V. Ramana (UT, El Paso)
PRESENTER: Md. Taibur Rahman (Student Researcher)

ABSTRACT

Additively manufactured nanoparticle films are being considered for high temperature sensor applications. Such films can monitor critical parameters such as strain and pressure in harsh environments and hard to reach places in Fossil Energy (FE) systems. Current work focuses on carrying out a detailed electrical and mechanical characterization of nanoparticles and their films for the use in sensor applications. Impedance and microstructural changes of the metal nanoparticle films fabricated using an Aerosol Jet based advanced additive manufacturing method are presented. High temperature in-situ characterization was performed on Ag, NiCr, and Ni nanoparticles and films. Transmission electron microscopy (TEM), selective area electron diffraction (SAED), X-ray diffraction, and SEM studies are performed to understand the microstructural changes and oxidation behavior of these materials. The results show that at the time scale of the experiments, the Ag shows minimal/no oxidation as seen under the impedance measurements and confirmed by XRD/XPS studies. Further, NiCr nanoparticles show a satisfactory oxidation performance up to about 400 °C. These results are used to select materials for the Aerosol Jet printing method for the FE sensors. A custom strain sensing set up was developed and integrated with an oven to test the printed sensors at low frequencies and temperatures up to 500 °C. A reliability test set up has also been constructed to estimate the interfacial fracture energy for the printed sensors for their reliable operation. The results presented in this work establish additive printing as a viable technology for sensors on arbitrary surfaces in FE systems.

03-20-2017 – 1400A

FE0026348 – NOVEL TEMPERATURE SENSORS AND WIRELESS TELEMETRY FOR ACTIVE CONDITION MONITORING OF ADVANCED GAS TURBINES

ORGANIZATION: Siemens Corporation **PRINCIPAL INVESTIGATOR**: Anand A. Kulkarni

TEAM MEMBERS: Joshua McConkey (Siemens Energy), John Fraley (CREE)

PRESENTER: Anand A. Kulkarni

ABSTRACT

The objective of the program is to integrate durable, non-intrusive, ultra-high-temperature thermocouples with high temperature wireless telemetry to enable materials prognostics and active condition monitoring of hot gas path turbine blades in industrial gas turbines. The concept of Condition monitoring sought here comprises engine and component monitoring sensor data transmitted wirelessly from a rotating component, and Operation-Based Assessment (OBA), followed by an integration and interpretation of these data to achieve life consumption prediction and Performance Monitoring. Siemens and Wolfspeed are developing a Smart turbine blade for long-term monitoring of combustion engine operation targeting durability in operating temperatures up to 1400°C with wireless deployment of 550°C. Phase 1 efforts involved scaling up the thermal spray process to develop high temperature ceramic thermocouples, development of wireless telemetry system components, and demonstration of integrated sensor/wireless telemetry approach on stationary lab test rig. Phase 2 will mostly focus on validation testing of sensor-wireless telemetry package in spin rig along with an advanced OBA model utilizing artificial intelligence. Significant efforts would be carried out towards download of the technology onto components to be tested an actual gas turbine engine for active condition monitoring.

03-20-2017 – 1430A

FE0026393 – MFIX-DEM PHI: PERF AND CAPABILITY IMPROVEMENTS TOWARDS INDUSTRIAL GRADE OPEN-SOURCE DEM FRAMEWORK W INTEGRATED UNCERTAINTY QUANTIFICATION

ORGANIZATION: Arizona State University **PRINCIPAL INVESTIGATOR**: Aytekin Gel

TEAM MEMBERS: Yang Jiao (ASU), Heather Emady (ASU), Charles Tong (LLNL), Jonathan Hu (SNL),Shaohua Chen (ASU), Manogna Adepu (ASU)

PRESENTER: Manogna Adepu (Student Researcher)

ABSTRACT

The objectives of the project are to improve the performance and physical modeling capabilities of MFiX-DEM while tightly integrating these improvements with an intuitive graphical user interface driven uncertainty quantification framework, and to effectively promote industrial adoption of MFiX-DEM. More specifically, in the 2016-1 release version of MFIX-DEM, each solid phase is only allowed to possess a single particle size, making it extremely difficult to simulate a true polydisperse system, in which each particle can possess a distinct particle diameter. We have developed a new feature for MFIX-DEM to easily handle an arbitrary number of solid phases, each possessing a distinct particle-size distribution, which can be prescribed by the user as input. The implementation was tested and validated with in-house hopper bin discharge experiments, a commonly used set-up with many industrially relevant applications. As part of the physical modeling capability enhancements, the wall-bed conduction heat transfer model was also validated using a rotary drum configuration, which is another setup often used by the industry. The end goal of Phase 1 research is to pave the way to create a user-friendly, powerful open-source multiphase flow simulation environment seamlessly integrated with a capability for the credibility assessment of the results and easily usable by diverse users.

03-20-2017 – 1500A

FE0023118 – DISTRIBUTED WIRELESS ANTENNA SENSORS FOR BOILER CONDITION MONITORING

ORGANIZATION: University of Texas at Arlington **PRINCIPAL INVESTIGATOR**: Haiying Huang

TEAM MEMBERS: Jian Luo, Ankur Jain, Jiuyuan Nie, Franck Mbanya Tchafa

PRESENTER: Haiying Huang

ABSTRACT

Monitoring the operational condition of coal-fired boilers is an important task with potential benefits, such as in-situ process control, real time health assessment of structures, reduced downtime etc. We identified three key parameters, namely temperature, strain, and soot accumulation, for conditioning monitoring of the steam pipes in a coal-fired boiler. This project focus on developing a distributed antenna sensor array for wireless measurements of these parameters during operation. Materials development, sensor design, multi-variant analysis, and wireless interrogation without electronics were studied to realize distributed condition monitoring of coal fired boilers at a low cost. The fabrication and characterization of the antenna sensors using high-temperature materials, i.e. alumina as substrate and platinum paste as electrodes, will be presented. The challenges and solutions of achieving a sensor pattern with controlled geometric features will be discussed. For multi-modality sensing, we will present experiment results that demonstrate simultaneous sensing of temperature and mechanical strain using a single patch antenna sensor. Finally, wireless interrogation of the passive antenna sensor using a Frequency-Modulated Continuous-Wave (FMCW) Radar will be presented. The FMCW radar enables dynamic interrogation of passive antenna sensors at a low cost and thus remove a major technical challenge in transferring the wireless antenna sensor technology from research labs to real-life applications.

03-20-2017 – 1530A

FE0012321 – INVESTIGATION OF "SMART PARTS" WITH EMBEDDED SENSORS FOR ENERGY SYSTEM APPLICATIONS

ORGANIZATION: University of Texas at El Paso **PRINCIPAL INVESTIGATOR**: Yirong Lin

TEAM MEMBERS: Ahsan Choudhuri, Ryan Wicker, Yirong Lin

PRESENTER: Yirong Lin

ABSTRACT

Built-in sensor in energy system components, parts, and devices could provide the advantages of in-situ real time sensing that is achievable using traditional sensors post fabrication. While there has been a surge of developing embedded sensors for monitoring critical parameters such as strain, temperature, vibration, etc, the feasibility of applying these parts in harsh energy system environment is still yet unknown. Therefore, the research effort of this project will contribute to the goal of not only design and fabricate parts used in energy systems but also test the "smart part" in realistic energy system to determine its durability, repeatability, and stability. The goal of this proposed research is to design, fabricate, and evaluate "smart parts" with embedded sensors for energy systems. The "smart parts" will be fabricated using Electron Beam Melting (EBM) 3D printing technique with built-in piezoceramic sensors. The objectives of the proposed project are: 1) Fabricate energy system related components with embedded sensors, 2) Evaluate the mechanical properties and sensing functionalities of the "smart parts" with embedded piezoceramic sensors, and 3) Assess in-situ sensing capability of energy system parts. The influence of sensing embedding on the overall smart parts property will be assessed, in addition, the sensor performance in various energy conversion environment will be assessed.

03-20-2017 – 1600A

FE0026330 – METAL 3D PRINTING OF LOW-NOX FUEL INJECTORS WITH INTEGRATED TEMPERATURE SENSORS

ORGANIZATION: University of Texas at El Paso **PRINCIPAL INVESTIGATOR**: Ahsan Choudhuri
TEAM MEMBERS: Ryan Wicker
PRESENTER: Phillip Morton

ABSTRACT

This work necessitates the exploration of design and prototyping of a Dry Low-NOx (DLN) fuel injector with integrated temperature sensing capabilities using the Electron Beam Melting (EBM) additive manufacturing (AM) process. The lack of assembly requirements and the virtually unlimited geometrical complexity renders the EBM process particularly attractive for fabricating complex energy system components. EBM has received considerable attention due to its high energy density and energy efficiency that allows full density metal components of comparable or even better quality than those produced by traditional methods. Additionally, the unique layer-by-layer fabrication technique allows the embedding of sensors within complex components early in the design process. A generic Low-NOx fuel injector (Fig. 2) with integrated temperature sensors (Ceramic Insulated High Temperature Thermocouple: OMEGA® Nextel/XC-14-J-12) will be used as the test component for the proposed effort. Several injector test articles will be fabricated and tested using Inconel 718, Inconel 625, and/or Titanium alloys.

The proposed effort has three specific objectives: [1] Development of design methodologies for Low-NOx fuel injectors with embedded temperature capabilities for EBM based 3D Manufacturing; [2] Development of optimum EBM process parameters and powder removal techniques to remove sintered powder from internal cavities and channels of Low-NOx fuel injectors with embedded temperature sensors; and [3] Testing of the EBM fabricated Low-NOx fuel injector with integrated temperature measurement capabilities in a High Pressure Laboratory Turbine Combustor

03-20-2017 – 1630A

FE0012272 – ADDITIVE MANUFACTURING OF SMART PARTS WITH EMBEDDED SENSORS FOR IN-SITU MONITORING IN ADVANCED ENERGY SYSTEMS

ORGANIZATION: Missouri University of Science and Technology **PRINCIPAL INVESTIGATOR**: Hai-Lung Tsai
TEAM MEMBERS: Hai Xiao, Ming Leu, Junhang Dong
PRESENTER: Hai Xiao

ABSTRACT

The refractory liners and high temperature pipes are among the most-stressed and vulnerable components in most energy generation units and their operating conditions need to be continuously monitored to maximize the operation lifetime while avoiding catastrophic failures. However, there is a serious lack of available techniques for in situ long-term monitoring because of the extremely harsh environments involved. The research and development work of this project aims to develop and demonstrate the novel concept of “smart parts” with embedded sensors for in situ monitoring of multiple parameters in high temperature and high pressure harsh environments. This presentation summaries our up-to-date progresses in the following areas: (a) novel, robust, embeddable optical carrier based distributed microwave wave interfereometric (OCMI) sensors for harsh environment sensing; (b) comprehensive thermal and mechanical models of the sensor-integrated “smart parts”; (c) multifunctional protective layers between the OCMI sensor and the host materials for thermal, mechanical and chemical protection of the sensors; and (d) additive manufacturing of the smart parts with embedded sensors. In addition to refractory liners and pipes, the research results can be applied to monitoring other critical components in energy systems for improved efficiency, enhanced reliability and reduced emission.

MONDAY, MARCH 20 TRACK B CROSSCUTTING RESEARCH ABSTRACTS

03-20-2017 – 1030B
FE0024120 – PREDICTING THE OXIDATION/CORROSION PERFORMANCE OF STRUCTURAL ALLOYS IN SUPERCRITICAL CO2
ORGANIZATION: Electric Power Research Institute Inc. **PRINCIPAL INVESTIGATOR**: John Shingledecker
TEAM MEMBERS: David Thimsen, Steve Kung, Brett Tossey, Ian Wright, Adrian Sabau
PRESENTER: John P. Shingledecker

ABSTRACT

Supercritical CO_2 (sCO_2) Brayton cycles are being considered for future fossil energy systems. These sCO_2 systems offer the possibility of improved efficiency combined with smaller turbo-machinery size to a traditional Rankine steam system if operated at fluid temperatures of about 700°C. The objective of this cross-cutting materials project is to provide computational predictions of the oxidation performance of structural alloys in supercritical CO_2 in severe operating environments at high temperatures. Short and long-term isothermal laboratory testing of structural candidate alloys at high temperatures (650-750°C) and pressures (200bar) have been completed. This talk will focus on the data generated including oxide scale thickness kinetics, morphology, and the potential for carburization. Various mathematical models, including an EPRI developed model for exfoliation, will be explored to evaluate the data and materials use limits for the use of small channel heat-exchangers envisaged for these systems. In the final long-term confirmatory tests, actual heat-exchanger subcomponents have been tested and the results will also be reported.

03-20-2017 – 1100B
NETL-R&IC – ALLOY PERFORMANCE IN SCO2 ENVIRONMENTS: EFFECTS OF SCO2 EXPOSURE
ORGANIZATION: NETL - Research and Innovation Center **PRINCIPAL INVESTIGATOR**: Omer N. Dogan
TEAM MEMBERS: G. Holcomb, J. Hawk, R. Oleksak, K. Rozman, C. Carney, J. Tylczak
PRESENTER: Omer N. Dogan

ABSTRACT

Supercritical CO_2 (sCO_2) cycles are investigated for fossil fuel power generation to increase efficiency (compared to steam cycles), lower cost (capital and operations and maintenance [O&M]), and reduce the environmental impact (reduced water usage, capture ready CO_2). How the current power plant materials will perform in sCO_2 conditions is needed to be demonstrated. This project aims to determine whether the available power plant materials (including advanced ultra-super critical [A-USC] materials) are suitable for fossil fuel sCO_2 service. Investigation establishes the effect of environment (working fluid, temperature, and pressure) on selected materials by exposing mechanical testing samples to the simulated sCO_2 conditions and analysis of the exposed samples.

03-20-2017 – 1300B

FE0011585 – DEVELOPING NOVEL MULTIFUNCTIONAL MATERIALS FOR HIGH-EFFICIENCY ELECTRICAL ENERGY STORAGE

ORGANIZATION: University of Tennessee **PRINCIPAL INVESTIGATOR**: Feng-Yuan Zhang
TEAM MEMBERS: Jingke Mo, Stuart Steen, Zhenye Kang, William Barnhill, Bo Han, Gaoqiang Yang
PRESENTER: Feng-Yuan Zhang

ABSTRACT

NETL is partnering with the University of Tennessee to develop a thin and well-tunable multifunctional component via micro/nano fabrication for high-efficiency electrical energy storage, which is critical for the long-term utilization of coal in energy applications to provide reliable, affordable electricity and modernize the electrical grid.

Novel titanium liquid/gas diffusion layers (LGDLs) with well-tunable pore morphologies were developed by employing micro/nano-manufacturing and showed significant performance improvements in proton exchange membrane electrolyzer cells (PEMECs). In addition, the reduction in LGDL thickness from the 350 µm of conventional LGDLs to 25 µm will substantially reduce the weight and volume of PEMEC stacks, which can lead to new avenues for future development of low-cost and higher-performance PEMECs. The well-tunable features of LGDL including pore size, pore shape, pore distribution, and thus porosity and permeability, will be valuable in developing PEMEC models and validating simulations of PEMECs with optimal and repeatable performance.

This project will further optimize novel multifunctional materials to promote the efficiency of energy storage technologies. Improvements to energy storage technologies will promote improved utilization of power plant assets that can provide operational flexibility and result in lower capital and operating costs.

03-20-2017 – 1330B

FE0023061 – VERTICALLY ALIGNED CARBON-NANOTUBES EMBEDDED IN CERAMIC MATRICES FOR HOT ELECTRODE APPLICATIONS

ORGANIZATION: University of Nebraska - Lincoln **PRINCIPAL INVESTIGATOR**: Yongfeng Lu
TEAM MEMBERS: Qiming Zou, Dawei Li
PRESENTER: Yongfeng Lu

ABSTRACT

The research goal of this project is to develop carbon nanotube-ceramic (CNT-C) composite structures in which vertically aligned CNTs (VA-CNTs) are embedded in ceramic matrices for hot electrode applications in magnetohydrodynamics (MHD) power systems. It is expected that the CNT-C composite structures would withstand the extreme environments in MHD generators and extract power directly from seeded oxy-fuel combustion fluids. Therefore, the proposed CNT-C composite structures will have all thermal and electrical properties meeting the requirements of hot electrodes, and withstanding the extreme operating conditions of the MHD systems (stable at high temperatures, chemically inert, and electrically and thermally conductive). To accomplish the primary goal, the following objectives will be achieved: 1) super growth of VA-CNT carpets; 2) fabrication of CNT-boron nitride (CNT-BN) composite structures; 3) stability and resistance studies of the CNT-BN composite structures; and 4) thermionic emissions of the CNT-BN composite structures. Upon the successful completion of the proposed project, CNT-C composite structures, such as CNT-BN, will be obtained. A fundamental understanding of the high-temperature properties of the CNT-BN composite structures will be established, including thermal stability, oxidation resistance, chemical inertness, electrochemical passiveness, electrical conductivity, thermal conductivity, and thermionic emission property. The same concept of producing CNT-BN composite structures can be expanded to a broad range of ceramic materials and form a family of CNT-C composite structures suitable for hot electrode applications.

03-20-2017 – 1400B

FE0023541 – NOVEL SILICA NANOSTRUCTURED PLATFORMS WITH ENGINEERED SURFACE FUNCTIONALITY AND SPHERICAL MORPHOLOGY FOR LOW-COST HIGH-EFFICIENCY CARBON CAPTURE

ORGANIZATION: Delaware State University **PRINCIPAL INVESTIGATOR**: Cheng-Yu Lai
TEAM MEMBERS: Daniela Radu, Nicholas Pizzi
PRESENTER: Nicholas Pizzi (Student Researcher)

ABSTRACT

The project aims to develop a silica nanosphere platform as solid sorbent for post-combustion CO2 capture in fossil-fired plants. The spatial arrangement prerequisite toward stable CO2 capture demands two amine groups proximity. This will be achieved by rationally designing the amine functionalization toward spatially-controlled, high amine coverage.

We have demonstrated to date that the silica nanosphere platform could be used as solid sorbent with spatial control of CO2 capture amine functionality and high amine loading at least 20 mmol N/g sorbent, with hybrid absorption–adsorption capacity of at least 4.7 mmol CO2 per gram of NSN sorbent (published results). In addition, morphology studies of the silica material with various aspect ratios are investigated to accomplish a higher surface area and increase CO2 accessibility to the amine groups.

We aim to develop a universal methodology technology for fabricating silica nanomaterials with high CO2 capture capacity at low-cost and with high recyclability. It is envisioned that the technology is applicable to other sectors such as operation of alkaline fuel cells and heterogeneous catalysis. The project involves training students in materials science and carbon capture.

03-20-2017 – 1500B

FE0022952 – ENGINEERING ACCESSIBLE ADSORPTION SITES IN METAL ORGANIC FRAMEWORKS FOR CO2 CAPTURE

ORGANIZATION: Clark Atlanta University **PRINCIPAL INVESTIGATOR**: Dr. Conrad W. Ingram
TEAM MEMBERS: Dr. Dinadayalane Tandabany, Saki Golafale (Student Researcher), Taylor Sledge (Student Researcher)
PRESENTER: Saki Golafale (Student Researcher)

ABSTRACT

The goal of this project is to develop metal organic framework (MOFs) materials with improved sites accessibility, thus enhanced their CO_2 adsorption and selectivity properties. Our three specific objectives are as follows: **1)** To synthesize MOFs with metal ions adsorption sites in more accessible locations (toward the center of the organic linkers) in order to enhance their CO_2 adsorption characteristics; **2)** To synthesize MOFs with nitrogen containing-ligand linker as a possible improved alternative to amine-functionalized MOFs which are known to be effective adsorbents for the gas; and **3)** To understand the nature of the adsorption sites and mechanism(s) by computational studies relevant to the adsorption of CO_2 within our metal organic frameworks, that complement experimental observations. The proposed research will contribute to advances in the science of coal technologies in direct support of the Department of Energy's (DOE) Office of Fossil Energy and the National Energy Technology Laboratory (NETL) mission. This project will serve to train graduate and undergraduate students in chemistry in general, as well as in special focus areas of materials science, nanoscience science and adsorption (CO_2) technologies.

03-20-2017 – 1530B

FE0023040 – POST COMBUSTION CARBON CAPTURE USING POLYETHYLENIMINE (PEI) FUNCTIONALIZED TITANATE NANOTUBES

ORGANIZATION: Prairie View A&M University **PRINCIPAL INVESTIGATOR**: Raghava R. Kommalapati
TEAM MEMBERS: Ziaul Huque, Hongbo Du, Melisa L. Stewart and Xinhua Shen
PRESENTER: Melisa L. Stewart (Student Researcher)

ABSTRACT

This research aims to develop a solid adsorbent for capturing carbon dioxide (CO_2) from coal fired power plant post combustion flue gas. With successful development of this adsorbent, it has the potential to replace the current liquid amine that is being used for CO_2 capture. Our research progress has been successful with the wet impregnation of polyethyleneimine (PEI) onto the protonated titanate nanotubes (PTNTs) that were synthesized using anatase, rutile and P-25 Degussa powders. Analysis of the titanate nanotubes using scanning electron microscopy (SEM) and transmission electron microscopy (TEM) confirmed the tubular shape as well as their nano size. Hydrothermal synthesis was used to produce the titanate nanotubes, with 0.1M hydrochloric acid wash and distilled water wash being used to achieve the PTNTs. Through SEM and TEM analysis, it was observed that the structure of the PTNTs was maintained after loading PEI of varying molecular weights. Synthesis temperatures and time have been seen to impact the length and diameter of these nanotubes, where 130 and 140°C have not shown much structural difference; however, at 150°C, there is a mixture of nanotubes and nanosheets, which is dependent on synthesis time. A customized experimental set up is being used for testing the adsorption capacity of the adsorbents. The adsorption capacity for the various adsorbents was found to be 50-70mg/g. ANSYS simulation of the CO_2 adsorption from the CO_2/N_2 mixture in the fixed bed showed that the pressure gradient inside porous domain was mainly determined by permeability and resistance coefficient.

03-20-2017 – 1600B

FE0011194 – SERRATION BEHAVIOR OF HIGH-ENTROPY ALLOYS

ORGANIZATION: University of Illinois at Urbana Champaign **PRINCIPAL INVESTIGATOR**: Karin Dahmen
TEAM MEMBERS: Peter Liaw, Students: Shuying Chen, Rui Feng, Will McFaul, Shu Li, Zong Wang and Nicholas Cross
Collaborators: Jien-Wei Yeh, Yong Zhang, and Jonathan T. Uhl
PRESENTER: Karin Dahmen

ABSTRACT

The prime goal of this project is to provide fundamental understanding of the serration behavior for high-entropy alloys (HEAs) through mechanical experiments, theoretical analyses, and slip-avalanche modeling. It is also to develop and test new serration-based methods to predict the mechanical performance, failure stress, or creep behavior for HEAs' long-term fossil-energy applications. To achieve the goal, we establish the deformation mechanisms of HEAs, through a combined program of statistical modeling and experimental investigations of the serration statistics of slowly-deformed HEAs, under tension and compression, for a wide range of strain rates, temperatures, numbers of samples, and various compositions.

03-20-2017 – 1630B

FE0011245 – REDUCED COST BOND LAYERS FOR MULTI-LAYER THERMAL/ENVIRONMENTAL BARRIER COATINGS

ORGANIZATION: Auburn University **PRINCIPAL INVESTIGATOR**: Jeffrey W. Fergus
TEAM MEMBERS: Honglong Wang, Wenzhuo Deng, Ahmet Bakal, Kai Roebecke, Ralf Fischer
PRESENTER: Jeffrey W. Fergus

ABSTRACT

The major goal of the project is to evaluate the resistance of thermal barrier / environmental barrier coating materials in gas turbine engineers to corrosion by calcium-magnesium-aluminum-silicates (CMAS) ingested into the engine. In particular, the performance of pyrochlore lanthanide zirconates, which have been shown to have lower thermal conductivity and better resistance to CMAS corrosion as compared to yttria stabilized zirconia, are being studied. Improved thermal barrier / environmental barrier coating materials will allow for higher operating temperatures, and thus improved energy conversion efficiencies, as well as longer lifetimes for gas turbine engines.

MONDAY, MARCH 20 TRACK C GASIFICATION SYSTEMS ABSTRACTS

03-20-2017 – 1030C
FE0012062 – DRY SOLIDS PUMP – COAL FEED TECHNOLOGIES
ORGANIZATION: Gas Technology Institute **PRINCIPAL INVESTIGATOR**: Timothy W. Saunders
TEAM MEMBERS: Joe Caravella, Tom Emerson, Harold Lacquement, Michael Kutin
PRESENTER: Timothy W. Saunders

ABSTRACT

The objective of the Dry Solids Pump (DSP) Coal Feed Technology project is to develop an innovative pump feed system and verify that it will reduce the cost of coal gasification plant construction and operations for power production with carbon capture. The project will mature DSP technology to support a first of a kind commercially relevant demonstration in 2018. The specific project objectives are: 1. Demonstrate high-pressure solids feed system operation with U.S. sub-bituminous and lignite coals. 2. Install and test component upgrades to the DSP that improve overall performance compared to the current prototype DSP. 3. Perform a techno-economic study comparing the DSP feed system to a dry solids lock-hopper feed system. This project has prepared the DSP and pump test facility for operations at 400 tons per day (tpd) pump capacity and 1200 psi max discharge pressure. The project will conduct scraper upgrade optimization and demonstration testing using Ill#6 coal. The project will perform pump component design activity, analyze test data, and modify or replace pump components to improve pump performance. The project has designed, fabricated, and tested component hardware in small scale component test rigs. Component test data has been analyzed to select components for testing in the DSP to support Techno-Economic Analysis (TEA). The project will conduct test operations with selected coals, collect and analyze data and models to support TEA. Based on operation and associated test data at 400 tons per day the project will prepare conceptual design of a 1000 tpd DSP.

03-20-2017 – 1100C
FE0023684 – INTEGRATED WATER-GAS-SHIFT PRE-COMBUSTION CARBON CAPTURE PROCESS
ORGANIZATION: TDA Research **PRINCIPAL INVESTIGATOR**: Gokhan Alptekin
TEAM MEMBERS: University of California – Irvine, Uniersity of Alberta, Gas Technology Institute, CB&I. Indigo Power Systems
PRESENTER: Gokhan Alptekin

ABSTRACT

The overall objective of this work is to develop an integrated WGS/pre-combustion carbon capture technology to eliminate CO2 emissions from Integrated Gasification Combined Cycle (IGCC) power plants. Our specific goal is to demonstrate the techno-economic viability of the new process by: 1) demonstrating it in large-scale slipstream tests, and 2) carrying out a high fidelity engineering design. TDA's process uses an advanced physical adsorbent to selectively remove CO2 from coal-derived synthesis gas above its dew point. The sorbent's performance has been well-characterized in representative bench-scale experiments and several slipstream field tests using actual coal-derived synthesis gas (DE-FE-0000469; DE-FE-0013105). We also carried out proof-of-concept evaluations for the integrated WGS/CO2 removal process and showed that our process can remove carbon with a much higher process efficiency than using the SelexolTM solvent (DE-FE-0007966; DE-FE-0012048). In this work, we are working on to develop a slipstream test unit to further demonstrate the merits of the integrated process; an 8-bed high temperature PSA system is being fabricated to run the full cycle sequence and demonstrate all critical design parameters including sorbent capacity, CO2 removal efficiency, extent of WGS conversion and H2 recovery.

03-20-2017 – 1300C
FE0023543 – OTM-ENHANCED COAL SYNGAS FOR CARBON CAPTURE POWER SYSTEMS AND FUEL SYNTHESIS APPLICATIONS
ORGANIZATION: Praxair, Inc. **PRINCIPAL INVESTIGATOR**: Juan Li
TEAM MEMBERS: Praxair OTM Research Group
PRESENTER: Juan Li

ABSTRACT

The project goal is to develop and demonstrate OTM combined reformer technology that can be integrated into coal-fired power plants to enhance the coal syngas quality, reduce the amount of ASU oxygen, and allow for coal and natural gas integration. Due to low parasitic power requirements and high carbon conversion efficiency, the OTM combined reformer has the potential to improve the power plant efficiency and lower the cost of electricity and carbon capture cost. The project objectives include:

1. A detailed techno-economic analysis of an OTM-enhanced IGCC plant with CO_2 capture. Cases with and without natural gas integration will be addressed. A case that is optimized to produce 5000 bbl/day of Fisher-Tropsch liquids from the coal and natural gas feedstocks will also be analyzed.
2. Development of a reactively-driven OTM membrane with integrated catalyst to support secondary reforming modes of operation.
3. Development of a membrane porous support structure and ceramic seal that is robust under high pressure service (200-425 psig).
4. Integration of the required components into a scalable OTM panel array module, tested in a multi-module OTM converter (100 – 500 tube scale) where natural gas and/or simulated coal syngas is converted in the OTM reactor, cooled, water-gas shifted, and fed to an integrated sorbent-based CO_2 separation system provided by TDA Inc.

03-20-2017 – 1330C
FE0026142 – LOW COST AIR SEPARATION PROCESS FOR GASIFICATION APPLICATIONS
ORGANIZATION: TDA Research **PRINCIPAL INVESTIGATOR**: Gokhan Alptekin
TEAM MEMBERS: University of California – Irvine, Uniersity of Alberta, Gas Technology Institute
PRESENTER: Gokhan Alptekin

ABSTRACT

The objective of this work is to develop a new chemical absorbent-based air separation process which can deliver low-cost oxygen to Integrated Gasification Combined Cycle (IGCC) power plants. The new sorbent operates at high temperature, hence eliminating the thermodynamic inefficiencies inherent in the conventional cryogenic air separation units (ASU). Unlike the sorbents used in commercial Pressure Swing Adsorption (PSA) systems, our sorbent selectivity removes oxygen (not nitrogen); which allows the effective utilization of the large amounts of energy in the high pressure oxygen-depleted steam. As a result, the new air separation system is highly efficient and delivers a low cost oxygen product. The specific objectives of this project are to increase the technical maturity and commercial viability of the new technology by: 1) demonstrating continuous oxygen generation in a prototype test system, and 2) carrying out a high fidelity process design and economic analysis. We are working with the University of California, Irvine (UCI), the University of Alberta (UOA) and the Gas Technology Institute (GTI) to meet these objectives.

03-20-2017 – 1400C

FE0026186 – DEVELOPMENT OF TWO-PHASE DENSE FLUID EXPANDER FOR ADVANCED CRYOGENIC AIR SEPARATION AND LOW-GRADE HEAT RECOVERY

ORGANIZATION: Air Products and Chemicals, Inc. **PRINCIPAL INVESTIGATOR**: Scott Marchessault
TEAM MEMBERS: Robert Benton, Ravi Pantula
PRESENTER: Scott Marchessault

ABSTRACT

Cryogenic air separation represents the state-of-the-art technology to produce oxygen to feed coal gasification units. Given the maturity of this technology, it is difficult to identify opportunities to improve process efficiency and reduce the cost of the oxygen produced. However, Air Products believes such an opportunity exists and proposed to conduct a research and a feasibility investigation into the use of a two-phase dense fluid expander (DFE) to improve the overall efficiency of cryogenic air separation. Demonstration of this novel concept should allow two important process improvements: 1) elimination of the need for the DFE discharge to be single phase; and 2) expansion of the operating region of the current devices, increasing the degree of power recovery and enabling the implementation of new process concepts. These new process concepts include power recovery from compression waste heat (up to 5% power reduction) and refrigeration extraction by replacing let-down valves with two-phase DFEs (1-3% power reduction). Considering the maturity of cryogenic air separation, these new process options represent a step change in power reduction and significant savings in operating costs for these units.

The first objective of this work was to better understand the limitations associated with two-phase dense fluid expansion from aerodynamic, thermodynamic, and mechanical perspectives. This work was completed in 2016. The next project phase will address the second objective: to apply this knowledge to construct a prototype device to further explore the basic properties of two-phase dense fluid expansion while developing primary data for techno-economic analyses.

03-20-2017 – 1500C

FE0023915: PILOT SCALE OPERATION AND TESTING OF SYNGAS CHEMICAL LOOPING FOR HYDROGEN PRODUCTION
FE0026185: CHEMICAL LOOPING COAL GASIFICATION SUB-PILOT UNIT DEMONSTRATION AND ECONOMIC ASSESSMENT FOR IGCC APPLICATIONS

ORGANIZATION: Ohio State University **PRINCIPAL INVESTIGATOR**: L.S. Fan
TEAM MEMBERS: Babcock & Wilcox Power Generation Group for both, WorleyParsons for FE0026185
PRESENTER: Andrew Tong

ABSTRACT

The Syngas Chemical Looping (SCL) process developed at The Ohio State University (OSU) uses an iron-based oxygen carrier to convert syngas into high-purity hydrogen while simultaneously capturing carbon dioxide that is readily sequestrable. A 250 kW_{th} – 3 MW_{th} pilot demonstration unit has been designed and constructed at the National Carbon Capture Center (NCCC) in Wilsonville, Alabama. The focus of this project is to operate the unit for extended syngas processing for hydrogen generation. OSU is also developing a chemical looping coal gasification (CLG) process using an iron-based oxygen carrier to produce syngas without the need for an air separation unit. The present presentation will introduce the SCL and CLG process concepts and discuss in detail the scale up and operation of both technologies at the 250kW_{th}-3MW_{th} and 15 kW_{th} scales, respectively. Process performance assessments for integrating the chemical looping reactor systems into an IGCC power plant will be presented.

03-20-2017 – 1530C

FE0026622 – RTI WARM SYNGAS CLEANUP OPERATIONAL TESTING AT TAMPA ELECTRIC COMPANY'S POLK 1 IGCC SITE

ORGANIZATION: RTI International **PRINCIPAL INVESTIGATOR**: Raghubir Gupta

TEAM MEMBERS: Brian Turk, Gary Howe, Atish Kataria, David Barbee, David Denton

PRESENTER: Raghubir Gupta

ABSTRACT

RTI has developed an advanced warm syngas desulfurization process (WDP) that utilizes a dual transport-bed reactor design and a proprietary attrition-resistant, high-capacity, regenerable sorbent. A U.S. DOE funded WDP pre-commercial test unit was designed and constructed at Tampa Electric Company's Polk 1 IGCC facility and was operated for >3,500 hours utilizing ~20% of their total syngas as feed. The primary objective of this work was to obtain sufficient operational testing to mitigate the technical risks associated with scale up and integration of WDP and CO_2 capture technologies, enabling subsequent commercial demonstration. WDP technology was shown to directly achieve up to 99.9% removal of total sulfur (as H_2S or COS) from coal/petcoke derived syngas at temperatures as high as 600°C, pressures up to 80 bar (~30 at Polk), and inlet sulfur concentrations ranging from a few thousand to 14,000 ppmv. The project also incorporated a sweet water-gas-shift process for hydrogen enrichment and an activated amine process for 90+% total carbon capture. The integration of these downstream processes enabled further reduction of total sulfur to sub-ppmv concentrations (up to 99.999% removal), suitable for stringent applications such as chemicals and fuels. Techno-economic assessments indicate significant (up to 50%) capital and operating cost reductions for the entire syngas cleanup block when WDP is integrated with a broad spectrum of conventional and emerging carbon capture technologies. The pre-commercial testing program was successful and the technology is now being made available globally for commercial licensing from Casale SA (RTI's licensing cooperation partner).

03-20-2017 – 1600C

FE0024000 – APPLICATION OF CHEMICAL LOOPING WITH SPOUTING FLUIDIZED BED FOR HYDROGEN-RICH SYNGAS PRODUCTION FROM CATALYTIC COAL GASIFICATION

ORGANIZATION: University of Kentucky **PRINCIPAL INVESTIGATOR**: Kunlei Liu

TEAM MEMBERS: Jinhua Bao, Liang Kong, Zhen Fan, Amanda Warriner, Heather Nikolic, Lisa Richburg

PRESENTER: Jinhua Bao

ABSTRACT

To overcome drawbacks of current molten-slag gasification technology using an entrained flow gasifier and low-temperature catalytic gasification [such as costly air separation unit (ASU) and expensive stand-alone water-gas shift (WGS) process, low carbon conversion rate and fast decay of catalyst], the UKy team has proposed to develop a pressurized catalytic steam-coal gasification integrated with chemical looping for coal derived syngas production, which utilizes hot iron-based solid particles to transport oxygen and heat from air-iron combustion in the Oxidizer for coal partial oxidation and gasification in the gasifier (Reducer) at relatively high temperature (1000-1100 °C). Meanwhile, large iron-based solid particles act as cost-effective multi-purpose catalyst (catalyst-OC) for promoting char gasification, water-gas-shift reaction and produced syngas reforming, all of which take place in a compact spouted-bed fuel reactor with fly ash recirculation. The three key features of the proposed process will provide high H2/CO ratio syngas, avoid conventional ASU step, and thus meet the priority objectives: (1) flexible platform that combines catalytic steam coal gasification with chemical looping for poly-generation of electricity and syngas; (2) multi-faceted catalyst-OC to provide oxygen/heat for gasification, and active site for improvement of gasification, WGS reaction and CH4/tar reforming; (3) a novel one-pot gasifier with coal conversion to syngas and in-situ water-gas shift reaction.

03-20-2017 – 1645C
NETL-R&IC – ADVANCED REACTION SYSTEMS
ORGANIZATION: NETL - Research and Innovation Center **PRINCIPAL INVESTIGATOR**: James C. Fisher II Ph.D. MBA
TEAM MEMBERS: Djuna Gulliver, Jonathan Lekse, William Rogers, Jeffery Hoffman
PRESENTER: James C. Fisher II

ABSTRACT

This will provide an overview of the Advanced Reaction Systems FWP being carried out by NETL's in-house research staff at the Research and Innovation Center (RIC). This presentation will provide information about the overall vision and expectations of the FWP including short and long term goals. The current focus is to complete a system analysis that represents the current state-of-the-art 1 MW combined heat and power system. This analysis, coupled with market studies, will provide a baseline that will be used to connect qualitative goals to the long term vision and determine a pathway for the small scale modular systems to change the energy land scape of the US.

03-20-2017 – 1700C
NETL-R&IC – MICROBIAL ENHANCED COALBED SYSTEMS
ORGANIZATION: NETL - Research and Innovation Center **PRINCIPAL INVESTIGATOR**: Djuna Gulliver
TEAM MEMBERS: Mark McKoy, Daniel Ross, Daniel Soeder, Yael Tucker
PRESENTER: Djuna Gulliver

ABSTRACT

Microbial enhance coalbed methane is a process that utilizes the microbial community native to coalbeds to naturally convert currently unusable coal into readily available methane. One methodology involves injection of nutrients into the coal seams to stimulate biogenic coal degradation and Methanogenesis. Identification of major taxonomy and functional pathways of biogenic coal degradation and subsequent methane production will lead to a better understanding of the coal-to-methane conversion, the microorganisms responsible for this conversion, and the nutrients required to bolster this conversion in situ. This study examines the taxonomy of 5 major coal basins and the metagenome of the Central Appalachian Basin. The presence of methanogens suggests Methanogenesis can occur. Furthermore, hydrocarbon degradation pathways were found, suggesting a route for biodegradation of coal.

03-20-2017 – 1715C
NETL-R&IC – ADVANCED REACTION SYSTEMS
ORGANIZATION: NETL - Research and Innovation Center **PRINCIPAL INVESTIGATOR**: James C. Fisher II Ph.D. MBA
TEAM MEMBERS: Djuna Gulliver, Jonathan Lekse, William Rogers, Jeffery Hoffman
PRESENTER: Jonathan W. Lekse

ABSTRACT

This presentation will provide an overview of Task 3 of the Advanced Reaction Systems FWP, Reaction Intensification: Testing Systems and Enabling Materials. This task ties together several diverse avenues of research that each address the overall goal of improving system performance. Research areas that will be covered in this presentation include non-traditional reactor design, reaction intensification using microwaves, advanced material and manufacturing technologies, oxygen carrier development, and advanced Fischer-Tropsch catalyst design. The current status of these research efforts as well as their goals will be presented.

03-20-2017 – 1730C

NETL-R&IC – VIRTUAL REACTOR DESIGN, VALIDATION, AND OPTIMIZATION THROUGH CFD MODELING

ORGANIZATION: NETL - Research and Innovation Center **PRINCIPAL INVESTIGATOR**: Dirk Van Essendelft

TEAM MEMBERS: Terry Jordan, Tingwen Li, William Rogers, Justin Weber, Jonathan Tucker, Greg Breault, Kyle Buchheit

PRESENTER: Dirk Van Essendelft

ABSTRACT

NETL is developing the Optimization Toolset (OT) as part of the Radically Engineered Modular Systems (REMS) program under the Advanced Reaction Systems FWP. The goal of this research is do develop and utilize user friendly tools to optimize and analyze multiphase unit operations by applying advanced optimization techniques to computational fluid dynamics (CFD) simulations using NETL's MFIX suite of codes. This will allow researchers and engineers to quickly identify operating conditions, geometries, and boundary conditions that lead to more efficient and less costly processes. NETL is already applying the OT to difficult problems, determining optimal performance conditions, and developing new technology. The OT together with advanced manufacturing techniques has also greatly sped up the pace of knowledge generation and understanding of multiphase processes.

03-21-2017 – 1030A

SC0008269 – ADVANCED CERAMIC MATERIALS AND PACKAGING TECHNOLOGIES FOR REALIZING SENSORS OPERABLE IN ADVANCED ENERGY GENERATION SYSTEMS

ORGANIZATION: Sporian Microsystems Inc. **PRINCIPAL INVESTIGATOR**: Yiping Liu
TEAM MEMBERS: Jason Fish, Sam Hotaling, Tim Trentler
PRESENTER: Jason Fish

ABSTRACT

There is a need for condition monitoring sensors capable of functioning in the harshest environments associated with advanced power systems that will directly contribute to improving operational efficiency through system control, reducing emissions, protecting capital equipment investment and promoting safety. These harsh environments include extreme temperatures (800-1800°C), high pressures (500-1000psi), and highly corrosive/erosive exposures. In the past several years, Sporian Microsystems, Inc. has established a solid track record of successful research and development of high-temperature (HT) sensors and packaging architectures for high temperature (up to 1350°C, 2450°F) turbine engine and other advanced power systems environments. Sporian's sensor technology is based on the combination of advanced high temperature packaging and recently developed polymer-derived silicon-carbide-nitride-based (SiCN) ceramics. Sporian worked with OEMs to identify desirable applications including: 1) 1800°C temperature sensor and 2) 1600°C temperature/pressure sensor suite. Commercial applications of advanced high-temperature sensing systems would be in demand for energy generation and propulsion industries as well as other generating asset OEMs. Utilities and end users will all stand to benefit from these high-efficiency, low emissions power systems.

03-21-2017 – 1100A

FE0012370 – HIGH-TEMPERATURE SAPPHIRE PRESSURE SENSORS FOR HARSH ENVIRONMENTS

ORGANIZATION: University of Florida **PRINCIPAL INVESTIGATOR**: Mark Sheplak
TEAM MEMBERS: William Oates, David Mills, David Arnold, Alexandra Garraud, Haocheng Zhou, Austin Vera, Peter Woerner, Jakob Consoliver
PRESENTER: Alexandra Garraud

ABSTRACT

As engineers seek to design more efficient turbines, a direct measurement within the hot section would help to better understand the thermal-fluid phenomena, as well as to implement active control methods. Currently, the control loop is not based on direct flame zone measurement, but rather is based on correlations to measurements in cooler regions. In order to characterize and control complex three-dimensional, unsteady flows in turbine systems, dynamic pressure, skin friction, and temperature sensors that can survive high temperatures are required. Unfortunately, commercially available sub-millimeter sensors capable of in situ measurements of these quantities in high-temperature environments do not exist. Dynamic high-temperature sapphire optical pressure sensors show great potential to revolutionize measurements in harsh environments by placing the sensors in close proximity to flow phenomena while shifting the electronics to a remote location.

We will present the advancement on the design, optimization and characterization of a sapphire-based sensor measuring pressure through a fiber optic lever method, expecting to perform up to 1200°C. Laser-machining is required to etch a cavity and turn the sapphire substrate and membrane onto a functional pressure sensor. The progress on the sensor fabrication, material modeling/experimental characterization and the high-temperature compatible packaging will be shown. In parallel, a high temperature planar wave tube for acoustic characterization is developed. Once finished, the pressure calibration at increasing temperatures will be carried out. In the future, high-temperature validation of sensors in hot jet environment will be performed.

03-21-2017 – 1300A

FE0026334 – ADVANCED CONTROL ARCHITECTURE AND SENSOR INFORMATION DEVELOPMENT FOR PROCESS AUTOMATION, OPTIMIZATION, AND IMAGING OF CHEMICAL LOOPING SYSTEMS

ORGANIZATION: Ohio State University **PRINCIPAL INVESTIGATOR**: Andrew Tong

TEAM MEMBERS: Babcock & Wilcox Power Generation Group, American Electric Power

PRESENTER: Andrew Tong

ABSTRACT

Chemical looping is considered a near-term technology with the potential to simplify CO_2 capture both efficiently and economically for power and chemical plant applications. The OSU syngas chemical looping process (SCL) represents the advanced energy system for the conversion gaseous fuels to H_2 and power with in-situ CO_2 capture. The goal of this project is to develop advanced process automation control architecture and imaging and optimization sensor software which significantly increase the operational reliability and efficiency of the chemical looping technologies. A high level controller (HLC) consisting of decision-making and controller-selection logic integrated with sliding mode controllers (SMCs) will be used to develop distributed intelligence automation scheme for the chemical looping process startup and shutdown. A commercial real time, closed-loop optimization software, FocalPoint Optimization System, will be specifically tailored to chemical looping processes for optimizing the process operating conditions. Additionally, an electrical capacitance volume tomography (ECVT) sensor software will be developed to image a packed moving bed of oxygen carriers at the operating temperatures of the reducer reactor. The present paper will discuss the operational results of the SMC development and testing in the 25 kW_{th} sub-pilot unit and ECVT sensor performance for gas-solid flow measurement at high temperatures.

03-21-2017 – 1330A

FE0012451 – DEVELOPMENT OF INTEGRATED BIOMIMETIC FRAMEWORK WITH INTELLIGENT MONITORING, COGNITION AND DECISION CAPABILITIES FOR CONTROL OF ADVANCED ENERGY PLANTS

ORGANIZATION: West Virginia University Research Corporation

PRINCIPAL INVESTIGATOR: Debangsu Bhattacharyya

TEAM MEMBERS: Richard Turton, Fernando Lima, Mario Perhinschi, Urmila Diwekar

PRESENTER: Debangsu Bhattacharyya

ABSTRACT

The objective of this project is to develop algorithms and methodologies for a novel, biomimetic control system for optimal control of advanced energy plants. The project seeks to develop computational techniques to accomplish: (i) self-organization of control structure for maximizing the plant operating profit, (ii) distributed, adaptive, and intelligent controllers with cognition and decision capabilities, and (iii) seamless integration in a highly interacting, multiagent environment.

Algorithms for biomimetic, self-organizing control structure selection are being developed by mimicking the organization of human brain. Design of the biomimetic controllers is inspired by the cooperative decision-making process of ants. For adapting to unexpected disturbances, the immune system of superior organisms is being mimicked and adaptive control laws for intelligent monitoring, cognition, and decision capabilities are being developed. Tasks at each level are prioritized and optimized by a biomimetic multi-agent optimization approach. At the end of this project, algorithms and methodologies will be available for developing an integrated biomimetic control framework that can be exploited for optimal control of highly complex and strongly interacting advanced energy plants.

03-21-2017 – 1400A

FWP-AL-14-450-012 – ENGINEERED COMPLEX SYSTEMS: A DOMAIN SPECIFIC LANGUAGE FOR CLOUD-BASED MODELING OF COMPLEX
ADVANCED POWER SYSTEMS

ORGANIZATION: Ames National Laboratory **PRINCIPAL INVESTIGATOR**: Dr. Kenneth "Mark" Bryden
TEAM MEMBERS: Mr. Zachary Reinhart, Ms. Tina Akinyi, Dr. Kris Bryden
PRESENTER: Zachary Reinhart (Student Researcher)

ABSTRACT

To provide for future power consumption needs while meeting higher regulatory standards, low carbon fossil energy advanced power plants are needed. Current and proposed advanced power plants are increasingly complex, leading to long design and deployment cycles. Integrated modeling has the potential to reduce this cycle time, but current integrated modeling approaches require the creation of a global ontology as well as redevelopment of the component models into a preset integration framework or monolithic integrated model, making model creation time consuming. Federated model sets have the potential to speed integrated model development by allowing component models to exist as independent, self-describing information entities that can be selected from a library, easily connected, and managed by a federation management system.

However, the current draft implementation of federated model sets requires model builders to do significant software development to integrate models. In this discussion, we will present a domain specific language for federated model sets that allows system builders to rapidly assemble model sets without significant software development. The syntax is designed to be simple and accessible to system builders without significant programming experience. The model library and message contract system will be discussed. These services, along with supporting tools, will enable the system to infer many of the necessary connections between models, further lessening the workload of the system builder.

03-21-2017 – 1500A

FE0026171 – PASSIVE WIRELESS SENSORS FABRICATED BY DIRECT-WRITING FOR TEMPERATURE AND HEALTH MONITORING OF ENERGY SYSTEMS IN HARSH-ENVIRONMENTS

ORGANIZATION: West Virginia University **PRINCIPAL INVESTIGATOR**: Edward M. Sabolsky

TEAM MEMBERS: David Reynolds, Kostas Sierros

PRESENTER: Nandhini Ranganathan, Michael Comparetto (Student Researchers)

ABSTRACT

West Virginia University propose to demonstrate a wireless, high-temperature sensor system for monitoring the temperature and health of energy-system components. The active sensor and electronics for passive wireless communication will be composed entirely of electroceramic materials (conductive ceramics) which are capable of withstanding the harsh-environments of fossil energy-based technologies. This work will focus primarily on the direct-writing and testing of temperature (thermocouples and thermistors) and health (strain/stress and crack propagation sensors) that function between 500-1700ºC. A "peel-and-stick"-like transfer process to deposit the entire sensor circuit to various energy-system components will be developed. These sensors systems may be applied to many systems such as solid-oxide fuel cells (SOFCs), chemical reactors, furnaces, engines, boilers, and gas turbines (for both energy and aerospace applications).

The specific project objectives are as follows: ***1)*** Investigate phase formation, sintering/grain growth, and electrical properties of polymer-derived electroceramic composites between 500-1700ºC; ***2)*** Define processes to direct-write through ink-jet and robo-casting the polymer-derived electroceramic composites onto oxide surfaces and organic carrier films*;* ***3)*** Develop methods to form monolithic "peel-and-stick" preforms that will efficiently transfer the sensor circuit to surfaces after thermal treatment; ***4)*** Design passive RF wireless LCR circuits and reader antennas for high-temperature sensor communication and testing at temperatures up to 1700°C; ***5)*** Investigate the passive wireless sensor system developed (and method of transferring sensor system) for temperature and stress/strain measurements on SOFC repeat units and gas turbine blade prototypes as example applications.

03-21-2017 – 1530A

FE0012383 – SMART REFRACTORY SENSOR SYSTEMS FOR WIRELESS MONITORING OF TEMPERATURE, HEALTH, AND DEGRADATION OF SLAGGING GASIFIERS

ORGANIZATION: West Virginia University **PRINCIPAL INVESTIGATOR**: Edward M. Sabolsky
TEAM MEMBERS: Debangsu Bhattacharyya, David Graham and Vinod Kulathumani
PRESENTER: Edward M. Sabolsky, Debangsu Bhattacharyya, David Graham and Vinod Kulathumani

ABSTRACT

In the research project, West Virginia University developed smart refractory brick, which contains embedded temperature, strain/stress, and spallation sensors throughout the volume of high-temperature refractory brick. The proposed work included a method to interconnect the sensors to the reactor exterior, where the sensor signals will be processed by low-power electronics and transmitted wirelessly to a central processing hub. The collected data was used for model-based estimation of refractory degradation, a technique that can help to monitor the health of the refractory in real-time. The developed smart refractory and refractory sensor system concept can be applied to many other applications, such as conventional coal-fired boiler technology, biomass gasification, and steel and glass manufacturing.

The specific project objectives were as follows: ***1)*** Investigate chemical stability, thermomechanical properties, and electrical properties of refractory oxide-silicide composites at temperatures between 750-1450ºC; ***2)*** Define processes to pattern and embed the electroceramic composites within high-temperature refractory materials to incorporate temperature and strain/stress sensors into refractory bricks; ***3)*** Develop methods to interface the electrical sensing outputs from the smart refractory with an embedded processor and to design a wireless sensor network to efficiently collect the data at a processing unit for further data analysis; ***4)*** Develop algorithms for model-based estimation of temperature profile in the refractory, slag penetration depth, spallation thickness, and resultant health by using the data from the wireless sensor network.

03-21-2017 – 1600A

NETL – SCENARIO SIMULATIONS OF POTENTIAL COST SAVINGS FROM R&D IN SENSORS AND CONTROLS

ORGANIZATION: National Energy Technology Laboratory **PRINCIPAL INVESTIGATOR**: Don Hanson
TEAM MEMBERS: Dave Schmalzer
PRESENTER: Chris Nichols

ABSTRACT

This research activity will define the benefits of advanced materials and improved/novel sensors that can improve heat rates and reduce forced outage rates in the existing fossil fuel electricity generating fleet. As intermittent renewables increase their share of electricity generation, current fossil units are being called upon to operate in cycling modes more frequently, as opposed to the baseload modes for which many were designed. Increased cycling on units which were designed for baseload exacerbates damage from component fatigue and creep in highly stressed environments. Using Argonne's unique modeling capability with the EISM model, energy market scenarios will be developed and run which demonstrate the impact of current operational cycles on the existing fossil fleet. The EISM model provides a unique combination of unit-level modeling, electricity dispatch and market-level integration which is not found in other energy market models. Then ANL will develop model inputs which simulate the effects of successful R&D in the materials, sensors and controls area which could mitigate the damage from these cycling operations. Results from both sets of model runs (Baseline and with R&D) will be compared to show the impacts of R&D. Deliverables will include a whitepaper and summary presentation of the results and methodology, as well as full access to the model by NETL.

03-21-2017 – 1030B

FE0024065 – NEW MECHANISTIC MODELS OF LONG TERM EVOLUTION OF MICROSTRUCTURE AND MECHANICAL PROPERTIES OF NICKEL BASED ALLOYS

ORGANIZATION: Oregon State University **PRINCIPAL INVESTIGATOR**: Jamie Kruzic
TEAM MEMBERS: P. Alex Greaney, T. Matthew Evans, Agnieszka Truszkowska, Qin Yu
PRESENTER: P. Alex Greaney

ABSTRACT

Nickel-based superalloys are used in fossil energy systems because of their ability to provide high strength and corrosion resistance in hostile environments at elevated temperatures. Material failures due to plastic and/or creep deformation occur by the emergence of deformation localization, microvoids, and cracks at heterogeneities in the material microstructure that are evolving over time.

While many traditional deformation modeling approaches (e.g., finite element) have difficulty capturing these emergent phenomena, the discrete element method (DEM) has proven very effective for the simulation of granular materials where properties and response vary over multiple microstructural scales. The DEM framework has the central advantage that it naturally captures the heterogeneity and geometric frustration inherent to deformation processes. While DEM has recently been adapted for successfully modeling the fracture of brittle solids, to date it has not been used for simulating metal deformation. The goal of our research is to develop a totally new crystal plasticity modeling framework for deformation and creep in nickel based superalloys that is based on DEM and is well-suited for the incorporation of heterogeneities and simulation of emergent damage. Here we present our progress in reformulating DEM to model the key elastic, plastic, and visco-plastic deformation characteristics of nickel-based superalloy polycrystals. The anticipated long term benefit of this project will be the availability of a modeling methodology that can be used by fossil energy system designers that will improve their capability to design safe energy systems without excessive and costly over-design or unsafe under-design.

03-21-2017 – 1100B

FE0024054 – COMPUTATIONAL DESIGN AND PERFORMANCE PREDICTION OF CREEP-RESISTANT FERRITIC SUPERALLOYS

ORGANIZATION: University of Tennessee **PRINCIPAL INVESTIGATOR**: Peter K. Liaw
TEAM MEMBERS: David C. Dunand, Gautam Ghosh, Michael Rawlings, Gian Song, Shao-Yu Wang, Song-Il Baik
PRESENTER: Peter K. Liaw

ABSTRACT

Novel ferritic superalloys based on the Fe-Al-Cr-Ni-X (X = Ti, Hf, Ta, and Zr) systems have been developed for the application of ultra-supercritical fossil-energy (FE) power plants under the condition of the steam temperature of 760 °C and the pressure of 35 MPa, in order to improve the efficiency of plants and reduce the greenhouse gases emission. Previously, the Fe-Al-Cr-Ni-X system has shown the potential of forming great creep-resistant alloys, due to the formation of hierarchical structure (B2 and $L2_1$) precipitates. In this project, studies on further improving the creep-resistance by alternating Ti with Hf and Zr have been conducted. The elastic properties of the single-crystal body-centered-cubic (bcc) iron, B2-phase NiAl, and $L2_1$-Ni_2TiAl are calculated and determined by first-principles calculations. The CALculation of PHAse Diagrams (CALPHAD) had been performed for predicting the microstructures of the alloy systems. Besides, advanced microstructural characterization tools (e.g, electron microscopy techniques, local-electrode-atom probe, and neutron diffraction) and creep tests were conducted for microstructural characterization and creep-resistance investigation. From the above investigations, it is shown that Fe-Al-Cr-Ni-Hf and Fe-Al-Cr-Ni-Zr systems do not form hierarchical structures or even, the $L2_1$ phase. Current creep tests show that alloys without hierarchical structures or $L2_1$ precipitates do not have comparable creep resistance with Fe-Al-Cr-Ni-Ti alloys. With all these results, we are going to determine the optimistic composition in the Fe-Al-Cr-Ni-Ti system, and hopefully is able to develop and integrate modern computational tools and algorithms to design high-temperature alloys for applications in FE power plants.

03-21-2017 – 1300B

FE0024056 – COMPUTATIONAL DESIGN AND DISCOVERY OF NI-BASED ALLOYS AND COATINGS: THERMODYNAMIC APPROACHES VALIDATED BY EXPERIMENTS

ORGANIZATION: Pennsylvania State University **PRINCIPAL INVESTIGATOR**: Zi-Kui Liu
TEAM MEMBERS: Brian Gleeson, Austin Ross, Bi-Cheng Zhou, Thomas Gheno, Greta Lindwall
PRESENTER: Zi-Kui Liu

ABSTRACT

This proposed collaborative project between the Pennsylvania State University and the University of Pittsburgh seeks to develop a thermodynamic foundation for the accelerated design of Ni-base alloys and coatings, i.e., the Ni-Al-Cr-Co-Si-Hf-Y system. Central to this foundation is the novel combination of atomic-scale first-principles calculations with continuum-scale thermodynamic modeling to arrive at consistent descriptions of the key phases in the Ni-base system in terms of composition- and temperature-dependent Gibbs energy, enabling prediction of tunable properties, including phase compositions and fractions, solubility limits and driving forces. In this proposed project, we develop an experimentally-verified database to determine the effects of major and minor alloying constituents on the stability and, hence, reactivity of trace Hf and Y additions in Ni-base systems. Computation based guidance on optimizing the levels of Y and/or Hf additions in multi-component Ni-based alloys is a much needed and significant outcome of this study. The project scope includes composition ranges that correspond to typical MCrAl-based (where M is Ni, Co or Ni+Co) coating compositions.

The information derived from this project is essential for the efficient design and performance prediction of alloys, coatings and coating/alloy combinations.

03-21-2017 – 1330B

NETL-RIC – USE OF DATA ANALYTICS IN ADVANCED ALLOY DEVELOPMENT: TRENDS AND MODELING

ORGANIZATION: NETL - Research and Innovation Center **PRINCIPAL INVESTIGATOR**: Vyacheslav Romanov

TEAM MEMBERS: Jeffrey Hawk, Terry Jordan, Narayanan Krishnamurthy, Jinichiro Nakano, Roger French, Jennifer Carter, Laura Bruckman, Amit Kumar and Mohamed Elsaeiti

PRESENTER: Vyacheslav Romanov

ABSTRACT

The overarching project goal is developing expertise in 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. Research objectives are to adapt and develop software tools, so that it is possible to curate, archive and analyze large volumes of raw data, with the focus on advanced alloys. Predictive models will be validated against experimental data. Certain analytical models that could be used in simulation and visualization will be designed to account for the features and relationships uncovered using data analytics. The developed analytical tools and user interfaces will allow the FE experts and technology developers to train the system and to extract hypotheses and recommended technological approaches out of the simulated and experimental data, in response to their questions and requests, through the integration of guided experimental research with computational sciences and engineering across time and length scales. It will provide the foundations of fundamental scientific understanding for advancing broad areas of science dealing with properties and behaviors of advanced materials and power plant components

03-21-2017 – 1400B

NETL-R&IC – OXIDATION AND MICROSTRUCTURAL EVOLUTION: COMPUTATIONAL INVESTIGATIONS & MODEL DEVELOPMENT

ORGANIZATION: NETL - Research and Innovation Center **PRINCIPAL INVESTIGATOR**: Youhai Wen

TEAM MEMBERS: Tianle Cheng, Jeff Hawk, David Alman

PRESENTER: Youhai Wen

ABSTRACT

One of the key challenges in modeling oxidation kinetics is the lacking of a thermodynamically consistent phase-field model for micro-elasto-viscoplasticity. Existing continuum phase-field models for plasticity seek to solve plastic strain by minimizing the shear strain energy. In our approach, the total free energy is minimized through constrained variational method and we show that the flow rules derived from the Ginzburg-Landau type equations can recover Odqvist’s law for viscoplasticity and Prandti-Reuss theory. Strain hardening rules and algorithm to deal with free surfaces and cracks/voids are incorporated into the model. The results are compared with analytical and existing numerical solutions.

03-21-2017 – 1500B

FE0011247 – RATIONAL DESIGN OF MIXED-METAL OXIDES FOR CHEMICAL LOOPING COMBUSTION OF COAL VIA COMPUTATIONAL EXPERIMENTAL STUDIES

ORGANIZATION: North Carolina State University **PRINCIPAL INVESTIGATOR**: Fanxing Li
TEAM MEMBERS: Erik Santiso (Co-PI), Amit Mishra, and Nathan Galinsky
PRESENTER: Fanxing Li

ABSTRACT

This project aims to rationalize oxygen carrier design strategies for the chemical looping with oxygen uncoupling (CLOU) process. In CLOU, an oxide based oxygen carrier spontaneously releases its lattice oxygen for solid fuel combustion, producing concentrated CO_2. After oxygen release, the reduced oxygen carrier is reoxidized with air in a separate reactor, producing heat. The ability for facile oxygen release allows improved combustion kinetics and simpler heat management when compared to conventional chemical looping processes. This presentation discusses perovskite-structured oxygen carriers with a general formula of $A_xA'_{1-x}Mn_yB_{1-y}O_{3-\delta}$ (A/A' = Sr, Ca, Ba; B = Al, V, Fe, Co, Ni). Results indicate $CaMnO_3$ provided satisfactory oxygen uncoupling properties; however, irreversible phase decomposition was observed. The effects of A-site and B-site dopants on $CaMnO_3$ were explored with the primary intention to prevent irreversible phase decomposition and to enhance the CLOU kinetics. These oxygen carrier materials were tested for oxygen release properties, redox stability, and activity for coal char conversion. Sr and Fe doped $CaMnO_3$ exhibited superior stability and solid fuel combustion activity. Density Functional Theory (DFT) calculations were also carried out to interpret the experimental data. Oxygen vacancy formation energy is determined, through DFT and experimental studies, to be an effective descriptor for oxygen carrier particle design and optimizations.

03-21-2017 – 1530B

NETL-R&IC – UPDATE ON THE TECHNO-ECONOMIC VIABILITY OF AUSC SYSTEMS

ORGANIZATION: NETL - Research and Innovation Center **PRINCIPAL INVESTIGATOR**: Wally Shelton
TEAM MEMBERS: Eric Lewis, Dale Keairns (Deloitte Consulting), Mark Woods, Richard Newby (KeyLogic)
PRESENTER: Travis Shultz

ABSTRACT

The U.S. Department of Energy (DOE) National Energy Technology Laboratory's (NETL) Systems Engineering & Analysis Directorate (SEA) develops and analyzes advanced energy technologies and systems at scales ranging from process to national infrastructure in support of the DOE's mission and goals. On behalf of the Office of Fossil Energy's Crosscutting Technology Research Program, SEA's Energy Process Analysis Team has conducted a techno-economic analysis of advanced pulverized coal (PC) plants incorporating Advanced Ultrasupercritical Steam Cycle (AUSC) technology. Incorporation of the higher Rankine cycle steam conditions results in efficiency improvements of 3.4 % points without carbon capture and 2.7% points with 90% carbon capture, relative to baseline supercritical PC plants. Cost-of-electricity (COE) decreases of $3.7/MWh (4.5%) without carbon capture and $10.4/MWh (7.8%) with 90% carbon capture were estimated. Significant limitations of the study will be discussed, as well as follow-on studies leveraging this work.

03-21-2017 – 1600B

NETL – R&IC – INSTITUTE FOR THE DESIGN OF ADVANCED ENERGY SYSTEMS (IDAES)

ORGANIZATION: National Energy Technology Laboratory, Lawrence Berkeley National Laboratory, Sandia National Laboratory, Carnegie Mellon University, West Virginia University

PRINCIPAL INVESTIGATOR: David C. Miller

TEAM MEMBERS: Deb Agarwal, John Siirola, John Eslick, Dan Gunter, Larry Biegler, Mingzhao Yu, David Molina Thierry, Bethany Nicholson, Carl Laird, John Eason, Anthony Burgard, Jinliang Ma, Chrysanthos Gounaris, Chris Hanselman, Nick Sahinidis, Marissa Engle, Zach Wilson, Debangsu Bhattacharyya, Paul Akula, Ignacio Grossmann, Qi Chen, Emma Johnson, Ignacio Grossmann, Cristiana Lara, Ben Omell, Joel Theis, Jean-Paul Watson, Benjamin Sauk, Josh Boverhof, David Woodruff, You-Wei Cheah, Keith Beattie

PRESENTER: Anthony Burgard

ABSTRACT

NETL's Institute for the Design of Advanced Energy Systems (IDAES) seeks to be the premier resource for the identification, synthesis, optimization, and analysis of innovative advanced energy systems at scales ranging from process to system to market to support the transformation of the national energy landscape to meet the Department of Energy's (DOE's) three enduring strategic objectives: energy security, economic competitiveness, and environmental responsibility. IDAES is developing and demonstrating the next generation of rigorous, computational approach to help enable development of new concepts for energy systems. Due to the complexity of energy systems, and importance of understanding uncertainty, the Institute's models will be multi-scale and dynamic while incorporating intrusive uncertainty quantification (UQ). These tools are being applied to the development of new, innovative energy systems, which are capable of meeting environmental, economic, and security objectives. IDAES and its capabilities will be applicable to the development of the full range of advanced fossil energy systems, including chemical looping, as well as integration with other new technologies such as supercritical CO_2. IDAES will bring many benefits, including the ability to identify novel new advanced energy systems; analyze various concepts; and support ongoing development, scale up, and deployment of new energy technology.

03-22-2017 – 0800A

FE0026307 – EVALUATION AND DEMONSTRATION OF COMMERCIALIZATION POTENTIAL OF CCSI TOOLS WITHIN gPROMS ADVANCED SIMULATION PLATFORM

ORGANIZATION: Process Systems Enterprise (PSE) Limited **PRINCIPAL INVESTIGATOR**: Alejandro Cano

TEAM MEMBERS: Alfredo Ramos, Pieter Schmal, Debangsu Bhattacharyya, Nikolaos Sahinidis, David Mebane, Ananya Chowdhury, Xiaohui Liu

PRESENTER: Adekola Lawal

ABSTRACT

This project aims to identify market opportunities for the Carbon Capture Simulation Initiative (CCSI) tools by exploring the feasibility of integration of CCSI tools with PSE's advanced process modelling platform, *gPROMS*. The CCSI is a partnership among national laboratories, industry, and academic institutions that is developing and deploying state-of-the-art computational modeling and simulations tools to accelerate the commercialization of carbon capture technologies.

To achieve this, PSE partnered with Carnegie Mellon University and West Virginia University to assess and rank the CCSI tools according to their commercial potential, technical feasibility and technology readiness level when integrated with *gPROMS* platform capabilities. Detailed integration and commercialization plans for promising tools have been developed, drawing on technical expertise from the project team, PSE's client base and the project's industrial advisory board. A number of suitable applications across advanced energy technologies have also been explored.

The commercialization of the CCSI toolkit by this consortium will contribute towards increasing its accessibility, usability and utility towards supporting the objective of accelerating development and deployment of promising CCS technologies. In addition, this project will provide the opportunity to extend the application of the CCSI toolkit to other advanced energy technologies.

03-22-2017 – 0830A

FWP-AL-14-510-075 – THE SMARTER PROJECT - SCIENCE OF MULTICOMPONENT ALLOYS: ROADMAP FOR THEORETICAL AND EXPERIMENTAL RESEARCH

ORGANIZATION: Ames National Laboratory **PRINCIPAL INVESTIGATOR**: Matthew Joseph Kramer

TEAM MEMBERS: P.K. Ray, B. Thoeny, P. Singh, L. Wang and D.D. Johnson

PRESENTER: Matthew Kramer

ABSTRACT

We adopt a two-pronged approach towards establishing the science of multi-component alloys. The first part of this research focuses on the factors driving the phase selection and ordering processes in model High Entropy Alloy systems. Specifically, we will focus on the ZrNbHf alloys, TiZrHfAl alloys and the AlFeCoCrNi alloys. The phase stability of these alloys has been studied using a combination of High Energy X-Ray Diffraction and theoretical models based on the Korringa-Kohn-Rostoker Coherent Potential Approximation (KKR-CPA) code. Using this approach we have attempted to map the phase selection processes in these alloy systems as a function of temperature and composition. Additionally, we have explored the oxidation mechanisms in AlFeCoCrNi alloys over a range of temperatures and alloy chemistries. Transient oxidation experiments using an equiatomic AlFeCoCrNi alloy at 900 and 1000°C were employed to establish the initial pathways for the oxide scale development, and the surface oxide characterized using a combination of X-ray Photoelectron Spectroscopy and Energy Dispersive X-ray Analysis. Once the mechanism was established using transient oxidation experiments, long-term isothermal oxidation studies were carried out by varying the Al:Cr ratios in order to establish the compositional effects on oxidation.

03-22-2017 – 0900A

FE0023114 – DEVELOPMENT OF REDUCED ORDER MODEL FOR REACTING GAS-SOLIDS FLOW USING PROPER ORTHOGONAL DECOMPOSITION

ORGANIZATION: Florida International University **PRINCIPAL INVESTIGATOR**: Dwayne McDaniel

TEAM MEMBERS: Paul Cizmas, George Dulikravich, Seckin Gokaltun

PRESENTER: Janhavi Chitale (Student Researcher)

ABSTRACT

Solving the governing equations describing the multiphase flow in reactors, which is a system of highly coupled partial differential equations, is a computational intensive task. This research concentrates on improving a reduced-order model (ROM) code based on the proper orthogonal decomposition (POD) method. A test case is developed to test performance of the ROM for chemically reacting flows with heat transfer against the full model. To generate the geometry of the experimental set up, a Cartesian grid cut cell technique is employed. Converging diverging grid enhanced the quality of the results. A user defined function is coupled with MFIX to calculate the mass fraction of the species based on the rate of reaction.

Another goal of the reduced kinetics model of chemical reaction is to validate its accuracy while simplifying its computational complexity. A modified form of the entropy inequality, which is a combination of the energy balance and the entropy inequality, is used to check if it is violated when reduced form of kinetic reactions are used to represent combustion. Results for numerical simulations for laminar flame generated by combustion of Methane are compared against the available experimental data for species mass fractions at different cross sections. Development of ROM for chemically reacting multiphase flows is in the process.

03-22-2017 – 0930A

NETL-R&IC – MFIX SUITE MULTIPHASE CODE DEVELOPMENT AND VALIDATION

ORGANIZATION: NETL - Research and Innovation Center **PRINCIPAL INVESTIGATOR**: William Rogers

TEAM MEMBERS: Multiphase Flow Science Team

PRESENTER: Jeff Dietiker

ABSTRACT

The objective of this work is to develop and support a validated suite of multiphase flow computational fluid dynamics models (MFiX Suite) capable of predicting the behavior of novel reactor configurations, including predictions of hydrodynamics, heat transfer, and chemical reactions. A large-scale, reacting MFIX-MPIC model employing complex chemical reactions and realistic geometry will be developed. The model will be an extension of the large-scale DEM model whereby the MPIC model may support a parcel/particle ratio more representative of a laboratory-scale system. New and improved physical submodels will be identified and/or developed to accurately model reacting multiphase flows and will be incorporated into the MFIX model suite. Enhancement of the MFIX-Graphical User Interface (MFIX-GUI) will be performed to improve the usability and accuracy of the model input, execution, and post-processing steps. Well-characterized laboratory-scale data will be generated to aid in understanding physical processes for development of mathematical models and for use in code validation. These efforts support the design, construction, operation, and maintenance of laboratory-scale cold-flow experiments for data generation within the Multiphase Flow Analysis Laboratory. A range of small-scale test units will be created and exercised to generate the data. This approach will help to provide cost-effective, well-characterized data in a timely fashion. Data from the tests will be suitable for validation of the MFiX suite of codes.

03-22-2017 – 1030A
FE0026220 – HIGH FIDELITY COMPUTATIONAL MODEL FOR FLUIDIZED BED EXPERIMENTS
ORGANIZATION: University of Texas at El Paso **PRINCIPAL INVESTIGATOR**: Dr. Vinod Kumar
TEAM MEMBERS: A Rodriguez, A Schiaffino, A Chattopadhyay, VMK Kotteda, W Spotz, V Kumar
PRESENTER: Dr. Vinod Kumar

ABSTRACT

A framework is developed to integrate MFiX with advanced linear solver packages in Trilinos. The framework consists of MFIX, Fortran. C, Cpp wrapppers. The MFIX wrapper interprets the structure of the matrix and vector from MFiX while the Fortran wrapper transfers this information to the C wrapper. C-wrapper acts as a mediator and manages the data structures between Fortran and Cpp wrappers. The Cpp wrapper passes the matrix and vector information to packages in Trilinos to get the unknown vector. This vector is transferred back to MFiX via Cpp, C, Fortran and MFIX wrappers. Besides the built-in solvers, the framework provides various advanced direct as well as iterative linear solvers. This simple, reliable and robust framework is tested on various computer architectures. In the present work, the distributed memory parallel MFiX suite is integrated with Trilinos and simulated flow in fluidized bed problems in two and three dimensions. MFiX includes four iterative solvers: successive over relaxation method, Bi-Conjugate gradients stabilized (BiCGStab) method, generalized minimal residual method (GMRES) and conjugate gradient method. The system of equations result in fluidized problems are non-symmetric in nature. Therefore, BiCGStab or GMRES method is used to solve the equations. Therefore, these methods are considered to solve the system of equations. The stopping criteria for the iterative solvers in MFiX and Trilionos is same. The flow from MFiX and the integrated solver, MFiX-Trilinos is compared. It is observed that they are qualitatively same. The performance of the solvers in MFiX and Trilinos is evaluated.

03-22-2017 – 1100A
FWP-AL-14-330-058 – KINETIC THEORY MODELING OF TURBULENT MULTIPHASE FLOW
ORGANIZATION: Ames National Laboratory **PRINCIPAL INVESTIGATOR**: Rodney O. Fox
TEAM MEMBERS: Bo Kong
PRESENTER: Bo Kong

ABSTRACT

Polydisperse gas-particle flows are common in many fields of engineering, such as in fluidized beds and risers, which are widely used in a variety of chemical processes. Due to the various physical and chemical interactions between particles and gas, such as particle collisions and breakage, gasification and chemical reactions, the individual particle size and the overall size distribution of particles changes as the flow develops. In this work, quadrature-based moment methods (QBMM) are applied to solve numerically the kinetic equation of the joint NDF with the hydrodynamic approximation for particle velocity, which is valid when particles are in the moderately dense and dense regime, such as in fluidized bed. By reconstructing the size-conditioned velocity distribution function, the spatial fluxes in the moment equations are treated using a kinetic-based finite-volume method. This approach was implemented in an open-source CFD package and then tested in a fluidized bed case. The results demonstrate that the ability of the code to capture the size segregation and size change due to aggregation and breakup, and that our approach is an effective way to model complicated polydisperse gas-particle flows.

03-22-2017 – 1300A

FE0023031 – DISTRIBUTED FIBER SENSING SYSTEMS FOR 3D COMBUSTION TEMPERATURE FIELD MONITORING IN COAL-FIRED BOILERS USING OPTICALLY GENERATED ACOUSTIC WAVES

ORGANIZATION: University of Massachusetts Lowell **PRINCIPAL INVESTIGATOR**: Xingwei Wang
TEAM MEMBERS: Chengyu Cao, Xinsheng Lou
PRESENTER: Xingwei Wang

ABSTRACT

Researchers from University of Massachusetts Lowell, University of Connecticut and General Electric, will attempt to monitor and optimize real-time spatial and temporal distributions of high-temperature profiles in a fossil fuel power plant boiler system. Distributed optical fiber sensing has the potential to measure high temperatures while the optically generated acoustic signals can measure regions where the fibers cannot survive (e.g., 2000 °C). The reconstructed 3-D temperature profile will provide critical input for the control mechanisms to optimize the combustion process, thus achieving higher efficiency and fewer pollutant emissions. To accomplish this, project personnel will first develop a methodology to (1) establish a boiler furnace temperature distribution model and guide the design of the sensing system; (2) develop the sensors with one active sensing element on each fiber as well as a temperature distribution reconstruction algorithm for proof-of-concept; and (3) develop the distributed sensing system to integrate multiple active sensing elements. The entire sensing system, when fully integrated and tested in the university labs, will be tested in GE's test facility. This novel distributed sensor can have broader applications including measurement of strain, flow, velocity, crack growth, and corrosion for monitoring structural health.

03-22-2017 – 1330A

FE0022993 – ROBUST METAL-CERAMIC COAXIAL CABLE SENSORS FOR DISTRIBUTED TEMPERATURE MONITORING IN FOSSIL ENERGY POWER SYSTEMS

ORGANIZATION: University of Cincinnati **PRINCIPAL INVESTIGATOR**: Junhang Dong
TEAM MEMBERS: Hai Xiao (Clemson University)
PRESENTER: Adam Trontz (Student Researcher) and Shixuan Zeng (Student Researcher)

ABSTRACT

The goal of this project is to develop a new type of low-cost, robust metal-ceramic coaxial cable (MCCC) Fabry-Perot interferometer (FPI) sensors and demonstrate its capability for real-time distributed monitoring of high temperatures up to 1000oC in gases relevant to coal-based power plants. The specific technical objectives of this project include: (i) developing metal and ceramic materials with properties suitable for constructing the novel metal-ceramic coaxial cable and microwave reflectors, (ii) fabricating single FPI and multi-point FPIs in one MCCC, (iii) developing instrument and algorithm for microwave sensing single processing, (iv) demonstrating the MCCC-FPI sensors for temperature measurements up to 1000oC, (v) examining the MCCC-FPI sensor stability in high temperature gases relevant to coal-based power plants, and (vi) improving the spatial resolution for truly distributed sensing using the multi-point MCCC FPI sensor with joint time-frequency domain signal processing method. Success of this project will lead to a new paradigm of distributed sensors to overcome the long-standing challenges of real-time distributed temperature monitoring for high temperature facilities in the fossil energy power systems.

03-22-2017 – 1400A
FE0012274 – REDUCED MODE SAPPHIRE OPTICAL FIBER AND SENSING SYSTEM
ORGANIZATION: Virginia Polytechnic Institute and State University
PRINCIPAL INVESTIGATOR: Gary Pickrell
TEAM MEMBERS: Dan Homa, Anbo Wang
PRESENTER: Dan Homa

ABSTRACT

In this program, the Center of Photonics Technology at Virginia Tech developed a Raman scattering-based distributed temperature sensing system based on a micro-structured sapphire fiber sensor with reduced modal volume. Real-time, accurate, and reliable temperature monitoring at distributed locations was achieved to help further revolutionize technologies such as the integrated gasification combined cycle configuration of turbines and ultra-supercritical steam cycle designs. A new modal reduction waveguide was designed and fabricated via a novel and precise etching technique that was optimized to create a unique and robust sapphire fiber that significantly reduced the modal volume by greater than 95%. The proposed sapphire fiber waveguide design will improve the signal quality and spatial resolution of fiber optic sensing technologies and overcome the harsh environment challenges that severely limit the integration of mature optical fiber sensing technologies into new power plant control systems. Overall, this technology is expected to lower operating costs by allowing more accurate measurement of the conditions inside a gasifier or boiler to better control its operation.

03-22-2017 – 1500A
NETL-R&IC – ADVANCED OPTICAL FIBER SENSOR DEVELOPMENT FOR FUTURE FOSSIL ENERGY APPLICATIONS
ORGANIZATION: National Energy Technology Laboratory **PRINCIPAL INVESTIGATOR**: Paul Ohodnicki
TEAM MEMBERS: Michael Buric, John Baltrus, Joseph Tylczak, Gordon Holcomb, Zsolt Poole, Bo Liu, Yuhua Duan, Yuning Wu, Ben Chorpening
PRESENTER: Paul Ohodnicki

ABSTRACT

The NETL Research & Innovation Center currently has a major research initiative on the topic of advanced optical fiber based sensors for future fossil energy applications that specifically targets the goal of embedding multi-parameter, and multi-point sensors within the harshest locations within fossil energy systems. This work is cross-cutting in nature and spans a broad range of activities including functional materials for chemical sensing, high temperature optical fiber materials, application relevant exposure testing of both optical fiber and enabling sensor materials, embedding of fiber sensors in high temperatures using additive manufacturing processes, and first principles calculations to understand properties under application relevant conditions. This presentation will overview the broad range of relevant efforts currently being pursued and will also highlight key successes and future research directions for the overall initiative moving forward.

03-22-2017 – 1530A
SC0011936 – ADAPTIVE ELECTRICAL CAPACITANCE VOLUME TOMOGRAPHY FOR REAL TIME MEASUREMENT OF SOLID CIRCULATION RATE AT HIGH TEMPERATURES
ORGANIZATION: Tech4Imaging LLC **PRINCIPAL INVESTIGATOR**: Qussai Marashdeh
TEAM MEMBERS: Ohio State University
PRESENTER: Qussai Marashdeh

ABSTRACT

The research goals are to develop a high resolution tomography system using Electrical Capacitance Volume Tomography (ECVT) to accurately measure circulation rates of high temperature solids. This is accomplished by using Adaptive ECVT sensors that can provide an order magnitude more measurement data. Upon successful completion of the project, the energy industry would have an available tool to better control and optimizes solid mass circulation rates for better efficiencies.

03-22-2017 – 1600A
FWP-AL-12-470-009 – MERGED ENVIRONMENTS FOR SIMULATION AND ANALYSIS: TESTING AND DEMONSTRATING A STIGMERGIC CONTROL STRATEGY BASED ON DISTRIBUTED CONSTRUCTION
ORGANIZATION: Ames National Laboratory **PRINCIPAL INVESTIGATOR**: Dr. Kenneth “Mark” Bryden
TEAM MEMBERS: Dr. Paolo Pezzini, Mr. Daniel Bell, Dr. Kris Bryden
PRESENTER: Dr. Paolo Pezzini

ABSTRACT

The increasing availability of small, inexpensive, and intelligent sensors creates the opportunity for new decentralized, multi-agent control strategies for energy systems. These types of control strategies are inspired by the construction behavior of social insects that accomplish tasks without a centralized authority, such as stigmergy. The composition of the agents (i.e., what sensors are used to create an agent and control a particular actuator) and the reuse of sensors can provide lower level and faster decisions compared to traditional centralized approaches. This talk discusses the development and testing of a stigmergic multi-agent control strategy and compares its performance against a traditional multivariable control approach using an advanced gas turbine—fuel cell hybrid power system (i.e., the Hyper facility at NETL). Results show that traditional multivariable architectures designed to provide more adaptability have convergence issues when multiple operating points are not substantially distinct. A dynamic scaling approach using the stigmergic algorithm was tested at the NETL Hyper facility and showed how the model-free characteristic of the multi-agent design can provide more flexible decisions. This provides an adaptable approach that does not require system identification and controller tuning at each operating point in the system. In conclusion, a stigmergic algorithm based on the multiagent concept can provide a better approach when the dynamic coupling of diverse components in an advanced energy system (e.g., in an advanced hybrid cycle, supercritical CO_2 plants, etc.) cannot be easily simulated.

03-22-2017 – 1630A

FE0012302 – EVOLVING ROBUST AND RECONFIGURABLE MULTI-OBJECTIVE CONTROLLERS FOR ADVANCED POWER SYSTEMS

ORGANIZATION: Oregon State University **PRINCIPAL INVESTIGATOR**: Kagan Tumer
TEAM MEMBERS: Shauharda Khadka, Drew Wilson
PRESENTER: Shauharda Khadka (Student Researcher)

ABSTRACT

Designing advanced power systems that are more efficient, reliable, and robust requires us to overcome two critical challenges. First, such systems are inherently complex and highly nonlinear, making them next-to-impossible to model and control with traditional methods. Second, as many of these advanced power system designs are hybrid in nature, they are inherently multi-objective, requiring new control methods. In this work, we address the first challenge by using bio-inspired controllers based on evolutionary algorithms to control the advanced power systems. We then address the second challenge by transforming the multidimensional objective space to allow for linear combinations of objectives to find many effective solutions, which leads both to robust performance to sensor and actuator noise. Our results to date show that the evolved neuro-controller is robust to both sensing and actuator noise up to 10% of the signal magnitude. In addition, the controller provides reconfigurability to changing plant conditions. Finally, our preliminary results show that a memory-augmented neural architecture improves both the robustness and the reconfigurability of the controller.

03-22-2017 – 0800B
FEAA90 – PHYSICS-BASED CREEP SIMULATIONS OF THICK SECTION WELDS IN HIGH TEMPERATURE AND PRESSURE APPLICATIONS

ORGANIZATION: Idaho National Laboratory **PRINCIPAL INVESTIGATOR**: Thomas M. Lillo
TEAM MEMBERS: Wen Jiang
PRESENTER: Tom Lillo and Wen Jiang

ABSTRACT

The long-term mechanical behavior of thick section welds in high temperature and high pressure applications often defines the operational limits and system inspection requirements. Material testing to determine this long term behavior is impractical, and accelerated testing methodologies do not exist for many long term metallurgical phenomena. The long-term mechanical behavior of materials is often dependent on many parameters such as grain growth, microstructural evolution (precipitation, precipitate growth, dissolution of meta-stable phases, sub-structure development, etc.), creep cavitation, cyclic loads, temperature history and oxidation/corrosion. Conventional fusion-welded joints add complexity since the microstructure and local composition can vary significantly from that of the base material. Ultimately, accurate modeling is required to predict long-term creep behavior of fusion welds.

The objective of this project is to develop a simulation and modeling capability that can accurately simulate the time-dependent deformation behavior of fusion welded joints in g'-strengthened, nickel-based alloy Alloy 740H under operating conditions expected in the A-USC fossil fuel power plant. A unique computational framework, Multiphysics Object-Oriented Simulation Environment (MOOSE), will be applied to predict high temperature materials behavior associated with dislocation glide and climb in a well-characterized, weld microstructure. The growth of γ' during long term service and the resulting changes to the interaction with moving dislocations, e.g. γ' shearing, γ' bypass by dislocation climb and/or Orwan dislocation looping of γ' particles, will be incorporated and supported through experimental creep testing (short- and long-term tests) and microstructural characterization of welds in thick plates of Alloy 740H.

03-22-2017 – 0830B

FEAA114 – ADVANCED ALLOY DESIGN CONCEPTS FOR HIGH-TEMPERATURE FOSSIL ENERGY APPLICATIONS

ORGANIZATION: Oak Ridge National Laboratory **PRINCIPAL INVESTIGATOR**: Yukinori Yamamoto

TEAM MEMBERS: Bruch Pint (ORNL), Suresh Babu, Ben Shassere, Sean Kuo (Univ. Tennessee), Bernd Kuhn (Forschungszentrum Jülich, Germany)

PRESENTER: Yukinori Yamamoto

ABSTRACT

The goal of this project is to identify and apply breakthrough alloy design concepts and strategies for steel alloys to be used as high-temperature structural applications in fossil-fired power generation systems. The developed alloys should incorporate the balanced properties including improved creep strength, environmental resistance, and weldability, intended for upper limit temperatures higher than that of the materials currently in service.

A scale-up effort of newly developed, creep-resistant Fe-30Cr-3Al-2Nb base alloys was conducted by using ~40kg vacuum-induction-melted ingots. No technical issue was found in its hot-deformability through forging and rolling process above 1000°C. However, the rolled plate with ~13mm thickness exhibited a crack susceptibility during cooling after solution heat treatment at 1250°C, similar to commercial thick-plate productions of high-Cr ferritic stainless steels. Effect of cooling rate as well as minor alloying additions were discussed. Parallel to the scale-up effort, property evaluation of the "engineering" model alloys containing Mn, Si, and C were initiated, in order to simulate commercial grade steel products. Balance of Laves-phase forming elements such as W, Nb, Mo, and Ti were tailored for the increased volume fraction of Laves-phase precipitates in the temperature range of 700-800°C, combining with very little change of the Laves-phase solvus temperature in the BCC matrix. One of the optimized alloys showed significantly improved creep properties up to 750°C, with promising surface protection in both steam-oxidation and ash-corrosion environments.

03-22-2017 – 0900B

FWP-FEAA118 – WELDABILITY OF CREEP-RESISTANT ALLOYS FOR ADVANCED FOSSIL POWER PLANTS

ORGANIZATION: Oak Ridge National Laboratory **PRINCIPAL INVESTIGATOR**: Zhili Feng

TEAM MEMBERS: Xinghua Yu, Wei Zhang, Yanfei Gao

PRESENTER: Xinghua Yu

ABSTRACT

Welding is extensively used in construction of fossil power plants. The performance of the weld region can be critical to the safe and economical operation of fossil power plants. Degradations in performance such as reduced creep strength and premature failure in the weld region (e.g. Type IV failure in Grade 91 steels) are examples of longstanding welding and weldability problems for boiler and other components. In order to understand the premature failures and to predict long-term performance of welded structures in power plants, the current study is focused on developing a long-term integrated multi-scale, multi-physics model based on fundamental understanding of the welding process, phase transformations, and the operative creep mechanism. Our modeling tools include the CALPHAD method and mean field approach for microstructure simulation and finite element analysis for micro-scale to meso-scale creep deformation and damage simulation. The progress of integrated model development will be presented.

03-22-2017 – 0930B

FWP-AL-15-450-013 – COMPUTATIONAL DESIGN OF MULTISCALE SYSTEMS

ORGANIZATION: Ames National Laboratory **PRINCIPAL INVESTIGATOR**: Richard LeSar
TEAM MEMBERS: Kenneth Bryden
PRESENTER: Richard LeSar

ABSTRACT

Our primary goal is to use computational materials modeling to accelerate the development, certification, and insertion of new materials into both existing and new technologies at all points in the design workflow. One of our biggest challenges is that materials behavior is complex, being governed by coupled physical processes that range in scales from nanometers of atomic interactions to the meters of manufactured products. Available models to describe these systems are largely independent and based on different physics for each of these scales. Multiscale modeling attempts to link together these independent models to form a unified computational tool for understanding the behavior of the overall system. The goal of our program is to accelerate the development of multiscale materials simulation tools by creating a way to easily link autonomous models together. We are basing our approach on a standardized interface, called the basic model interface (BMI), which is a set of standardized functions that make a model self-describing and fully controllable within a modeling framework. We will review our successful implementation of the BMI into two independent methods, a Lattice Boltzmann model of continuum flow and a molecular dynamics code at the atomistic scale. The primary focus of this talk will be, however, on the implementation of a BMI into an independent code developed and maintained by someone else, specifically the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) molecular dynamics code developed at the Sandia National Laboratories. LAMMPS is widely used in the materials modeling community.

03-22-2017 – 1030B

FWP49022 – GAS TURBINE MATERIALS LIFE ASSESSMENT AND NON-DESTRUCTIVE EVALUATION

ORGANIZATION: Argonne National Laboratory **PRINCIPAL INVESTIGATOR**: J.G Sun
TEAM MEMBERS: K. Natesan, A. Kulkarni, Z. Zeng
PRESENTER: J.G. Sun

ABSTRACT

This is a collaborative project between the Siemens Corporation and Argonne National Laboratory (ANL) to focus on the research for advanced gas turbine materials. Gas turbines are critical components within conventional combined cycle power systems and in the gasification systems that are being developed and demonstrated around the world. In such applications, the demand from fuel flexibility and using fuels derived from coal, biomass and waste poses a new set of challenges for the materials used to construct gas turbine hot gas paths. To meet the combined targets of maximizing efficiencies and minimizing CO_2 emissions, it is necessary to consider these materials challenges. The two objectives of this project are: (1) develop predictive models for deposition, corrosion and component life assessment in gas turbines operating on novel fossil fuel gases and, (2) develop/demonstrate advanced nondestructive evaluation (NDE) inspection tools and technologies for hot gas path components to enable on-going assessment of the remaining lives of components during their use.

For the first objective, work is ongoing to evaluate the corrosion effects on turbine materials from syngas and steam/CO_2 environment. The intent is to evaluate corrosion damage through metallographic analysis to develop a materials model capable of thermo-kinetic modeling of contaminant flux. The ultimate deliverable of the task is establishment of corrosion maps for high temperature metallic and ceramic systems. Eighteen sets tasks were planned to evaluate four turbine alloys and seven coatings at 950°C and 1010°C in both air combustion and oxy-fuel environments. Fourteen tests have been performed so far. Weight changes of samples were recorded, and the corrosion depths were measured by scanning electron microscope cross-section analysis. Most Siemens developed coatings successfully protected alloy substrates from high temperature corrosion in both air and oxy-fuel gas environments in the fourteen tests. The other four tests will be continued. The effects of temperature and gas environments on alloy and coatings will be evaluated and the life-times of these coatings will be assessed after all tests finished.

For the second objective, work is underway to develop and validate advanced NDE methods for the health monitoring and life prediction of ceramic thermal barrier coatings (TBCs). This work has successfully demonstrated an advanced pulsed thermal imaging–multilayer analysis (PTI-MLA) method that can accurately measure coating properties such as thermal conductivity and thickness over entire TBC coated surface. To further advance its industrial applications, one effort has been on evaluation of a low-cost infrared camera for cost-effective NDE characterization of TBCs and another on development of an image construction method to display measured TBC property distributions on the entire surface of complex 3D components. Experimental results for measured TBC properties on a turbine blade will be presented.

03-22-2017 – 1100B
FWP-49943 – DEVELOPMENT OF NONDESTRUCTIVE EVALUATION (NDE) METHODS FOR STRUCTURAL AND FUNCTIONAL MATERIALS
ORGANIZATION: Argonne National Laboratory **PRINCIPAL INVESTIGATOR**: J. G. Sun
TEAM MEMBERS:
PRESENTER: J. G. Sun

ABSTRACT

The objective of this project is to develop nondestructive evaluation (NDE) technologies as part of the overall effort to develop high-temperature structural and functional materials for advancing the utilization of fossil fuel resources. The focus of such materials under this project includes ceramic thermal barrier coatings (TBCs) applied on hot-gas-path components in advanced gas turbines and additive manufactured (AM) metallic components. These materials are made through complex manufacturing processes and may have complex structures and/or compositions. Because of their important roles in system safety and reliability, NDE is necessary to assess the quality of as-processed materials, monitor their degradation during service, and provide data for reaching rational decisions on replace/repair/re-use of these components. A TBC system consists of a thermally insulating ceramic topcoat (the TBC) made of yttria stabilized zirconia, a thin oxidation-resistant metallic bond coat, and a metal substrate. TBC degradation is caused by sintering of the ceramic TBC layer at high temperatures which results in gradual cracking and eventual delamination at the TBC/bondcoat interface. This entire TBC life can now be accurately assessed by an Argonne developed NDE method: pulsed thermal imaging–multilayer analysis (PTI-MLA). PTI-MLA can quantitatively measure important TBC properties such as thermal conductivity and thickness over entire coated component surface, and the conductivity is very sensitive to TBC sintering and cracks. While we have proposed a TBC life prediction approach based on measured average TBC conductivity by PTI-MLA, a new investigation is conducted for the detection of crack initiation and growth during TBC life. To further extend PTI-MLA applications in industry, we also evaluated a low-cost, room-temperature infrared camera and developed models for accurate TBC property measurements. For AM materials, one concern is their property anisotropy and the present of defects. Such material anisotropy was examined using a PTI method that can measure thermal diffusivity in all three dimensions. This presentation describes these recent developments and experimental results.

03-22-2017 – 1300B
FE0024009 – CERAMIC HIGH TEMPERATURE THERMOELECTRIC HEAT EXCHANGER AND HEAT RECUPERATORS IN THE POWER GENERATION SYSTEMS
ORGANIZATION: West Virginia University Research Corporation **PRINCIPAL INVESTIGATOR**: Xueyan Song
TEAM MEMBERS:
PRESENTER: Xueyan Song

ABSTRACT

This project will develop compact and highly efficient all-oxide ceramic thermoelectric (TE) generators to work as compact heat exchanger and simultaneously recover the high temperature waste heat from high temperature power systems such as solid oxide fuel cells. With the combination of enhanced performance of oxide materials and the innovative designs of TE generators, the proposed all-oxide TE device will potentially over-perform the state-of-the-art TE materials that are made of conventional metallic or semiconductor materials for high temperature applications. Overall, the TE devices proposed in this project will be highly efficient, lightweight, reduced in size, highly stable in air at high temperatures, and non-toxic, for powering sensors at temperatures in the 600-980 degrees Celsius range. In addition, the new devices will be easy to fabricate and thus will facilitate mass production with a high potential for use in large-scale operations.

03-22-2017 – 1330B
FE0023974 – ADDITIVE MANUFACTURING OF FUEL INJECTORS
ORGANIZATION: Edison Welding Institute, Inc. **PRINCIPAL INVESTIGATOR**: Mahdi Jamshidinia
TEAM MEMBERS: Solar Turbines Inc.
PRESENTER: Mahdi Jamshidinia

ABSTRACT

The overall objective of this project is to develop and qualify the mechanical performance of Alloy X (similar to Hastelloy X) fuel nozzles made using the laser powder bed fusion (L-PBF) additive manufacturing process. Gas turbine components require very specific design and material considerations. Dimensional tolerances need to be met along with the material and metallurgical properties. These components operate in very high temperature and stress environments, so the margin for design error is very small. Since additive manufacturing is still relatively new to the gas turbine industry, EWI and Solar Turbines Incorporated will evaluate the impact on several variables in additive manufacturing a fuel injector tip. These variables include evaluating different types of powder material from various suppliers, AM parameter and heat treat sensitivity. The fuel nozzle tip currently has a long lead time and is very difficult to cast. AM will reduce the scrap, therefore, lowering the cost, and greatly improving the lead time. The AM flexibility will allow Solar Turbines Incorporated to design features into the components that may improve turbine performance and durability. It may also result in lower costs by reducing manufacturing time and eliminating scrap material. This project will establish the baseline methodology for developing material property design curves for other high temperature alloys of interest to the industrial gas turbine industry.

03-22-2017 – 1400B
FE0024090 – HIGH TEMPERATURE CERAMIC HEAT EXCHANGER FOR SOLID OXIDE FUEL CELL
ORGANIZATION: Mohawk Innovative Technology, Inc. **PRINCIPAL INVESTIGATOR**: Hooshang Heshmat
TEAM MEMBERS: Jose Luis Cordova
PRESENTER: Jose Luis Cordova

ABSTRACT

NETL is partnering with Mohawk Innovative Technology, Inc. (MiTi) to develop a high effectiveness, low pressure drop *ceramic* heat exchanger for use as a cathode air preheater for solid oxide fuel cell (SOFC) applications. At the operating conditions of SOFCs, the use of stainless steels and/or chromium-containing metallic alloys commonly found in commercial heat exchangers may result in chromium volatilization, which is a known cathode degradation mechanism that reduces SOFC performance and life. By using ceramics such as alumina or alumina-silicate and eliminating the use of metals in heat exchangers, this project provides a necessary element for the practical commercialization of SOFC technology. The novel ceramic heat exchanger design presented leverages a geometry previously demonstrated by MiTi to produce high effectiveness and low pressure drop heat exchange elements. Heat exchanger performance and design calculations are based on state of the art SOFC operating conditions. A thermal-based tradeoff analysis for ceramic material selection is performed, and a modular heat exchanger design and its heat exchange elements are presented. The modular concept allows for incremental aggregation of modules to target a broad range of operating conditions typical of present and upcoming SOFC applications (e.g., 25 to 400 kWe). Results are presented of heat transfer and pressure drop performance tests that were obtained for a complete 5 kWth prototype in both stand-alone conditions and integrated to an actual SOFC stack.

03-22-2017 – 1500B

NETL-R&IC – MICRO CHANNEL HEAT EXCHANGERS BASED ON ALLOY 230: EXPOSURE CHARACTERISTICS AND MECHANICAL BEHAVIOR

ORGANIZATION: NETL - Research and Innovation Center **PRINCIPAL INVESTIGATOR**: Omer N. Dogan
TEAM MEMBERS: M. Kapoor, J. Hawk, S. Akanda
PRESENTER: Omer N. Dogan

ABSTRACT

The sCO_2 cycles rely heavily on heat recuperation for increased efficiency. Compact heat exchanger designs are proposed to reduce equipment size and enhance heat transfer between the high-temperature and low-temperature fluids in sCO_2 power cycles. Components containing small features in compact heat exchangers are typically joined together by diffusion bonding or brazing. Although the goal is to form a monolithic structure, depending on the alloy composition and microstructure, the interface region of the bonded structure may have a chemical composition and microstructure different from the parent alloy. This can be a source of mechanical and/or chemical instability for the structure in the application environments. Sometimes, post bonding heat treatment may be practical to eliminate or reduce the chemical gradient and microstructural variation in the structure. Transient-liquid-phase-bonding (TLP) is one such joining techniques for compact heat exchangers and was studied in Ni-based-superalloy-H230 for use in a heat exchanger operating at 720°C and 25 MPa pressure. Tensile testing of the stacks at 760°C indicated a yield strength of ~ 86% that of the bulk H230. sCO_2 exposures of these stacks carried out in an autoclave at the operating conditions for up to 1500 h showed a similar corrosion behavior on the bond regions and base metal.

03-22-2017 – 1600B

FE0026260 – OPTIMIZATION OF ADVANCED STEELS FOR CYCLIC OPERATION THROUGH AN INTEGRATION OF MATERIAL TESTING, MODELING AND NOVEL COMPONENT TEST VALIDATION

ORGANIZATION: Electric Power Research Institute **PRINCIPAL INVESTIGATOR**: John Siefert
TEAM MEMBERS: Jonathan Parker, Ian Perrin, Graham Pritchard, Amit Shyam, Ian Dempster
PRESENTER: John Siefert

ABSTRACT

Legacy and continued generation of creep data for advanced 9Cr steels widely specified for critical components in the power generation industry continue to exhibit variations in performance (either strength, ductility or both). Specifically, there is a marked trend for some of these steels (P92 as one example) to remarkably low creep ductility values of less than 10% and as established by a reduction of area measurement. The observed variation in creep ductility for P92 is particularly alarming because this suggests that the material may exhibit low damage tolerance in end-use applications where mechanical notches are present in parent material due to poor design or in weldment applications where a metallurgical notch is present. The primary objective in this study is to increase the creep strength and the creep ductility for a conventional heat of P92 steel through an elevated temperature normalization and rapid quenching process prior to tempering. Detailed microstructural examinations are planned to validate the elimination and/or reduction in boron nitride, which has shown to be a key nucleation site for creep cavities in previously evaluated, long-term tests on multiple heats of P92 steel. Improved performance in regards to component behavior will be assessed through conventional creep tests, notch bar creep tests, sequential creep-fatigue and fatigue-creep tests, large specimen cross-weld creep tests and pressurized creep tests under various loading and thermal cycling conditions. The expected results of the project will be demonstration at the lab scale of an improved version of P92 for use in cycling fossil energy power plants.

03-22-2017 – 1630B

FWP-14-017626 – EXPLORING ENERGY-WATER ISSUES IN THE UNITED STATES

ORGANIZATION: Sandia National Laboratories **PRINCIPAL INVESTIGATOR**: Vincent Tidwell

TEAM MEMBERS: Barbara Moreland, Calvin Shaneyfelt

PRESENTER: Vincent Tidwell

ABSTRACT

The availability of freshwater supplies to meet future demand is a growing concern, particularly in the energy sector. Water availability metrics are needed to inform future water development decisions. With the help of water managers, water availability was mapped for over 1300 watersheds throughout the 31-conterminuous states in the Eastern U.S. complimenting a prior study of the Western U.S. The compiled set of water availability metrics are unique in that they consider multiple sources of water (fresh surface and groundwater, wastewater and brackish groundwater), accommodate institutional controls placed on water use, and are accompanied by cost estimates to access, treat and convey each unique source of water. Although the East is generally considered “water rich” water managers have identified a number of watersheds as Areas of Concern where water supply challenges exist due to drought related impacts, environmental flows, groundwater overdraft, and salt water intrusion. Important differences are realized between the Eastern and Western U.S. in terms of water availability and the basic culture of water management.

03-22-2017 – 1030C

FE0026443 – PILOT-SCALE TESTING OF AN INTEGRATED CIRCUIT FOR THE EXTRACTION OF RARE EARTH MINERALS AND ELEMENTS FROM COAL AND COAL BYPRODUCTS USING ADVANCED SEPARATION TECHNOLOGIES

ORGANIZATION: University of Kentucky **PRINCIPAL INVESTIGATOR**: Jack Groppo
TEAM MEMBERS: Rick Honaker, Jim Hower, Cortland Eble
PRESENTER: Rick Honaker

ABSTRACT

The approach that will be used in this investigation emphasizes collaboration with coal companies actively mining in the Illinois Coal Basin to develop and implement a sampling and characterization program that will be representative of both current (mine face and preparation plant) and future mining in the region. The approach identifies and characterizes coal and coal-related material in the Illinois Coal Basin that contain elevated concentrations of Rare Earth Elements (REEs) by using archived core databases, analyzing existing cores from a variety of sources, including state geological surveys and mining companies, as well as new cores extracted from areas of interest and preparation plant process streams. Sampling locations will focus primarily on economic coal beds, particularly those with current mining and/or exploration activity, as well as those with sufficient reserves to sustain commercial development for the foreseeable future. Specific coal beds of primary interest are Springfield, Herrin and Baker, although other deeper coal beds may be considered, provided core data justified further sampling and the known reserve base is sufficient.

03-22-2017 – 1100C

FE0027167 – HIGH YIELD, ECONOMICAL AND ENVIRONMENTALLY BENIGN PRODUCTION OF RARE EARTH ELEMENTS FROM COAL ASH

ORGANIZATION: Physical Sciences Inc. **PRINCIPAL INVESTIGATOR**: Prakash B. Joshi
TEAM MEMBERS: Physical Sciences Inc., Andover, MA; Equinox Chemicals LLC, Albany, GA; Center for Applied Energy Research, Lexington, KY
PRESENTER: Dorin V. Preda

ABSTRACT

Physical Sciences Inc. and its team members, Equinox Chemicals LLC, and Center for Applied Energy Research (University of Kentucky) have optimized physical and chemical processes that enabled recovery of trace REYSc elements from coal ash with high yield (>18%) and high enrichment (>30% REY content in the final product) on a Phase 1 project. Ponded ash (>500 ppm REYSc) from Dale power plant in Ford, KY was selected as the ash source for demonstration of key process elements on pilot scale as well as a potential source for a commercial scale plant in Phase 2. The team developed a detailed techno-economic model of the REYSc recovery process based on ash feedstock and reagent inputs and REE concentrate, and co-product outputs of commercial value, taking into account capital and operating expenses. Key elements of the ash characterization, physical separation and chemical processing as well as results of the techno-economic modeling will be presented.

03-22-2017 – 1300C

FE0027102 – PLASMA ARC GASIFICATION BASED RARE EARTH ELEMENT RECOVERY FROM COAL FLY ASH

ORGANIZATION: Southern Research **PRINCIPAL INVESTIGATOR**: Jay Renew, P.E.
TEAM MEMBERS: Ken Jeffers, P.E.
PRESENTER: Ken Jeffers, P.E.

ABSTRACT

Southern Research and its collaborators are developing an innovative, environmentally-friendly thermal extraction process using plasma arc technology for concentrating rare earth elements (REEs) in coal fly ash (CFA). The proposed technology includes two process options. For Option 1, plasma smelting is used to separate ash into slag and metal (iron) portions where it is intended that the REEs will collect into the iron phase. In Option 2, the molten iron from smelting is volatilized, and the vapors are condensed and collected sequentially to produce REE-enriched metal fractions. The initial project work included acquiring CFA samples from several coal-fired power plants fueled on eastern bituminous coal and characterizing the ash for REE content. A comprehensive feasibility study was conducted including bench-scale experiments using a plasma furnace to determine the fate of REEs in the separation between the slag and metal layers, evaluation of enhancements to promote the partitioning of REEs to the metal layer, and the plasma volatilization of the iron phase was modeled, including the sequential condensation of REE-enriched vapors. Finally, a design package will be prepared for a pilot-scale system. Project benefits include creating a new beneficial use market for coal ash, reducing waste ash volume, and concentrating REEs without the use of environmentally-damaging chemicals.

03-22-2017 – 1330C

FE0027155 – ECONOMICALLY VIABLE AND ENVIRONMENTALLY BENIGN HIGH-PERFORMANCE TECHNOLOGY TO RECOVER RARE EARTH ELEMENTS FROM COAL BY-PRODUCTS

ORGANIZATION: Tusaar Corp **PRINCIPAL INVESTIGATOR**: Dr. Gary Carlson
TEAM MEMBERS: Elizabeth Alexander (Research Chemist), Raelynn Kadnuc (Research Chemist) , Gautam Khanna (CEO), Timothy Lanyk (Senior Process Engineer), Dr. Dean Stull (Consultant), George Yates (Senior Application Specialist)
PRESENTER: Dr. Gary Carlson

ABSTRACT

The main goal of this project is to develop a rare earth element (REE) extraction process for coal by-product materials (fly ash) utilizing a proprietary technology involving leaching processes and proprietary sorption media with the ability to process up to 2 kilogram batches and deliver a product with greater-than 2.5wt% REO. Project activities focus on two unique project requirements - firstly the extraction/leaching of target metals from source materials and secondly, concentration of extracted metals into an end product acceptable for further processing. Specific objectives include: (1) possible beneficiation of coal by-product source material, (2) coal by-product leaching, (3) radioactive material separation, (4) REE sequestration and recovery, and (5) waste water treatment for heavy metal removal.

It is expected that successful execution of this project will lead to possible reduction of US dependence and other western countries on China REO production, which currently controls over 95% of the heavy rare earth market. An additional benefit of successful project completion will be the separation of uranium and thorium from fly ash materials therein enabling the use of additional fly-ash material sources into more applications where it currently cannot be used. Since fly ash is produced in large quantities across the US, additional, beneficial uses of coal fly ash is an important factor in the continued use of coal fired power plants for energy production.

03-22-2017 – 1400C

NETL-R&IC – OVERVIEW AND ACCOMPLISHMENTS OF R&ICS RARE EARTH ELEMENTS FROM COAL AND COAL BY-PRODUCTS

ORGANIZATION: NETL - Research and Innovation Center **PRINCIPAL INVESTIGATOR**: Evan J. Granite

TEAM MEMBERS: Elliot Roth, Tracy Bank, Mary Anne Alvin, Karol Schrems

PRESENTER: Evan J. Granite

ABSTRACT

Coal is an important resource, both in the United States and around the world. The US generates approximately 30% of its electricity through coal combustion and, at the current overall rate of consumption, has more than a 250-year supply of coal. In the US, most coal is burned for power generation, but substantial quantities are also used in the manufacture of steel, chemicals, and activated carbons. Numerous industries—such as mining, power, rail transportation, manufacturing, chemical, steel, activated carbon, and fuels—are involved in the production, transportation, and use of coal. Rare earths are commercially produced from ores containing monazite (rare earth phosphate mineral) or bastnäsite (rare earth carbonate-fluoride mineral) as well as from ion exchangeable clays. They are also found in coal; combustion byproducts such as ash, coal preparation residues, gasification slags, and mining byproducts; and the strata above and below some coal seams, thereby making every process in the mining and utilization of coal a potential source of rare earth elements.

The NETL Research and Innovation Center (NETL-RIC) recently initiated research to support the measurement of concentration, identification of rare earth compounds, and recovery of rare earths from abundant domestic coal byproducts. Some of the early and exciting results will be discussed.

03-22-2017 – 1500C

FE0026952 – NOVEL MEMBRANE AND ELECTRODEPOSITION-BASED SEPARATION AND RECOVERY OF RARE EARTH ELEMENTS FROM COAL COMBUSTION RESIDUES

ORGANIZATION: Duke University **PRINCIPAL INVESTIGATOR**: Heileen Hsu-Kim

TEAM MEMBERS: Zachary Hendren, James Hower, Desiree Plata, Mark Wiesner

PRESENTER: Heileen Hsu-Kim

ABSTRACT

The goal of this project is to develop and demonstrate bench-scale technology to separate and concentrate rare earth elements (REEs) from coal fly ash and other coal combustion residues (CCRs). For this project we are studying 12 types of coal ash samples, selected as a representative collection of CCRs generated at U.S. power utilities. We are developing hydrometallurgical-based technology to extract and concentrate REEs. Part of this technology involves membrane-based filtration in combination with electrodeposition for the separation of REEs from acid leachates of CCRs. Specific objectives of the work are to: 1) Perform collection and characterization of CCR feedstocks; 2) Determine the technical and economic feasibility of the proposed separation methods; and 3) Evaluate and test hydrometallurgical extraction techniques and REE separation methods from CCR extracts. A variety of nanofiltration, electrodeposition, and other ion separation configurations have been tested with leachates of the CCR samples. The expected benefits of this project will be the development of technologies to recover REEs from a highly abundant waste material (coal combustion residues) and the development of methods to determine the most promising CCR materials for REE recovery. The outcomes will include a new approach for REE extraction that utilizes advanced separation technologies to enable environmentally benign processes relative to conventional approaches that use hazardous chemicals for separations.

03-22-2017 – 1530C
FE0027012 – RECOVERY OF RARE EARTH ELEMENTS (REES) FROM COAL ASH WITH A CLOSED LOOP LEACHING PROCESS
ORGANIZATION: Battelle Memorial Institute **PRINCIPAL INVESTIGATOR**: Rick Peterson
TEAM MEMBERS: Mike Heinrichs, Kathryn Johnson, Jackie Gerst
PRESENTER: Rick Peterson

ABSTRACT

The primary project objective is to validate the economic viability of recovering REEs from the coal byproduct coal ash using Battelle ·s patented closed-loop Acid Digestion Process (ADP). This will be accomplished by selecting coal sources with the potential to provide REE concentrations above 300 parts per million by weight, collecting characterization data for coal ash samples generated via three different methods, and performing a Techno-Economic Analysis (TEA) for the proposed process. Three sources of coal ash are targeted for evaluation of the economics of REE recovery in this project: (1) coal ash from power generation stations, to include fly ash and/or bottom ash, (2) ash generated in a lower temperature ashing process, and (3) ash residual from Battelle · s coal liquefaction process.

The proposed technology offers a breakthrough for the economic recovery of REEs from coal products by minimizing significant waste streams, through reagent. The process produces a concentrated solid form of rare earth oxides for easy delivery to a REE purification facility. The principal benefit of this project will be the validation of an economical process for recovery of REEs from in-country resources, specifically coal byproducts. Despite critical applications for rare earth elements, ranging from catalysts and optics to magnets in motors and generators, over 90% of the global supply of rare earths is produced by China.

03-22-2017 – 1600C
FE0026927 – RECOVERY OF RARE EARTH ELEMENTS (REES) FROM COAL MINE DRAINAGE
ORGANIZATION: West Virginia University Research Corporation **PRINCIPAL INVESTIGATOR**: Paul Ziemkiewicz
TEAM MEMBERS: Aaron Noble, Xingbo Liu
PRESENTER: Paul Ziemkiewicz

ABSTRACT

A research team at West Virginia University is studying the feasibility of recovering rare earth elements (REE) treating AMD sludge as a primary feedstock. The study utilized field sampling, preliminary laboratory extraction data and basic processing assumptions to generate the necessary input parameters for a feasibility study. A regional AMD solids production model was constructed to estimate the potential of AMD to support an REE industry. Annual TREE content of AMD solids in the Northern Appalachian Coal Basin was estimated to be 1,180 t/year with an in-situ value of $184 million. Based on these results, we can conclude that AMD solids are a promising feedstock for REE recovery. Laboratory experiments indicated nearly 100% extraction of REE from AMD solids under acid leaching and re-precipitation as pH was adjusted upward. This confirmed that REEs occur in AMD solids as hydroxides/oxy-hydroxides and their dissolution /precipitation response is similar to that of iron hydroxide: $Fe(OH)_3$. Ongoing work focusses on efficient extraction of REE from the iron hydroxide matrix. Solvent extraction and pH adjustment experiments are underway. Using solvent extraction alone, the ratio of the REE yttrium to major ions increased from 0.05% in the leaching solution to 1.03% in the extractant. In order to further improve extraction selectivity, pH adjustment is being refined to identify points where REEs separate from $Fe(OH)_3$.

03-22-2017 – 1630C

FE0001202 – A POLLUTION-PREVENTION AND ECONOMICALLY-VIABLE TECHNOLOGY FOR SEPARATION OF RARE EARTH ELEMENTS FROM POWDER RIVER BASIN (PRB) COAL ASHES

ORGANIZATION: University of Wyoming **PRINCIPAL INVESTIGATOR**: Maohong Fan
TEAM MEMBERS: Hanjing Tian, Eric Williams, Gabrielle Gaustad, Hertanto Adidharma, Maciej Radosz, Zaixing Huang, Kai Li, ChooiKim Lau, Yan Luo, Kaiying Wang, Andrew Thomas Jacobson
PRESENTER: Maohong Fan

ABSTRACT

Rare earth elements (REEs) are critical materials in various fields including energy production and environmental protection. The market for REEs will continue to grow quickly. Global demand for REEs in 2025 is projected to reach ~300,000 tons. Thus, people are increasingly interested in searching developable REEs- resources, and among them are coal by-products. Wyoming is rich in coal, thus it has a lot of coal by-products also, including fly ashes. Supported by U.S. DOE, the UW-WVU-RIT team has been developing new pollution-avoidance or pollution-prevention, and cost-effective technologies with enhanced performance and great scalability for recovering high-value REEs from coal ashes with the goal of enriching the REEs from 300 ppm in coal ashes (eventually coal and other coal utilization byproducts) to 2 wt% targeted by DOE. The concentrations of the REEs-containing solids generated by the team are higher or much higher than the targeted 2 wt-% (elements based). In addition, factorial tests are being conducted to minimize the cost and maximize the REEs recovery efficiency of the new REEs extraction processes. The overall progress shows that recovery of REEs from coal fly ashes with the new extraction technology is promising.

03-22-2017 – 1715C

FE0027006 – INVESTIGATION OF RARE EARTH ELEMENT EXTRACTION FROM NORTH DAKOTA COAL-RELATED FEEDSTOCKS

ORGANIZATION: University of North Dakota **PRINCIPAL INVESTIGATOR**: Steven A. Benson
TEAM MEMBERS: Daniel Laudal, Michael Mann, Dan Palo, and Shane Addleman
PRESENTER: Steven Benson

ABSTRACT

As part of the US Department of Energy effort to identify alternative domestic sources of Rare Earth Elements (REE), the University of North Dakota was awarded a project to determine the feasibility of recovery of REE from North Dakota lignite coal and related feedstocks. Laboratory testing of a novel concentrating method has shown very high recovery of about 80-90% of the REEs from two potential feedstocks, ranging from 580 to 2300 ppm REE content on an ash basis, with excellent selectivity/recovery of the critical and heavy REE. Details of a processing scheme to economically concentrate the REE to the goal of 2 weight percent using a simple and environmentally benign method have been established. The project team has also developed the concepts for integration of the REE recovery process within an existing coal conversion facility that will provide cost-saving synergies and infrastructure to reduce costs. Based on the results of the Phase I work, the project team believes North Dakota lignite-related feedstocks to be a highly promising alternative domestic source of REE that will limit dependence on foreign supply.

03-22-2017 – 1730C

NETL-R&IC – DEVELOPMENT OF A NOVEL CFD MODEL FOR LARGE-SCALE REE EXTRACTION PROCESS

ORGANIZATION: NETL - Research and Innovation Center **PRINCIPAL INVESTIGATOR**: Evan Granite
TEAM MEMBERS: Liqiang Lu, Sofiane Benyahia
PRESENTER: Sofiane Benyahia

ABSTRACT

In past decades, the continuum approach was the only practical technique to simulate large-scale fluidized bed reactors because discrete approaches suffer from the cost of tracking huge numbers of particles and their collisions. This research improves significantly the computation speed of discrete particle methods by combining the following two ideas: First, the time-driven hard-sphere (TDHS) algorithm with a larger time-step is proposed allowing a speedup of 20-60 times; Second, the number of tracked particles is reduced by adopting the coarse-graining particle method (CGPM) gaining an additional 2-3 orders of magnitude speedup of the simulation. A new velocity correction term is introduced and validated in TDHS to solve the over-packing issue in dense granular flow. This novel model is validated by simulating several small and large-scale flow reactors where published experimental and numerical data are available. Then, a chemical reaction mechanism based on rare earth elements (REE) leaching from coal byproducts was implemented with CGPM to study the effects of several flow and design parameters on the leaching process. A counter-current reactor was studied and optimized to maximize the mass fraction of REE in the liquid solution. Finally, a large-scale version of this REE reactor is simulated to investigate the effects of scale-up on the process performance.

03-22-2017 – 1745C

NETL-R&IC – EVIDENCE OF MOBILIZATION OF REE: GEOLOGICAL ASPECTS OF REE FORMATION IN THE UNITED STATES

ORGANIZATION: NETL - Research and Innovation Center **PRINCIPAL INVESTIGATOR**: Tracy Bank
TEAM MEMBERS: Elliot Roth, Bret Howard, Evan Granite
PRESENTER: Tracy Bank

ABSTRACT

Sedimentary rocks that comprise the coal, overburden and underclay of two major Pennsylvanian coal deposits have been investigated as sources of rare earth elements (REE). Samples from the Lower Kittanning coal seam in the Allegheny Formation as well as the Buck Mountain coal in the Llewellyn Formation are included in this study. Data indicate that the studied rocks are enriched in total rare earth elements compared to both the North American Shale Composite (NASC) and the Post-Archean Australian Shale (PAAS). A strong positive correlation of total rare earth elements with Ti/Al and with P in the Buck Mountain samples (R2 = 0.58 and 0.33, respectively) indicates that elevated REE concentrations occur where coarse clastic input increased. These data support a detrital source of REE, possibly occurring as the mineral monazite. In the Kittanning samples, total REE correlate with high Th and V, but not Ti/Al (R2=0.0003) or P (R2 = 0.004), and geochemical and mineralogical evidence supports a different mechanism of REE enrichment. In this case, minor deposits of adsorbed REE, similar to the ion adsorbed REE deposits of China, may have formed but conditions during diagenesis allowed for crystallization of the REE, rendering them no longer exchangeable.

03-23-2017 – 0830A

FE0026308 – MODEL-BASED EXTRACTED WATER DESALINATION SYSTEM FOR CARBON SEQUESTRATION

ORGANIZATION: General Electric Company **PRINCIPAL INVESTIGATOR**: David Moore
TEAM MEMBERS: GEGRC: Ryan Adams, William Alberts, Elizabeth Dees, Rachel Gettings, Paul Smigelski, Albert Stella
PSU: Manish Kumar, Li Li
PRESENTER: Rachel Gettings

ABSTRACT

The focus of this research effort centered around water recovery from high Total Dissolved Solids (TDS) extracted waters (180,00 mg/L) using a combination of water recovery (partial desalination) technologies. The goals include: a) define the scope and test location for pilot-scale implementation of the desalination system, b) define a scalable, multi-stage extracted water desalination system that yields clean water, concentrated brine, and, salt from saline brines, and c) validate overall system performance with field-sourced water using GE pre-pilot lab facilities.
Conventional falling film-mechanical vapor recompression (FF-MVR) technology was established as a baseline desalination process. A quality function deployment (QFD) method was used to compare alternate high TDS desalination technologies to the base case, including, but not limited to: membrane distillation (MD), forward osmosis (FO), and high pressure reverse osmosis (HPRO). Technoeconomic analyses elucidated system-level cost savings for stand-alone or hybrid HPRO technologies.
Pre-pilot-scale tests were conducted using field production water to validate key process steps for extracted water pretreatment. Approximately 5,000 gallons of field produced water was processed through, microfiltration, ultrafiltration, and steam regenerable sorbent operations for use in desalination testing. Improvements in membrane materials of construction were considered as necessary next steps to achieving further improvement in HPRO element performance at high pressure. Several modifications yielded elements capable of withstanding ~5,000 PSI without gross failure.

03-23-2017 – 0900A

FE0026315 – ADVANCED INTEGRATED TECHNOLOGIES FOR TREATMENT AND REUTILIZATION OF IMPAIRED WATER IN FOSSIL FUEL-BASED POWER PLANT SYSTEMS

ORGANIZATION: Ohio University **PRINCIPAL INVESTIGATOR**: Jason Trembly
TEAM MEMBERS: Xingbo Liu, Xiujuan Chen, Dora Lopez, and David Ogden
PRESENTER: Jason Trembly

ABSTRACT

This objective of this project is to validate the technical/commercial promise of an advanced multistage process for treatment and reutilization of impaired water as make-up water in fossil fuel-based power plants (power plants) through small scale testing and prepare the technology for a future pilot scale test effort. Small scale testing efforts include evaluating the performance of a new supercritical water unit design for major constituent removal, electrochemical stripping (E-stripping) to remove minor constituents, and the ability to utilize corrosion resistant coatings to improve stainless steel performance in impaired water with high chloride content. Water desalination tests have demonstrated the ability to recover a reusable water product from brines containing 5-18wt% dissolved solids. Electrochemical stripping tests have proven effective in selective removal of value added components from the remainder of the dissolved matrix. Furthermore, a techno-economic study has shown the process has attractive competitive water treatment costs in comparison to currently commercially available technology.

03-23-2017 – 0930A
NETL-R&IC – DEWATERING OF HIGH SALINITY BRINES
ORGANIZATION: NETL - Research and Innovation Center **PRINCIPAL INVESTIGATOR**: Nicholas Siefert
TEAM MEMBERS: Jason Arena (ORISE), Timothy Bartholomew (ORISE/CMU), Meagan Mauter (ORISE/CMU)
PRESENTER: Jason Arena

ABSTRACT

In reverse osmosis (RO), the maximum concentration of a solution that can be dewatered is about 90 g/L total dissolved solids (TDS). This limitation has impeded the application of RO for dewatering high salinity brine produced at fossil power plants. When only electricity is available, the current standard in high salinity brine concentrating is mechanical vapor compression (MVC). MVC uses an electrically-driven compressor to extract steam from a brine fed to an evaporator. Ultimately, the extracted steam is condensed to pure water via heat exchange with the incoming brine. A drawback to MVC is low efficiency (<10%), meaning 10 times the minimum electrical work to desalinate the brine is needed. NETL researchers in collaboration with Carnegie Mellon University have developed the osmotically assisted reverse osmosis (OARO) in order to significantly increase the efficiency of brine concentration processes. OARO operates by the serial dilution of a saline sweep solution. This sweep solution has a salinity lower than the brine and is diluted from brine being dewatered by reverse osmosis. This presentation will outline the composition of GCS brines, demonstrate experimentally the feasibility of OARO at the bench scale, validate the membrane transport equations of OARO, present initial systems analysis results for kWh/m³ of electricity consumption, and compare both the OARO process and MVC against the minimum electrical work to dewater a high salinity brine.

03-23-2017 – 1030A
FE0026212 – LOW-ENERGY WATER RECOVERY FROM SUBSURFACE BRINES
ORGANIZATION: RTI International **PRINCIPAL INVESTIGATOR**: Young Chul Choi
TEAM MEMBERS: Gyu Dong Kim, Mustapha Soukri, Zachary Hendren, Marty Lail
PRESENTER: Young Chul Choi

ABSTRACT

High total dissolved solids (TDS) containing brine are generated throughout the fossil fuel cycle such as oilfield produced water, flue gas desulfurization blowdown and water generated from CO2 subsurface storage. Because of high TDS (180,000 ppm), membrane processes can't be applied and energy intensive thermal process is the sole solution to remove TDS from these waters.

This project aims to develop and demonstrate bench-scale feasibility of a low-cost, low-energy treatment process using non-aqueous solvent (NAS) extraction to recover water from these high TDS brines. Specific objectives to achieve the project goals are: (i) identification of candidate solvents; (ii) characterization and evaluation of solvent capabilities with respect to water recovery & salt rejection from brine; (iii) establishment and successful demonstration of bench-scale treatment process train for the production of potable water; (iv) optimize the overall process and perform techno-economic assessment for scale up.

Water absorbing-desorbing mechanisms were identified from literature review and preliminary test. Three promising mechanisms were tested using dozens of solvents. Among those mechanism, the low temperature water absorbing & high temperature water desorbing mechanism showed the highest water recovery and decent salt rejection. Using the selected mechanism, solvents were screened and solvents that could recover more than 5% of water from brine with high salt rejection (>94%) were identified. The recovered water could be reused with an appropriate post treatment to remove residual solvent in the water. And a preliminary process flow was also introduced using the identified solvent in order to design a pilot scale system.

03-23-2017 – 1100A

FWP-FE-663-15-FY1 – ADVANCED THERMALLY ROBUST MEMBRANES FOR HIGH SALINITY PRODUCED BRINE TREATMENT

ORGANIZATION: Los Alamos National Laboratory **PRINCIPAL INVESTIGATOR**: Kathryn A. Berchtold
TEAM MEMBERS: NETL-RIC
PRESENTER: Rajinder Singh

ABSTRACT

Managing and deriving value from the large quantities of extracted waters generated by CO_2-storage operations poses major technical, economic, and environmental challenges. Treatment of the extracted water from these sources is a significant challenge owing to high concentration of total dissolved solids (TDS), and presence of hydrocarbons and metals. While reverse osmosis is currently the most energy efficient technology deployed for desalination, it is inherently limited to lower salinity brines such as those encountered in sea water (TDS <40,000 mg/L). Current commercial technologies for treating high-salinity (TDS >30,000 mg/L) brine streams, e.g., evaporative crystallization and mechanical vapor compression, are considered too costly and energy inefficient to warrant their use on large scale. Therefore, novel energy efficient separation methods for treating high salinity produced water are of great interest.

A membrane-based desalination process applicable to these thermo-chemically challenging extracted waters and operating environments would provide an economic alternative to thermal desalination methods. Such a process would provide opportunities for waste heat utilization and increased power generation opportunities while reducing extracted water disposal costs and generating higher quality water for reuse. Polybenzimidazole (PBI)-based membranes have demonstrated thermo-chemical robustness and high water vapor transport characteristics owing to their hydrogen bonding ability, high water uptake, and high water mobility. These characteristics make PBI-materials excellent candidates for extracted water treatment. In this work, PBI membranes are being evaluated in sweep gas membrane distillation and pervaporation modes at elevated temperatures approaching 200 °C to understand their utilization potential for high-salinity brine treatment.

03-23-2017 – 1300A

FE0024074 – FOULING-RESISTANT MEMBRANE FOR TREATING CONCENTRATED BRINES FOR WATER REUSE IN ADVANCED ENERGY SYSTEMS

ORGANIZATION: RTI International **PRINCIPAL INVESTIGATOR**: Zachary Hendren
TEAM MEMBERS: Young Chul Choi, Rachael Gunter, Wenyan Duan, Alexander Dudchenko, David Jassby
PRESENTER: Zachary Hendren

ABSTRACT

The complex range and high concentrations of divalent salts, minerals, and metals that make up the total dissolved solids (TDS) found in brines generated throughout the fossil fuel lifecycle severely limit current treatment and disposal options. The high TDS levels in concentrated brines (often 8 times higher than that of seawater) make the current state-of-the art approaches to water treatment untenable. In this project, we demonstrate the bench-scale feasibility of a novel water treatment process using electrically conductive membrane distillation (ECMD) for the reuse of concentrated brines. This ECMD approach is projected to result in significantly lower costs for the treatment of high-TDS water relative to current approaches. Our approach addresses the two major challenges associated with this water: 1) the membrane distillation process removes the high TDS content and produces high quality effluent suitable for beneficial reuse, and 2) the charged CNT membrane coating prevents the formation of scale that would otherwise pose a significant operational hurdle.

This project's goal is to develop a new class of advanced, electrically conductive membranes that will mitigate the fouling issues that occur during water treatment of high concentration brines; thus paving the way for expanded water reuse and discharge options beyond what is currently feasible. The efficacy of the ECMD approach will be demonstrated on the bench scale by treating both synthetic and actual high TDS wastewaters that have high scaling potential.

03-23-2017 – 1330A

FE0024061 – DEVELOPMENT OF MEMBRANE DISTILLATION TECHNOLOGY UTILIZING WASTE HEAT FOR TREATMENT OF HIGH SALINITY WASTEWATERS

ORGANIZATION: University of Pittsburgh **PRINCIPAL INVESTIGATOR**: Radisav D. Vidic
TEAM MEMBERS: Omkar Lokare, Andrew Beck, Vikas Khanna
PRESENTER: Omkar Lokare

ABSTRACT

The main objective of this study is to evaluate the feasibility of using membrane distillation (MD) technology to treat high salinity wastewaters generated during unconventional gas production or CO_2 sequestration utilizing waste heat that is available in thermoelectric power plants or compressor stations (both natural gas and CO_2 compressors). Laboratory-scale studies with synthetic and actual wastewaters will be used to assess capabilities and limitations of MD technology and define key design and operating parameters for high salinity brines generated by unconventional gas extraction or active CO_2 reservoir management. This information will be utilized for a systems-level analysis and integration of MD process with low-grade heat sources (i.e., thermoelectric power plants and natural gas and CO_2 compressor stations). This study will also conduct a preliminary techno-economic assessment of the proposed integrated system in comparison to competing technologies as well as for the system that uses natural gas as fuel source for MD treatment of high salinity wastewaters in the formations where NG is the main target resource (i.e., Marcellus Shale) and those where it is not (i.e., Baken and Eagle Ford).

03-23-2017 – 1400A

FE0024084 – TREATMENT OF PRODUCED WATER FROM CARBON SEQUESTRATION SITES FOR WATER REUSE, MINERAL RECOVERY AND CARBON UTILIZATION

ORGANIZATION: Southern Research **PRINCIPAL INVESTIGATOR**: Jay E. Renew
TEAM MEMBERS: Kristen Jenkins
PRESENTER: Jay E. Renew

ABSTRACT

With pending regulations to limit carbon dioxide (CO_2) emissions from new and existing fossil energy sources, it is imperative for utilities to make advances in the systems that might be used for storing CO_2. It is anticipated that one issue resulting from the storage of CO_2, will be managing any produced waters from injection activities. The water produced from CO_2sequestration sites presents a significant challenge for reuse since such waters could contain very high total dissolved solids (TDS) concentrations up to 400,000 mg/L. The project will develop a total strategy and design for the management and reuse of produced water from carbon sequestration sites through evaporation. The project will evaluate a strategy for using waste heat from a power plant to drive the evaporation. Some of the project activities include development of process flow diagram for thermal evaporation system to concentrate high TDS produced, development optimized solidification and stabilization recipes targeted at the immobilization of metals, development of by-product reuse strategies, and conduct an economic and technology readiness evaluation of the proposed approach and identify areas of innovation that are needed to further reduce cost and improve process efficiency.

03-23-2017 – 1500A

SC0013863 – INTEGRATED SENSORS FOR WATER QUALITY

ORGANIZATION: Sporian Microsystems, Inc. **PRINCIPAL INVESTIGATOR**: Kevin Harsh
TEAM MEMBERS: Tim Trentler, Michael Cole, Christina Sack

PRESENTER: Laurel Frediani

ABSTRACT

There is a present and growing emphasis on reducing or maintaining the water-use footprint in the energy sector. One of the requirements for effectively managing water is monitoring through reliable, real-time, measurement-based data of water quality/composition within treatment systems and bodies of water associated with power generation facilities. Many existing water quality sensor technologies are large, difficult to install or deploy, and expensive -- all of which inhibits utilities' ability to deploy a network of such sensors. What is needed is the development of an integrated water sensor package that is low-cost, rapidly-deployable, wireless, and self-powered, that can relay real-time relevant in-situ water measurements. Ideally, such hardware would simultaneously monitor multiple water quality factors and contaminants at a reduced overall cost. Sporian is leveraging its mature water quality monitoring sensor and sensor system technology/hardware, including many of the needed water quality sensor types, to extend the sensing capability of these systems to include heavy metal contamination (RCRA 8s) through the use of Imprinted Polymer (IP) -based detection materials/schemes. The developing technology will support reducing or maintaining the water-use footprint in the energy sector, providing low cost to deploy reliable, real-time, measurement-based data for water management. Such a technology will be highly attractive for broad application within energy, industrial, agricultural, mining, and civilian drinking water and wastewater monitoring sectors that require sanitary water for consumption or whose processes affect water and need a sensor to assure proper contamination monitoring and abatement.

03-23-2017 – 1530A
SC0013811 – WIRELESS NETWORKED SENSORS IN WATER FOR HEAVY METAL DETECTION
ORGANIZATION: **PRINCIPAL INVESTIGATOR**: Dr. Hang Ruan
TEAM MEMBERS: Dr. Yuhong Kang, Dr. Richard Claus, Ms. Liz Gladwin, Ms. Michelle Homer
PRESENTER: Dr. Hang Ruan

ABSTRACT

NanoSonic will develop wireless sensors for use in analyzing heavy metal chemistry for power generation facilities and, more broadly, for commercial use. The company will develop wireless networked sensors using conformal nanomembrane-based chemical field effect transistors (ChemFETs) to detect heavy metals in water. NanoSonic will fabricate prototype nanomembrane ChemFET sensor elements, design and synthesize chemical-specific ionophores for selectively detecting targeted heavy metal elements, and demonstrate the performance of prototype sensor devices. NanoSonic will work with a local environmental monitoring company to produce a wireless sensor network for in situ environmental monitoring.

Project success will enable efficient monitoring of heavy metals in water for environmental surveillance, location of pollution sources using analysis from concentration gradients, and detection and mapping of chemical concentrations that are potentially harmful to people and/or destructive to agriculture.

03-23-2017 – 1600A
FE24008 – EVALUATING THE TECHNO-ECONOMIC FEASIBILITY OF FORWARD OSMOSIS PROCESSES UTILIZING LOW GRADE HEAT: APPLICATIONS IN POWER PLANT WATER, WASTEWATER, AND RECLAIMED WATER TREATMENT
ORGANIZATION: Carnegie Mellon University **PRINCIPAL INVESTIGATOR**: Meagan S. Mauter
TEAM MEMBERS: Dave Dzombak, Jeffrey J. Siirola
PRESENTER: Daniel B. Gingerich (Student Presenter)

ABSTRACT

In the future, power generation systems will face an increased need for fuel efficiency and more significant constraints on water consumption and wastewater discharge. A novel technique for water and wastewater treatment, forward osmosis (FO), has the potential to help power plants meet these needs by using heat recovered from flue gas to treat power plant wastewater for internal recycle and compliance with new environmental standards.

This project has four objectives. The first objective is to develop estimates of heat quantity, quality, and availability from US power generators in light of a changing electricity sector and regulatory environment. The second objective is to model cost-effective low-temperature heat recovery systems and integrate these models with FO draw solute recovery models. The third objective is to model FO water treatment processes to be used for treating plant wastewater effluent for compliance with the effluent limitation guidelines and internal recycling. The fourth objective is to demonstrate the technical and economic feasibility and environmental benefits of recovering low-temperature heat for water treatment in NETL coal and natural gas plant models.

03-23-2017 – 1630A

FE0024015 – AN INTEGRATED SUPERCRITICAL SYSTEM FOR EFFICIENT PRODUCED WATER TREATMENT AND POWER GENERATION

ORGANIZATION: University of Illinois **PRINCIPAL INVESTIGATOR**: Seyed Dastgheib

TEAM MEMBERS: Hafiz Salih, Ali Ashraf, Hong Lu, Keong Yong, SungWoo Nam

PRESENTER: Seyed Dastgheib

ABSTRACT

The goal of this project is to evaluate the feasibility of an integrated, supercritical (SC) power/water cogeneration system for treatment of produced waters with total dissolved solids (TDS) concentrations of 30,000-200,000 mg/L (ppm) in a zero-liquid discharge plant. The closed-loop steam cycle of conventional power plants is replaced with an open-loop steam cycle that heats the pretreated produced water above the SC point of water (374 °C and 221 bar) to precipitate the dissolved salts and produce SC steam that is further treated by a SC polishing unit to reduce its salt content from ~100 ppm to low levels suitable for power generation. Project tasks include process simulation and techno-economic evaluation of the integrated system; design, and baseline testing of the SC salt precipitation and steam purification systems; development and characterization of advanced materials for the steam purification system; and treatment of different produced water samples. The research team has demonstrated desalination of produced water samples to ~100 ppm by shock crystallization at SC conditions, and tested carbon membranes that are stable at SC conditions and can further reduce the TDS of the SC steam to sub-ppm levels through multi-cycle treatments. This project may offer a transformative approach to generating power from coal or natural gas and purifying water from high-TDS saline or produced water.

THURSDAY, MARCH 23 TRACK B CROSSCUTTING RESEARCH ABSTRACTS

03-23-2017 – 0830B

FE00025064 – MATERIALS FOR ADVANCED ULTRA-SUPERCRITICAL STEAM TURBINES - ADVANCED ULTRA-SUPERCRITICAL COMPONENT DEMONSTRATION

ORGANIZATION: Energy Industries of Ohio **PRINCIPAL INVESTIGATOR**: Robert Purgert

TEAM MEMBERS: Horst Hack (Electric Power Research Institute), Robert Schrecengost (GE Power), James Claeys (GE Power)

PRESENTER: Horst Hack

ABSTRACT

A "clean coal" technology, which reduces emissions by up to 35%, has been developed by an industrial consortium, led by The Energy Industries of Ohio (EIO). The U.S. Advanced UltraSupercritical (AUSC) program has been funded by the U.S. Department of Energy's National Energy Technology Laboratory (DOE-NETL), the Ohio Development Services Agency, industrial partners, and the Electric Power Research Institute (EPRI). After 15 years of development, this project is addressing the last technical challenges, in order to achieve commercial scale readiness. This U.S. based technology, supporting steam temperatures of up to 760°C, is the most advanced of its kind in the world, while other AUSC technologies being developed in Europe, Japan, India and China, have temperatures limits of no more than 720°C. The goal of the final phase of this project is to prove supply chain capability and operation of key items under AUSC conditions. Project scope will include casting, welding and fabricating components for a superheater, turbine and optional cycling header, to be operated under representative conditions, with steam temperatures up to 760°C.

This final component testing phase, called a "ComTest", will take place over the next 4 years. This is very timely, since many of our U.S. coal-fired power plants are reaching their end-of-life. ComTest will also support U.S. industry by developing the domestic capability to fabricate castings, forgings and extrusions from advanced high-temperature alloys, allowing for export opportunities, given the considerable international interest in AUSC technology.

03-23-2017 – 0900B

FWP FEAA125 – NI-BASED ALLOYS FOR ULTRA SUPER CRITICAL STEAM CYCLE TURBINE MATERIALS

ORGANIZATION: Oak Ridge National Laboratory **PRINCIPAL INVESTIGATOR**: Philip J. Maziasz

TEAM MEMBERS: Amit Shyam, Jeremy Moser, Kinga Unocic, Ying Yang, Xiang Chen

PRESENTER: Philip J. Maziasz

ABSTRACT

This project is about testing and qualifying materials supplied mainly by GE for use in the A-USC steam turbine components for ComTEST. Currently ORNL has been doing HCF testing at 750-800C and testing in a unique rig set up for testing in 100% steam or air. To date for triple-melted and forged 282, there are no effects of steam that can be detected. Long-term creep-rupture testing is ongoing at 1300-1450F, with 11,100h of a planned 25,000h currently achieved. Microstructural analysis of the rotor forging of Haynes 282 shows and extremely fine grain size, with the smallest grains lacking gamma prime precipitation. This causes a 25% reduction in the creep rupture strength. ORNL is also investigating the mechanical properties and microstructure of the largest casting of Haynes 282 alloy (17,000 lb, half valvebody) that has been done to date by GE and MetalTek. Tensile tests as a function of test temperature of the show YS of 87 ksi and 3% total elongation at room temperature, which compare well with wrought Haynes 282 alloy. At a slower cooling rate, strength is similar but ductility is only about 0.5%. Tests are being done now at higher temperatures and microstructure is being characterized. Creep rupture testing at 1300-1450F shows 5200h with no sign of rupture.

03-23-2017 – 0930B
FWP-FEAA117 – TECHNICAL QUALIFICATION OF NEW MATERIALS FOR HIGH EFFICIENCY COAL-FIRED BOILERS
ORGANIZATION: Oak Ridge National Laboratory **PRINCIPAL INVESTIGATOR**: Bruce A. Pint
TEAM MEMBERS: H. Wang
PRESENTER: Bruce A. Pint

ABSTRACT

This project is addressing materials issues relevant to qualifying and deploying a Ni-base alloy for a new application in an advanced ultrasupercritical coal-fired boiler. The goal is the deployment of Haynes International alloy Haynes® 282® for applications in superheaters, reheaters, and steam delivery pipes, by completing base metal, cross-weld and all-weld metal mechanical testing needed for an ASME Boiler and Pressure Vessel Code Case and the associated microstructural analyses needed for assurance of boiler-relevant lifetimes. To date, a total of 66 creep tests have been initiated with over 200,000 h of cumulative testing completed, approximately 40% of the total needed. Tensile testing has been completed on the three base metal heats from 20°-927°C. Cross-weld specimens using two different welding techniques have been received for testing. Stress allowables have been estimated for alloy 282 and show slightly higher values than alloy 740. This project is being performed with 20% cost share from Haynes International.

03-23-2017 – 1100B
FWP-FEAA116 – CORROSION ISSUES IN ADVANCED COAL-FIRED BOILERS
ORGANIZATION: Oak Ridge National Laboratory **PRINCIPAL INVESTIGATOR**: B. A. Pint
TEAM MEMBERS: S. S. Raiman
PRESENTER: B. A. Pint

ABSTRACT

This project is addressing corrosion and environmental effects issues in current and future coal-fired boilers ranging from waterwalls to superheater tubes. In order to be relevant to current materials issues, two tasks focus on (1) stress corrosion cracking (SCC) in waterwall or membrane panel tubes and the alloys and microstructures that may be more resistant to this type of degradation, and (2) the effect of shot peening on steam side oxidation of austenitic superheater tubes. To support advanced combustion concepts, the third topic is studying the effect of pressure on high temperature oxidation. Progress this year included completing SCC experiments in 200°C recirculating water with two different oxygen contents. The shot peening task is nearly complete with specimens exposed for up to 15,000 h in 1 bar 600°, 625° and 650°C steam. Initial work exploring the effect of steam pressure examined specimens exposed at 1-30 bar at 550°C. Future work in the water loop will explore pressure effects to much higher steam pressures with controlled water chemistry. An increase in understanding of these corrosion mechanisms is critical in future efforts to develop more accurate lifetime prediction models for current and future higher-performance coal-fired power systems.

03-23-2017 – 1330B
FWP-FEAA119 – MICROSTRUCTURE AND PROPERTIES OF NI-BASED COMPONENTS FABRICATED BY ADDITIVE MANUFACTURING
ORGANIZATION: Oak Ridge National Laboratory **PRINCIPAL INVESTIGATOR**: Sebastien Dryepondt
TEAM MEMBERS: Mike Kirka, Anand Kulkarni
PRESENTER: Sebastien Dryepondt

ABSTRACT

The goal of this project is to optimize additive manufacturing fabrication processes with an initial focus on gas turbine components made of high temperature NI-based Hastelloy X (HX) alloy. A collaboration between ORNL and Siemens will provide the unique opportunity of comparing results for HX alloy products made by three main AM techniques, electron beam melting (EBM) and selective laser melting (SLM) at ORNL, and laser metal deposition (LMD) at Siemens. Extensive microstructure characterization and mechanical testing has been conducted to determine the relationships among the deposition process, microstructure and mechanical properties. The mechanical properties of actual gas turbine components fabricated by additive manufacturing will be measured, and, as a final step, cost analyses of the three AM processes will be conducted to establish the potential gains of using EBM, LMD, or SLM over conventional fabrication routes. The technology developed in this project is anticipated to be transferable to the production of other similar size components for other advanced fossil energy applications.

03-23-2017 – 1500B
FWP-FEAA123 – ADVANCED MATERIALS ISSUES IN SUPERCRITICAL CARBON DIOXIDE
ORGANIZATION: Oak Ridge National Laboratory **PRINCIPAL INVESTIGATOR**: B. A. Pint
TEAM MEMBERS: J. R. Keiser, R. M. Connatser
PRESENTER: B. A. Pint

ABSTRACT

This project is addressing materials issues associated with scaling up supercritical carbon dioxide (sCO_2) Brayton cycle systems to higher temperatures for increased efficiency and larger size for commercial power production. The effort is intended to understand the applicable corrosion mechanisms in sCO_2 as a function of impurity (e.g. O_2, H_2O) levels in both closed and open systems. In order to study impurities at high pressures (200-300 bar), a new experimental rig is being designed to create controlled O_2 and H_2O impurities and monitor their concentration at high pressure. A laser based detector system has been designed, however, initial measurements found CO_2 becomes opaque in the supercritical state and design changes are in progress. While the new system is being built, initial experiments are comparing behavior in research grade and industrial grade (i.e. higher O_2 and H_2O levels) CO_2 at 1 and 300 bar for up to 5,000 h. Six commercial alloys have been selected for these studies: alloys 617, 230, 740H, 282, 247 and type 310H stainless steel. Model Ni-Cr and Fe-Ni-Cr alloys also are being exposed to assist in alloy design with a goal of lowering the material costs for new utility-size sCO_2 systems. Research sponsored by the U.S. Department of Energy, Office of Fossil Energy, Crosscutting Research Program.

03-23-2017 – 1530B

NETL-R&IC – STATUS OF NETL SUPERALLOY DEVELOPMENT: MELT PROCESSING & HEAT TREATMENT

ORGANIZATION: NETL - Research and Innovation Center **PRINCIPAL INVESTIGATOR**: Paul D. Jablonski
TEAM MEMBERS: Jeffrey A. Hawk
PRESENTER: Paul D. Jablonski

ABSTRACT

A-USC power plants will see steam temperatures approaching 760°C. Conventional 9% Cr martensitic steels will not work in this environment. Thus, Ni-based superalloys are considered both in the wrought and cast forms. Of particular interest is achieving thick-wall γ' strengthened nickel superalloys castings. Full size castings can be quite substantial and achieving uniform properties is critical for their use. NETL with the A-USC consortium addressed this problem by looking at solution and precipitation strengthened wrought variants but casting them into laboratory-scale ingots. Effort was expended to reduce segregation prior to subsequent heat treatments. One particular benefit of this approach was improved creep resistance. The status of NETL's efforts related to superalloy development will be reported on including melt processing and heat treatment.

03-23-2017 – 1600B

NETL-R&IC – ADVANCED ALLOY DEVELOPMENT: HEAT RESISTANT 9% CR STEELS: CREEP ANALYSIS COMPARISONS

ORGANIZATION: NETL - Research and Innovation Center **PRINCIPAL INVESTIGATOR**: Jeffrey A. Hawk
TEAM MEMBERS: Paul D. Jablonski, Omer N. Dogan, Gordon R. Holcomb, Youhai Wen, Michael C. Gao
PRESENTER: Jeffrey A. Hawk

ABSTRACT

Processes, Manufacturing, and Properties (PMP) within Advanced Alloy Development anticipates the need for not only generic but specific new energy efficient and high temperature capable materials for Ultra Super Critical (USC), A-USC and beyond constructions, such as materials for sCO_2 cycles and advanced turbines, etc., by providing material ready solutions (i.e., alloy design and scalable manufacturing methodology) that can be more quickly incorporated into the commercial sector. PMP envisions and develops structural materials that will lower the cost and improve the performance of fossil-based power-generation systems. The main benefits of this research include: (1) developing and manufacturing specific steels (for example, martensitic-ferritic 9% Cr steel like CPJ7 that approach 650°C operation), superalloys like Haynes 282 but with modified chemistry to decrease the gamma prime coarsening rate, and other advanced alloys for FE applications, (2) understanding the nuances of high entropy fundamentals (for example, using high entropy concepts to optimize and stabilize the alloy matrix for strength and oxidation resistance) and applying them to nickel superalloys and other advanced alloys, and (3) developing computational algorithms to accurately predict evolutionary changes within existing and new advanced heat resistant alloys that will more accurately define "end of life." This talk focuses on CPJ7 9% Cr steel in both the wrought and cast conditions.

03-23-2017 – 1630B

NETL – CONCENTRATED SOLID SOLUTION ALLOYS: COMPUTATIONAL MODELING AND EXPERIMENTAL VALIDATION

ORGANIZATION: AECOM **PRINCIPAL INVESTIGATOR**: Michael Gao
TEAM MEMBERS: Paul Jablonski, Jeffrey Hawk
PRESENTER: Michael Gao

ABSTRACT

The goal of the project is to accelerate design and development of high-performance alloys based on the high entropy concept by integrating computational modeling with key experiments. The objective of the modeling is to provide fundamental understanding of solid-solution high-entropy alloy formation and their intrinsic properties using various computational modeling at different length and time scales. The modeling techniques include empirical parameters, CALPHAD modeling, first-principles density functional theory calculations, Monte Carlo simulations, and molecular dynamics simulations. Shed light by the present study, the high-entropy-alloy formation criteria are critically re-evaluated, and new equimolar single-phase HEAs compositions with the FCC, BCC and HCP structures are suggested. The modeling also predicts the entropy sources (e.g., configurational entropy, vibrational entropy, and electronic entropy) and enthalpies as a function of temperature, elastic properties, and yield strength of example alloys. The experimental work include alloy fabrication, thermo-mechanical processing, microstructure characterization, mechanical properties tests, and environmental tests. Development of high-entropy high-performance alloys enables them to be used at higher temperatures with improved life time for wide ranges of applications.

03-23-2017 – 0830C

NETL-R&IC – ANALYSIS, SIMULATION, & EXPERIMENTAL VALIDATION FOR MHD ENERGY CONVERSION

ORGANIZATION: National Energy Technology Laboratory **PRINCIPAL INVESTIGATOR**: Rigel Woodside
TEAM MEMBERS: Clint Bedick, David Huckaby, Danylo Oryshchyn, Eric Zeuthen, Hyoungkeun Kim
PRESENTER: Rigel Woodside

ABSTRACT

Simulation and analysis tools are being developed for the predictive assessment of an MHD generator's thermodynamic and electrical performance under various operating conditions. Calculated results for a seeded oxy-fuel combustion product's electrical conductivity are presented. In order to validate the electrical conductivity predictions as a function of oxidant enrichment and potassium carbonate seeding concentration, a lab-scale oxy-methane burner and double Langmuir probes is being utilized. The latest results from this test campaign are presented and discussed. Additionally, CFD simulations are utilized to investigate the heat transfer from a high temperature supersonic flow to a cooled wall. For model validation, a high velocity kerosene-oxygen combustor capable of producing supersonic velocities is being utilized. In the experiment, overall wall heat losses are determined using a calorimetric method and the results are reported as a function of the input mass flow and combustion stoichiometry. Broad band radiometry and narrow band radiometric imaging are also utilized to quantify the radiance and flow patterns as the supersonic flow exits the system, leading to an over-expanded free jet. A planned experimental effort with a "back-powered" MHD channel section attached to this high velocity combustion system is also presented. This experiment aims to validate predictions of the effective conductivity in a channel, accounting for boundary layer voltage drops. Finally, the latest results from experimental and modeling efforts on the use of photoionization to enhance a plasma's electrical conductivity are presented.

03-23-2017 – 0900C

NETL-R&IC – EFFECT OF POTASSIUM CARBONATE ON ELECTRODE MATERIALS FOR ADVANCED COMBUSTION MHD GENERATORS

ORGANIZATION: National Energy Technology Laboratory **PRINCIPAL INVESTIGATOR**: Peter Hsieh, Rigel Woodside
TEAM MEMBERS: Eric Zeuthen, Hyoungkeun Kim, Kyei-Sing Kwong, Michael Johnson, David Cann
PRESENTER: Peter Hsieh

ABSTRACT

Electrode are exposed to extreme conditions in magnetohydrodynamic (MHD) generators. Testing of potential electrode materials under MHD-relevant conditions, specifically exposure to potassium carbonate at high temperatures, provides important data needed to design, build, and operate a MHD channel for direct power extraction in support of advanced oxy-fuel combustion.

We measured the mass loss of tungsten, 90% W-10% Cu, and 70% W-30% Cu samples exposed to a high-velocity oxy-kerosene flame, with and without potassium carbonate seeding. Oxidative evaporation was found to be the principal tungsten mass loss mechanism. Tungsten oxides, potassium tungstates, and other reaction products formed at the sample surface were further characterized through powder x-ray diffraction, energy-dispersive x-ray spectroscopy, and scanning electron microscopy.
A dense rare-earth oxide ceramic sample was fabricated via uniaxial pressing and sintering. Resistance to attack by molten potassium carbonate will be evaluated using a modified vapor attack test (ASTM C987) for the oxide ceramic sample and tungsten.

Measurement of electrode mass loss rates and resistance to corrosive attack as a function of electrode material and operating conditions offer valuable insights into the design and operation of MHD channels for electrical power generation. Lessons learned may also be applicable to the development of high-temperature electrode materials that are resistant to oxidation or attack by potassium compounds in their molten or vapor states.

03-23-2017 – 0930C

FE0026333 – COMBUSTION SYNTHESIS OF BORIDE-BASED ELECTRODE MATERIALS FOR MAGNETOHYDRODYNAMIC (MHD) DIRECT POWER EXTRACTION

ORGANIZATION: University of Texas at El Paso **PRINCIPAL INVESTIGATOR**: Evgeny Shafirovich
TEAM MEMBERS: Chintalapalle V. Ramana, Sergio Cordova, Leonardo Gutierrez-Sierra
PRESENTER: Sergio Cordova (Student Researcher)

ABSTRACT

NETL is partnering with the University of Texas at El Paso to develop a novel technology for advanced, low-cost manufacturing of boride-based ultra-high-temperature ceramics for direct power extraction applications. The project will determine optimal conditions of mechanical activation, self-propagating high-temperature synthesis (SHS), and pressureless sintering for fabricating doped zirconium diboride (ZrB_2) and hafnium diboride (HfB_2) that possess all the required properties needed to function as sustainable magnetohydrodynamic electrodes. The project will also determine thermophysical, electrical, mechanical, and oxidation properties of borides obtained by mechanically activated SHS followed by pressureless sintering. This effort will focus on the use of inexpensive materials such as zirconium dioxide (ZrO_2), hafnium oxide (HfO_2), boron trioxide (B_2O_3), magnesium (Mg), and sodium chloride (NaCl), which could lead to significantly lower production costs compared to synthesis from elements.

The technology developed in this project will solve certain problems associated with SHS, such as difficult ignition of low-exothermic mixtures and high porosity of products, while exploiting SHS advantages such as low cost, low energy consumption, and high product purity.

03-23-2017 – 1030C

FE0024062 – HIGH TEMPERATURE HIGH VELOCITY DIRECT POWER EXTRACTION USING AN OPEN CYCLE OXY COMBUSTION SYSTEM

ORGANIZATION: University of Texas El Paso **PRINCIPAL INVESTIGATOR**: Norman Love
TEAM MEMBERS: Ahsan Choudhuri
PRESENTER: Norman Love

ABSTRACT

NETL is partnering with the University of Texas at El Paso to develop high-temperature, high-velocity direct power extraction using an open-cycle oxy-combustion system. Researchers have designed and tested a lab-scale high-velocity and high-temperature oxy-fuel combustor, nozzle and injector. The 60-kW unit was tested for durations of up to five minutes, replicating steady-state operation. This combustor has been designed and built to accommodate high-velocity oxy-fuel flow reaching temperatures that exceed 3000 K.

The project will demonstrate the feasibility of MHD oxy-combustion system components for use in electrical power generation, and support the development of energy-efficient technologies that can be used in conjunction with carbon capture techniques. In addition, the outcome of the project will not only improve fundamental understanding of oxy-fuel combustion and flame stability, but also provide critical experimental data for validating modeling tools. For example, a numerical model has been developed to characterize heat transfer properties of the system and was validated with experimental results. Currently a 1-MW version of the initial unit has been designed using these data.

03-23-2017 – 1100C

FE0026325 – NOVEL HIGH TEMPERATURE CARBIDE AND BORIDE CERAMICS FOR DIRECT POWER EXTRACTION ELECTRODE APPLICATIONS

ORGANIZATION: Florida International University **PRINCIPAL INVESTIGATOR**: Zhe Cheng
TEAM MEMBERS: Arvind Agarwal, Andrés Behrens, Archana Loganathan
PRESENTER: Andrés Behrens (Student Presenter)

ABSTRACT

Direct power extraction (DPE) via magnetic hydrodynamic (MHD) power generation is an attractive technique for generating power from fossil fuels and nuclear energy due to its conceptual simplicity and high theoretical efficiency comparable to or even higher than the state-of-the-art combined-cycle power generation. However, the adoption for MHD technology has been limited so far, partly due to the challenge with electrode and wall materials used for MHD. The goal of this project will be to carry out basic research on high temperature ceramic materials so that the new fundamental knowledge obtained may be leveraged into DPE applications for cleaner and more efficient power generation. The overall objective of the proposed research is to develop nano carbide and boride ceramic solid solution and related composites materials via novel solution-based synthesis and related rapid densification processing technique and understand the fundamental composition-processing-structure-property relationships for such materials as potential hot electrodes for DPE systems. The proposed research will bring significant impacts not only to the development of high temperature MHD electrodes but also the general fields of advanced ceramics and high temperature materials science. It will also train minority graduate students and provide access to research for undergraduates here at FIU.

03-23-2017 – 1300C
FE0023142 – PRECURSOR-DERIVED NANOSTRUCTURED SIC-BASED MATERIALS FOR MHD ELECTRODE APPLICATIONS
ORGANIZATION: University of Washington **PRINCIPAL INVESTIGATOR**: Fumio S. Ohuchi
TEAM MEMBERS: Raj. Bordia (Co-PI, Clemson University) and YiHsun Yang (UW Graduate Student), Keelan Christensen (UW Graduate Student)
PRESENTER: Fumio S. Ohuchi

ABSTRACT

NETL is partnering with University of Washington (UW) to develop a novel class of SiC-based ceramic composite materials through a polymer-precursor-derived route with tailored compositions for channel applications in magnetohydrodynamic (MHD) generators. University of Washington will investigate the effect of precursor chemistry (specifically C/Si) and processing conditions (e.g., temperature) on the nanodomain structure, resultant stoichiometry, nature of the carbon phase (e.g., graphene sheets, carbon nanoparticles), and the resulting thermo-mechanical properties at elevated temperatures. A minor constituent X in Si-C-X is incorporated at the precursor stage during material synthesis, and its effect on the electrical properties, including electrical conductivity, thermionic emissions and arcing property for use in MHD generators, is investigated. Important parameters to be investigated are the domain size, the type and distribution of carbon, and the sizes and volume fractions of crystalline SiC and the constituent X. By developing SiC-based materials with nanostructured features and tailoring their compositions, the high-temperature resistance, electrical properties, and plasma resistance of SiC will improve relative to that for SiC produced by conventional powder processing approaches, such as solid state sintering. A successful outcome of this research will result in the emergence of reliable and affordable designed materials for MHD applications. The UW will also investigate the interaction of these materials with plasma as a first step toward understanding the plasma-induced degradation process using a newly developed High Density Plasma- Materials Testing Facility.

03-23-2017 – 1330C
FE0022988 – DISTRIBUTED FIBER SENSING SYSTEMS FOR 3D COMBUSTION TEMPERATURE FIELD MONITORING IN COAL-FIRED BOILERS USING OPTICALLY GENERATED ACOUSTIC WAVES
ORGANIZATION: University of Idaho **PRINCIPAL INVESTIGATOR**: Indrajit Charit
TEAM MEMBERS: Krishnan S. Raja, Steven Sitler, James Zillinger
PRESENTER: Indrajit Charit

ABSTRACT

Researchers from University of Massachusetts Lowell, University of Connecticut and General Electric, will attempt to monitor and optimize real-time spatial and temporal distributions of high-temperature profiles in a fossil fuel power plant boiler system. Distributed optical fiber sensing has the potential to measure high temperatures while the optically generated acoustic signals can measure regions where the fibers cannot survive (e.g., 2000°C). The reconstructed 3-D temperature profile will provide critical input for the control mechanisms to optimize the combustion process, thus achieving higher efficiency and fewer pollutant emissions. To accomplish this, project personnel will first develop a methodology to (1) establish a boiler furnace temperature distribution model and guide the design of the sensing system; (2) develop the sensors with one active sensing element on each fiber as well as a temperature distribution reconstruction algorithm for proof-of-concept; and (3) develop the distributed sensing system to integrate multiple active sensing elements. The entire sensing system, when fully integrated and tested in the university labs, will be tested in GE's test facility. This novel distributed sensor can have broader applications including measurement of strain, flow, velocity, crack growth, and corrosion for monitoring structural health.

03-23-2017 – 1500C
FE0011453 – MODIFIED KINETIC THEORY APPLIED TO THE SHEAR FLOWS OF GRANULAR MATERIALS
ORGANIZATION: University of Texas at San Antonio **PRINCIPAL INVESTIGATOR**: Zhi-Gang Feng
TEAM MEMBERS: Yifei Duan
PRESENTER: Yifei Duan (Student Researcher)

ABSTRACT

To improve the kinetic theory results for granular flows in the dense flow regime, we propose a Modified Kinetic Theory (MKT) model that utilizes the contact duration or cut-off time to account for the complex particle-particle interactions in the dense regime. The contact duration model, also called TC model, is originally proposed by Luding and McNamara1 to solve the inelastic collapse issue existing in the Inelastic Hard Sphere (IHS) model. This model defines a cut-off time tc such that dissipation is not counted if the time between two consecutive contacts is less than tc. We relate the TC model with the Discrete Element Method (DEM) by choosing the cutoff time tc to be the duration of contact calculated from the linear-spring-dashpot soft-sphere model of the DEM. We examine two types of granular flows, the simple shear and the plane shear flows, and compare the results of the classical Kinetic Theory (KT) model, the present MKT model, and the DEM model. We show that the MKT model entails a significant improvement over the kinetic theory model for simple shear flows at inertial regimes. Even for the plane shear flows, where shear rate and solid fraction are inhomogeneous, the results of the MKT model agree very well with the DEM results.

03-23-2017 – 1530C
FE0026191 – INTERFACING MFIX WITH PETSC AND HYPRE LINEAR SOLVER LIBRARIES
ORGANIZATION: University of North Dakota **PRINCIPAL INVESTIGATOR**: Gautham Krishnamoorthy
TEAM MEMBERS: Jeremy Thornock (U. Utah), Lauren Clarke (UND)
PRESENTER: Gautham Krishnamoorthy

ABSTRACT

High computational cost associated with the solution of large, sparse, poorly conditioned matrices is a serious impediment to increasing the utility of computational fluid dynamics models for resolving multiphase flows. This project will interface NETL's Multiphase Flow with Interphase Exchanges (MFiX) code with Portable Extensible Toolkit for Scientific Computation (PETSc) and High Performance Preconditioners (HYPRE) linear solver libraries with the goal of reducing the time to solution for the large, sparse, and often ill-conditioned matrix equations resulting during the solution process. The lack of robust convergence associated with the current iterative methods in MFiX can be alleviated through appropriate preconditioning techniques to Krylov subspace solvers and multigrid methods accessible from these libraries.

The overall objective of this project is to establish a robust well-abstracted solver interface that will enable MFiX to successfully interface with various solver libraries. Next, this extensibility will be demonstrated by interfacing MFiX with PETSc and HYPRE linear solver libraries with the goal of reducing the time to solution for large, sparse, linearized matrix equations resulting from the discretization of multiphase transport equations.

This project could reduce the time to solution by at least 50 percent when compared to current linear solver options in MFiX. It also could show that near linear scaling in parallel performance can be achieved to at least 1000 processors, which could translate to achieving good scalability on current high-performance computing systems such as the DOE leadership computing facilities as well as enabling the portability of MFiX with new hardware technologies.

03-23-2017 – 1600C

FE0026298 – MFIX DEM ENHANCEMENT FOR INDUSTRY-RELEVANT FLOWS

ORGANIZATION: University of Colorado **PRINCIPAL INVESTIGATOR**: Christine M. Hrenya

TEAM MEMBERS: Thomas Hauser, Dane Skow, Aaron Holt, Ray Grout, Deepthi Vaidhynathan, Hariswaran Sitaraman, Peiyuan Liu, William Fullmer, Ray Cocco, Allan Issangya

PRESENTER: William D. Fullmer

ABSTRACT

CFD-DEM is a powerful tool that can provide unparalleled insights into the behavior of gas-solid particulate systems. Unfortunately, CFD-DEM is not yet in widespread use among industrial scientists – the largest barrier being the disparity in size (e.g., number of particles) between most full-scale industrial systems and the current computational capabilities. To help bridge this gap, this project has (i) surveyed industrial CFD users with an emphasis on current areas of need; (ii) developed a suite of scalable benchmark problem to assess MFiX's scalability; (iii) performed serial and parallel profiling of the original 2015-1 version to highlight high impact areas of the code; (iv) introduced algorithmic changes and optimizations to improve code performance; (v) extensively reviewed the OpenMPI implementation with an eye to exploiting hybrid architectures of the latest hardware; (vi) performed an experimental investigation of opposing, horizontal air jets with an emphasis on propagating known errors and directly quantifying particle properties via empirical probability density functions to provide accurate uncertainty inputs to CFD-DEM simulations; and (vii) CFD-DEM validation studies of a horizontal jet system using the calculated and measured uncertainties to compile an exhaustive parameter identification and ranking table. This talk will focus primarily on the experimental investigation and subsequently CFD-DEM modeling of the opposing, horizontal air jets penetrating into a semi-circular fluidized bed of Geldard Group D particles.

TUESDAY, MARCH 21   JOINT POSTER SESSION

CROSSCUTTING RESEARCH PROJECT POSTERS

Poster 01
FE0027891 – INVESTIGATION OF HIGH TEMPERATURE SILICA BASED FIBER OPTIC MATERIALS
ORGANIZATION: Virginia Polytechnic Institute and State University
PRINCIPAL INVESTIGATOR: Gary Pickrell
TEAM MEMBERS: Dan Homa, Anbo Wang
PRESENTER: Dan Homa

ABSTRACT

In this program, the Center of Photonics Technology at Virginia Tech will lead the investigation into the high temperature stability of state of the art fused silica optical fibers. The most robust commercial optical fibers will be exposed to chemical constituents, such as H_2, O_2, H_2O, CO, and CO_2, to thoroughly assess the optical and mechanical stability at elevated temperatures approaching 1000°C. The impact of devitrification phenomena, dopant diffusion, glass chemistry and environmental susceptibility on the performance will be investigated for traditional fused silica based optical fibers. Furthermore, optical fibers will be drawn with novel cladding materials and under variable process conditions to provide the basis for the design and fabrication of the next generation of thermally tolerant optical fibers. This project will provide the roadmap and design approach for optical fiber sensor materials that will break through the performance barriers that limit the deployment of optical fiber sensors in harsh environments. The expanded portfolio and enhanced understanding of high temperature optical fiber materials will awaken the use of dormant and underutilized fiber optic sensing technologies that will enable more efficient, reliable, and safe operation of next generation energy conversion systems.

Poster 02
FE0027840 – RAMAN SPECTROSCOPY FOR THE ON-LINE ANALYSIS OF OXIDATION STATES OF OXYGEN CARRIER PARTICLES
ORGANIZATION: Washington State University
PRINCIPAL INVESTIGATOR: Hergen Eilers
TEAM MEMBERS: John Kirtley (Postdoc. Associate), Victoria Leichner (Student Researcher)
PRESENTER: Hergen Eilers

ABSTRACT

The need for cleaner energy systems, including CO2 capture technologies, is driving the current development of chemical looping technologies such as chemical looping combustion (CLC) and chemical looping gasification (CLG). Specific processes that are under development for using solid fuels are in-situ Gasification Chemical-Looping Combustion and Chemical Looping with Oxygen Uncoupling. Chemical looping is based on using oxygen carriers to provide the oxygen for the reaction with the fuel. In order to optimize the overall process performance, it is critical that the properties of the oxygen carriers are well-defined and maintained for their specific purpose during the different stages of the CLC process. One of the critical properties of the oxygen carrier is its oxidation state (e.g., content of Fe_2O_3 vs. Fe_3O_4) as it affects the fundamental operation of the CLC process. Unfortunately, the ability to make on-line measurements of the oxidation state of oxygen carriers is lacking and new sensors need to be developed. Our goal is to develop a non-contact, stand-off, time-gated Raman spectroscopy based sensor for the on-line analysis of the oxidation state of oxygen carrier particles and to demonstrate its feasibility. Oxygen carrier particles (OCPs) of interest include iron oxides, copper oxides, calcium sulfite, and calcium sulfate, with particle sizes typically less than 0.5 mm diameter. The expected operating conditions of the sensor include temperatures between 800 °C and 1000 °C, and pressures of about 10 atm. The expected results are to be of a statistical nature, providing relative concentrations of the different oxidation states.

Poster 03

FE00028992 – ENGINEERING METAL OXIDE NANOMATERIALS FOR FIBER OPTICAL SENSOR PLATFORMS

ORGANIZATION: University of Pittsburgh **PRINCIPAL INVESTIGATOR**: Kevin P. Chen
TEAM MEMBERS: Corning Inc.
PRESENTER: Kevin P. Chen

ABSTRACT

Objectives and goals of this project are to engineer metal oxide nanomaterials as optical sensing materials for fiber optic chemical measurements in high temperatures (400-900°C) harsh environments for fossil fuel energy applications using both silica and sapphire fibers as sensing platforms.
To engineer metal oxide nanomaterials, a scalable nanofabrication scheme will be developed to engineer refractive indices, surface areas, and chemical specificities of a wide range of transition metal oxides and their dopant variants for fiber optical chemical sensing in high temperatures (400-900°C). Functional metal oxide sensory materials with proper refractive indices and chemical sensitivities will be integrated on both silica fiber and sapphire fiber platforms. Using distributed fiber sensing schemes such as Rayleigh backscattering Optical Frequency Domain Reflectometry (R-OFDR), or fiber Bragg grating arrays, we will develop a unique distributed fiber optical chemical sensing technique to probe energy chemistry at high temperatures with high spatial resolution of 1-cm or better. Using the same distributed fiber sensing scheme, various metal oxides will be integrated on-fiber for real-time multi-species gas measurements in high temperatures (400-900°C) environments.
The success of this project will lead a new chemical sensing technology that can perform real-time multi-species gas sensing with unprecedented spatial resolutions at high temperatures beyond current operational temperature limits of electronic chemical sensors at ~400°C. This sensor technology will enable scientists and engineers to understand and to design optimal energy chemistry occurred in a wide range of fossil fuel reactors to improve their energy efficient and to reduce their environmental impacts.

Poster 04

FE0027581 – A GUIDELINE FOR THE ASSESSMENT OF UNIAXIAL CREEP AND CREEP-FATIGUE DATA AND MODELS

ORGANIZATION: University of Texas at El Paso **PRINCIPAL INVESTIGATOR**: Calvin M. Stewart
TEAM MEMBERS: Jack F. Chessa
PRESENTER: Mohammad Shafinul Haque (Student Researcher)

ABSTRACT

Recent drives to increase the efficiency of existing fossil energy (FE) power plants and the development of Advanced Ultrasupercritical (A-USC) power plants, have led to designs with steam pressures above 4000 psi and temperatures exceeding 1400°F. The complexity of the applied thermo-mechano chemical boundary conditions makes it critically important to consider creep and creep related failures. One primary concern to FE practitioners is a determination of which constitutive models are the “best”, capable of reproducing the mechanisms expected in an intended design accurately; as well as what experimental datasets are proper or “best” to use for fitting the constitutive parameters needed for the model(s) of interest. In this poster the work completed during the 1st quarter towards these questions are presented. Creep-rupture data for P91 and 316 SS are collected and statistical analysis in terms of Z-parameter are performed. Twelve time-temperature rupture models are collected and analyzed in the form of time-temperature parameterization, iso-stress lines, points of convergence, and master curves. A taxonomy classification for creep models is developed. Similarities between models are exploited to develop four new models by modifying the existing models. Experimental data for alloy P91 at four isotherms are used to determine material constants. In the process of finding material constants, a general model (metamodel) is derived where the submodels (existing and new models that are exploited to develop the metamodel) are special case such that instantaneous and efficient evaluation of the submodels can be performed simultaneously.

Poster 05

NETL – ENABLING TECHNOLOGIES FOR SURFACE ACOUSTIC WAVE (SAW) SENSORS IN HARSH ENVIRONMENTS

ORGANIZATION: NETL – R&IC **PRINCIPAL INVESTIGATOR**: Paul R. Ohodnicki

TEAM MEMBERS: Robert T. Fryer

PRESENTER: Robert T. Fryer

ABSTRACT

Zirconia-doped ceria (ZrO_2-doped CeO_2) (ZDC) thin films are being developed at NETL as a stable gas sensing layer for surface acoustic wave (SAW) sensor devices to alleviate shortcomings with state-of-the-art gas sensing layers like ZnO and SnO_2 films. SAW sensors are a leading choice for many harsh-environment applications as they're easily configured wirelessly and are well-suited for longstanding operation beyond 1000°C. Challenges remain, however, in film-substrate adhesion and interdiffusion, and in sensing response time, sensitivity, selectivity, and general effectiveness over wide-ranging temperatures. ZDC shows promise as a superior gas sensor layer given its exceptional ionic conductivity and thermodynamic stability in severely sub-stoichiometric compositions. Furthermore, ZDC films exhibit strong dependence of film resistivity on partial pressures — a relationship that enables the gas sensing function of SAW sensor devices; however, unlike other oxygen-ion conductors (e.g., ZnO, SnO_2, or undoped CeO_2), ZDC film resistivity exhibits near-temperature-independence, usefully enabling ZDC films for selective sensing of gas species with minimal cross-response from changes in temperature. To optimize ZDC film structure for stable sensor response during operation, several film properties (compositional, structural, morphological, electrical, optical) are being characterized as a function of processing, from ambient conditions up to 800°C/1000 psi, in an array of gases relevant for fuel gas streams (H_2, O_2, N_2, CO, CO_2, CH_4); specific focus surrounds the mechanism and effectiveness of sensor response, as well as their stabilities. Development of these stable films and associated sensors will improve sustainability by increasing efficiencies and high-temperature machinery lifetimes, reducing energy consumptions and greenhouse gas emissions, and more.

Poster 06

NETL-R&IC – DEVELOPMENT OF CONTROL STRATEGIES FOR THE DYNAMIC OPERATION OF A 10MWE SUPERCRITICAL CO2 RECOMPRESSION BRAYTON CYCLE

ORGANIZATION: National Energy Technology Laboratory **PRINCIPAL INVESTIGATOR**: Eric Liese

TEAM MEMBERS: Steve Zitney, Jacob Albright (ORISE)

PRESENTER: Eric Liese

ABSTRACT

The project involves development of control strategies for the dynamic operation of a 10MWe supercritical CO_2 recompression Brayton cycle (relevant to STEP program efforts). This objective is development of basic proportional-integral-derivative (PID)-based control, advanced regulatory control (ARC), and advanced process control (APC) strategies for a pressure-driven dynamic model of the system (using Aspen Dynamics). Specific cycle controls may include but are not limited to inventory control, flow split control, temperature control, bypass control, speed control, compressor surge control, and turbine control. Operational scenarios may include but are not limited to heat input turndown and ramp up, heat rejection disturbances, load-following operation, startup and shutdown. The work will support the identification of improved/optimized designs and operational strategies; for example, performance under part-load operation versus only at the nameplate rating. As part of this effort, the development and refinement of an Aspen Custom Modeler (ACM) multi-stage compressor model will continue, with emphasis placed upon accurate results near the critical point. Results are presented for the current Aspen Dynamics model looking at control options for maintaining system efficiency at reduced heat input conditions. Results are also presented for the custom multi-stage compressor model with operations near the critical point.

Poster 07

NETL-R&IC – ADVANCED SENSORS AND CONTROLS FWP, DIAGNOSTICS AND SENSOR APPLICATIONS IN R&IC RESEARCH

ORGANIZATION: NETL - Research and Innovation Center **PRINCIPAL INVESTIGATOR**: Ben Chorpening

TEAM MEMBERS: Juddha Thapa, Amy Falcon, Jared Charley, Michael Buric, Doug Straub

PRESENTER: Ben Chorpening

ABSTRACT

The overall goal of this research effort is to develop novel sensors and instrumentation technology, or significantly improve upon existing technology, to support improvements to the operation of power generation systems, both existing and in development by DOE. Benefits of this effort include application of advanced sensors and diagnostics to R&IC research on advanced power systems, providing measurements that are unavailable through conventional instruments, to aid research progress; and cost efficient advancement of the Technology Readiness Level of sensors being developed with FE support, through piggyback testing in NETL facilities.

Poster 08

NETL-R&IC – NETL INSIGHTS INTO HYBRID POWER SYSTEMS: OPPORTUNITIES AND OVERCOMING CHALLENGES

ORGANIZATION: NETL - Research and Innovation Center **PRINCIPAL INVESTIGATOR**: Lawrence Shadle

TEAM MEMBERS: Dave Tucker, Valentina Zaccaria, Nor Farida Harun, Dan Oryschyn, Lawrence Shadle, Mike Shelton, Ron Breault, Ben Chorpening

PRESENTER: Lawrence Shadle

ABSTRACT

The overall goal of this research effort is to develop necessary sensors and control technologies that significantly improve the potential for early deployment of the highly efficient power cycles. Fuel Cell-Turbine hybrids are arguably the most efficient power cycle conceived. Unfortunately, fuel cells were too expensive and too fragile to incorporate into this type of close coupled hybrid cycle until process controls were developed. The Hyper project was developed to overcome these challenges. The Hyper project is the world's only recuperated turbine coupled to a cyber physical solid oxide fuel cell capable of duplicating process dynamics and instabilities. This makes it ideal to evaluate the potential for sensors and advanced technologies to control the hybrid process. Research opportunities abound because of the cycle's high efficiency, operating flexibility, and low emissions. The challenges for the technology are in system integration and dynamic controls, including identifying potential design and sensors to accurately measure the onset of instabilities and poor performance. Several of these challenges have been recently addressed. This includes systems analysis that identify the optimum operating range and design constraints are having a 50:50 power split between fuel cell and turbine generators to maintain low capital investment, high process efficiency, and low operating and maintenance costs. The potential of employing the fuel cell as a thermal energy storage was identified during a test to evaluate fuel flexibility. This concept was evaluated. As much as 2.1 GJ of heat were found to be stored within a typical 300kW SOFC and simply changing the fuel composition can release significant quantities of heat within an 80 ms. In addition, the potential to utilize the hybrid system to extend the life of the SOFC was further evaluated. An analysis of the uncertainty in each of the factors in the SOFC degradation models was used to quantify the probabilities that the life of the SOFC was extended by an order of magnitude in the hybrid configuration over a standalone power system. Control schemes to evaluate this effect were demonstrated in the Hyper system.

Poster 09
NETL-R&IC – R&IC-SEA WATER MANAGEMENT RESEARCH
ORGANIZATION: NETL - Research and Innovation Center **PRINCIPAL INVESTIGATOR**: Erik Shuster
TEAM MEMBERS: Eric Grol
PRESENTER: Erik Shuster

ABSTRACT
The U.S. Department of Energy (DOE) National Energy Technology Laboratory's (NETL) Systems Engineering & Analysis Directorate (SEA) develops and analyzes advanced energy technologies and systems at scales ranging from process to national infrastructure in support of the DOE's mission and goals. SEA conducts a variety of efforts on behalf of the Office of Fossil Energy's Crosscutting Technology Research Program and is conducted research in the area of water management.

Water is essential for energy extraction and thermoelectric electricity generation and energy is essential for extracting, transporting, and treating water. This inextricable link between water and energy is known as the water/energy nexus. Current water management research being conducted by SEA includes the development of a national energy/water model for electricity generation that will be linked to EIA's NEMS, detailed systems level analyses used to develop metrics for desalination of extracted brines from carbon storage reservoirs to manage plume and pressure or produced water from oil/natural gas production, a scoping study on the use and/or reduction of nontraditional streams from coal-fired power plants, and a case study on power plant water use practices and data to identify future operational issues related to plant water use.

The objective is to gain a better understanding of the dynamics that make up this water/energy nexus. The outcome from these studies will provide knowledge of future water available, water quality, reductions in fresh water use and use of alternative water sources which is important for a sustainable future.

Poster 10
FE0027778 – CONTINUOUS WATER QUALITY SENSING FOR FLUE GAS DESULFURIZATION WASTEWATER
ORGANIZATION: University of Alabama at Birmingham **PRINCIPAL INVESTIGATOR**: Lee Moradi
TEAM MEMBERS: UAB EITD, Southern Research, Metrohm
PRESENTER: Samuel Misko (Student Researcher)

ABSTRACT

The University of Alabama at Birmingham (UAB) is developing an integrated on-line water sensor package for continuous water quality monitoring of flue gas desulfurization (FGD) wastewaters to include concentration measurements of multiple contaminants (i.e., trace metals: Se, As, Hg) and measurement of common water quality indicators (i.e., pH, temp, TDS, etc.).

The proof-of-concept prototype will successfully demonstrate the key features of the technology through in-field automated operation for extended periods (i.e., 1wks); accurate trace metal detection (i.e., Se, As, Hg) using a proprietary FGD sample preparation technique, low cost, small footprint detection with COTS (commercial off the shelf) voltammetry device, parts per trillion (ppt) limit of detection/qualification; continuous monitoring with high sampling frequency (i.e., more than one measurement per hour for trace metals); integration of COTS water quality indicators (i.e., pH, temp, TDS); and wireless transmission of measurements to on-site control room. All measurements will be validated for accuracy and reliability through comparison with the gold-standard analysis method provided by on-site ICP-MS total metals analysis.

This technology represents a robust sample preparation process to facilitate process monitoring of trace metal concentrations in FGD wastewater influent and post-phys/chem treatment effluent discharge for coal fired power plants; thereby reducing recurring operating and off-site laboratory analysis costs and providing a high level of confidence of compliance with limits set in the EPA ELG.

Poster 11
FE0027893 – DEVELOPING COST EFFECTIVE BIOLOGICAL REMOVAL TECHNOLOGY FOR SELENIUM AND NITRATE FROM FLUE GAS DESULFURIZATION (FGD) WASTEWATER FROM AN EXISTING POWER GENERATING FACILITY
ORGANIZATION: West Virginia State University **PRINCIPAL INVESTIGATOR**: Dr. Sanjaya
TEAM MEMBERS: Bagyalakshmi Muthan and Matthew Blackborn
PRESENTER:

ABSTRACT

The overall goal of our project is to investigate and determine a technically feasible and cost effective process for designing photosynthetic organisms capable of sequestering selenium (Se} and nitrates from flue gas desulfurization (FGD} wastewater. To that end, we will explore a variety of genomics, biochemical, genetic, and molecular approaches to understanding the molecular basis of Se and nitrate sensing, uptake, and sequestration by algae and plants. Purified FGD wastewater using this biological technique can be reused in power plants, contributing to freshwater conservation. To realize this goal, we have chosen to focus on the following 3 objectives: (1} investigate changes in transcripts and metabolism in algae and plants in response to FGD wastewater; (2} explore biotechnological strategies to increase sequestration of Se and nitrates in biomass to improve agricultural productivity; and (3} enhance student hands-on experience and participation in STEM research and education.

Poster 12
FE0027800 – THE FUNDAMENTAL CREEP BEHAVIOR MODEL OF GR.91 ALLOY BY INTEGRATED COMPUTATIONAL MATERIALS ENGINEERING (ICME) APPROACH
ORGANIZATION: Florida International University **PRINCIPAL INVESTIGATOR**: Yu Zhong
TEAM MEMBERS: Andrew Smith, Wei Zhang
PRESENTER: Yu Zhong

ABSTRACT

In the current project, we will mainly investigate the Gr.91 base alloy and weldment with the Integrated Computational Materials Engineering (ICME) approach. We will investigate the fundamental creep cracking mechanism of Gr.91 during the operation condition in the advanced technologies Fossil Fuel (FE) power plants and build the link among ***Composition – Processing Parameters – Phase Stability – Microstructure – Creep Resistance***. **The specific project objectives are as follows:** ***1.)*** Predict the phase stability and microstructure of Gr.91 base alloy and weldment with the computational thermodynamics and kinetics (CALPHAD) approach; ***2.)*** Carry out welding, heat treatment, and creep test for the Gr.91 alloy; ***3.)*** Develop a model which has excellent match with the experimental data from the current work and also from the previous existing work; ***4.)*** Predict how to improve the long-term creep resistance for the Gr.91 family alloys. At the end of the project, a model based on computational thermodynamics and kinetics will be developed to provide guidance on how to improve the creep resistance of Gr.91 alloys. It will address the data scattering problem of **the creep test results of the "same alloy"** from different groups. This model will not only be applied to the structural alloys in FE power plants, but in many different applications, such as nuclear reactors.

Poster 13

FE0027822 – DEVELOPMENT OF A PHYSICALLY-BASED CREEP MODEL INCORPORATING ETA PHASE EVOLUTION FOR NICKEL BASE SUPERALLOYS

ORGANIZATION: Michigan Technological University **PRINCIPAL INVESTIGATOR**: Walter W. Milligan
TEAM MEMBERS: Akhila Gorantla (Student), Paul G. Sanders, Calvin L. White
PRESENTER: Walter W. Milligan

ABSTRACT

Advanced fossil energy power generation cycles employ high performance polycrystalline nickel-base superalloys such as Nimonic 263. These types of alloys are principally strengthened by the gamma prime phase. During extended times at turbine operating temperatures, however, eta phase often forms in service. Although little is understood about the eta phase, it is known to form at the expense of gamma prime, and may negatively impact strength and creep resistance. The primary objective of this work is to develop a physically based creep model for Nimonic 263 that synthesizes known creep behavior based on gamma prime strengthening with a new understanding of the effects of eta phase on creep performance at long service times in fossil energy power plants.

Poster 14

SC0015922 – IMPROVED MODELS OF LONG TERM CREEP BEHAVIOR OF HIGH PERFORMANCE STRUCTURAL ALLOYS FOR EXISTING AND ADVANCED TECHNOLOGIES FOSSIL ENERGY POWER PLANTS

ORGANIZATION: QuesTek Innovations LLC **PRINCIPAL INVESTIGATOR**: Jiaodong Gong
TEAM MEMBERS: Jifeng Zhao, Abhinav Saboo, Greg Olsen, Jason Sebastian
PRESENTER: Jiaodong Gong

ABSTRACT

QuesTek Innovations LLC, a leader in the field of computational materials design, developed a robust creep modeling toolkit that expands its computational Materials by Design® technology, in order to predict the long term creep performance of materials for base alloys in fossil energy systems under wide thermal and mechanical conditions. The goal is to establish microstructure-sensitive models that capture the different creep mechanisms observed in ferritic steels and predict the creep properties as a function of the materials, microstructure, stress and temperature.

In Phase I period, the creep model(s) for calculating creep strain vs time have been demonstrated and validated on creep resistant ferritic steel alloys with evolving microstructure during creep. The models developed in this SBIR program should provide guidelines to designing a microstructure with improved creep properties. Accurate and efficient quantification of material properties for AUSC boilers will directly enhance the success of DOE's crosscutting research and new alloy development program and provide significant public benefits.

Poster 15
FE0027502 – ADDITIVE MANUFACTURING OF ENERGY HARVESTING MATERIAL SYSTEM FOR ACTIVE WIRELESS MEMS SENSORS
ORGANIZATION: University of Texas at El Paso **PRINCIPAL INVESTIGATOR**: Yirong Lin
TEAM MEMBERS: Norman Love, Ryan Wicker
PRESENTER: Victor Elicerio (Student Researcher)

ABSTRACT

The overall goal of proposed research is to design, fabricate, and evaluate an energy harvesting material system capable of working up to 1200 °C to harvest both vibrational and thermal energy for powering high-temperature wireless MEMS sensors. This multidisciplinary effort includes investigators with expertise in energy harvesting, sensors, 3D printing, and energy systems. The team's overarching goal is to study using modified binder jetting based 3D printing technique to fabricate engineered graphene/ceramic composites with high temperature vibration and thermal energy harvesting properties. We will use binder jetting based 3D printing technique to fabricate graphene/lithium niobate (LiNbO3) composites for energy harvesting in harsh environment. The following research objectives are proposed to investigate the energy harvesting material for wireless MEMS sensors: Objective 1: Establish theoretical models to predict the effective material property. Objective 2: Fabricate the ceramic-graphene composites using binder jetting 3D printing technique. Objective 3: Determine energy harvesting property at high temperatures.

Poster 16
FE0027776 – ICME FOR CREEP OF NI-BASE SUPERALLOYS IN ADVANCED ULTRA-SUPERCRITICAL STEAM TURBINES
ORGANIZATION: Ohio State University **PRINCIPAL INVESTIGATOR**: Stephen Niezgoda
TEAM MEMBERS: Yunzhi Wang, Pengyang Zhao
PRESENTER: Stephen Niezgoda

ABSTRACT

This program has three major objectives: (1) the application of advanced materials informatics for critical assessment of existing experimental data, (2) critical assessment of existing modeling capabilities and (3) development of new modeling capabilities that are critical for predicting long-term creep behavior of Ni-base superalloys for advanced ultra-supercritical (A-USC) steam turbines. Creep data is being aggregated with the assistance of our collaborator GE-GRC. Enterprise-scale materials data infrastructure and machine-learning framework supplied by our collaborator Citrine Informatics will be used to process and datamine the data to establish the processing-microstructure-property relationships. Existing creep-life models will be rigorously assessed using uncertainty quantification tools. Phase-field and FFT-based crystal plasticity will be integrated to develop a multiscale physics-based microstructure sensitive creep model to document effects of microstructural heterogeneities on creep life. The Ni-base superalloys have been identified as the critical materials enabling the A-USC steam turbine design that will allow for an efficiency increase from an average of 35% (current power plants) to 47% and a reduction of CO and other fuel-related emissions by as much as 29%. The proposed ICME approach will improve the efficiency and accuracy of current assessment of the alloy's long-term creep performance, accelerating the development of next- generation materials for A-USC steam turbine. This will allow the US manufacturers to maintain a competitive edge in the global market in building highly efficient coal-fired power plants. The ICME approach developed will be generic in nature and applicable to other high temperature materials where creep is the first-tier consideration.

Poster 17

FWP 1022427 – OPTICAL AND THERMODYNAMIC PROPERTIES OF PURE- AND LA-DOPED $SRTIO_3$

ORGANIZATION: NETL Research & Innovation Center **PRINCIPAL INVESTIGATOR**: Yuhua Duan

TEAM MEMBERS: Paul Ohodnicki, Benjamin Chorpening and Gregory Hackett

PRESENTER: Yuhua Duan

ABSTRACT

Lanthanum doped strontium titanate ($La_{1-x}Sr_xTiO_3$, La-STO) materials are essential for solid oxide fuel cell (SOFC) electrodes and high-temperature gas sensors. To better understand the thermodynamic and optical behaviors of La-STO with different La-doping levels at high temperature, the *ab initio* thermodynamics by combining the first-principles density functional theory with lattice phonon dynamics have been employed to investigate their electronic structures and thermodynamic evolutions versus temperatures. The results show that when doping La into STO, the band-gap vanished as extra electron fills into the STO conduction band. With increasing the La-doping levels, the La-STO structures become unstable with phonon soft modes. From the calculated dielectric constant matrix of La-STO with different La-doping levels, one can see that in three cases (2La-STO, 3La-STO, 6La-STO) their diagonal elements are not equal, which means that these crystal structures are uniaxial and anisotropic. With increasing La-doping levels, the calculated thermodynamic properties (ΔH, ΔG) with reference to DFT energy of pure STO are decreased. With increasing temperature (T), the $\Delta H(T)$ is increased while the $\Delta G(T)$ is decreased.

Poster 18

FWP 1022427 – BAND-GAP OPENING PROPERTIES OF GRAPHENE BINDING WITH LOW-CONCENTRATION FLUORINE

ORGANIZATION: NETL Research & Innovation Center **PRINCIPAL INVESTIGATOR**: Yuhua Duan

TEAM MEMBERS: Charter D. Stinespring and Benjamin Chorpening

PRESENTER: Yuhua Duan

ABSTRACT

To better understand the effects of low-level fluorine (F) in graphene-based sensors, the structure and impact of low-concentration of fluorine defects on the electrical properties of single- and multi-layer graphene films were investigated by density functional theory with van der Waals dispersion interactions. When F bonds to a carbon atom of graphene, the carbon atom is pulled slightly above the graphene plane creating what is referred to as a C_F defect, and a valence band (B_F) near the Fermi level is formed mainly from the *p* orbitals of the F atoms with some small contribution from the *p* orbitals of the bonded carbon atoms. Depending on the F binding sites, the B_F can serve as a valence band or a conduction band and only few configurations of the F-binding graphene can open a band gap. Such results indicate that the band gap opening for graphene with low F-adsorption level strongly depends on the F-binding configurations, which is different from the fully or highly partial fluorinated graphene. At low F-adsorption level, the interaction between neighboring pairs of F adatoms is negligible and the most important interaction is between the F and carbon atoms in the C_F defect. Such results are useful for sensor and nano-electronics developments.

Poster 19
FE0024059 - INTERMEDIATE TEMPERATURE NANOSTRUCTURED CERAMIC HOLLOW FIBER MEMBRANES FOR OXYGEN SEPARATION
ORGANIZATION: University of South Carolina **PRINCIPAL INVESTIGATOR**: Xingjian (Chris) Xue
TEAM MEMBERS: Chunlei Ren, Yun Gan, Myongjin Lee, Chunyang Yang, Guohui Dong
PRESENTER: Xingjian Xue

ABSTRACT

High-purity oxygen production is of particular importance for oxygen-intensive industries. Ceramic permeation membrane is an economically viable technique for high-purity oxygen production from air. However, such membranes are generally operated at high temperatures (>700°C), which could lead to various degradations and increase the cost of oxygen separation systems. While lowering the operating temperature to intermediate range (500–700°C) may potentially overcome these issues, it in turn would deteriorate the permeation performance of ceramic membranes. Therefore it is highly desired for ceramic membranes to be able to operate at lower temperatures while obtaining high permeation performance. *The objective of the proposed project is to study advanced fabrication technologies to develop intermediate temperature nanostructured ceramic hollow fiber membranes for air separation and oxygen production to satisfy the requirements of production rate and purity of oxygen that can support oxygen-intensive industries*. It is expected that the proposed research employing nanotechnology and advanced fabrication technology to fabricate nanostructured ceramic hollow fiber membranes will lead to low cost and high performance technology for high-purity oxygen production. The reduced operating temperature (less than 700°C) may significantly improve the durability of separation membranes while reducing the cost for the system and operations.

Poster 20
FE0024013 – ADVANCING COAL CATALYTIC GASIFICATION TO PROMOTE OPTIMUM SYNGAS PRODUCTION
ORGANIZATION: Virginia Polytechnic Institute and State University
PRINCIPAL INVESTIGATOR: Dr. Francine Battaglia
TEAM MEMBERS: Dr. Foster A. Agblevor (Utah State Univ.), Dr. Michael T. Klein (Univ. of Delaware)
PRESENTER: Ryan Soncini (Student Researcher)

ABSTRACT

A collaborative effort involving experiments, kinetic modeling, and computational fluid dynamics (CFD) is being conducted to address and recommend advanced catalytic gasification of coal. The novel approach is the use of a red mud derived catalyst with sub-bituminous coal to effectively gasify coal and produce clean hydrogen rich syngas. The gasification experiments are conducted for a range of temperatures utilizing bench-scale and pilot-scale reactors. The red mud catalyst is modified using nickel as the pyrolysis medium to lower gasification temperatures. Fuel composition is then analyzed to guide the development of detailed reaction kinetics models. The molecular kinetic modeling will provide the reaction pathways that will be converted to a set of reaction equations. A reaction module will be built using the equations and will be coupled with Cantera and C3M for use in CFD codes. Decoupling the transport and chemical source terms using a fractional step approach will provide an efficient method for solving the complex chemistry. The outcome of this research effort will demonstrate the capability of red mud to improve syngas composition as compared to inert fluidization media. It will be shown that using red mud increases hydrogen content and reduces methane concentrations in the produced syngas. An important aspect will be the development of catalytic coal gasification chemical kinetic models that can be integrated into CFD modeling environments such as MFiX and OpenFOAM. Such advancements will allow for improved efficiency in low-rank coal processes via the redmud catalyst, and can be investigated using high fidelity CFD modeling.

Poster 21

FE0024080 – PRODUCTION OF HIGH-PURITY O2 VIA MEMBRANE CONTACTOR WITH OXYGEN CARRIER SOLUTIONS

ORGANIZATION: Gas Technology Institute (GTI) **PRINCIPAL INVESTIGATOR**: Shiguang Li
TEAM MEMBERS: Gas Technology Institute (GTI), University of South Carolina (USC)
PRESENTER: Shiguang Li

ABSTRACT

The objective of the project is to achieve the proof of concept of an innovative oxygen production technology using hollow fiber membrane contactor (HFMC) with oxygen carrier solution as solvent and air as feed to produce high purity of O_2. The goal of this technology development is to achieve O_2 purity greater than 95% capable of being used in oxygen-intensive industries at a cost that is substantially below the current benchmarks for commercially available, stand-alone Air Separation Units.

In the process, air is sent to a membrane absorber and passes through small-diameter membrane tubes, while a lean O_2 carrier solution flows counter currently on the shell side of the membrane. The O_2 permeates through the membrane pores and is absorbed in the O_2 carrier solution. The O_2-rich carrier solution can be regenerated in a second membrane module (desorber) operated in a reverse process.

This technology has potential to produce oxygen with purity as high as 99.9% for applications in IGCC, oxy-combustion, and other advanced power generation technologies. It should offer tremendous opportunities to improve the efficiency and cost for air separation, and thus, on the overall oxygen-intensive industries.

Poster 22

FE0023999 – CATALYTIC PRB COAL-CO2 GASIFICATION FOR FUELS AND CHEMICALS WITH TWO DIFFERENT TYPES OF SYNGAS (1ST- CO + ZERO CH4; 2ND- H2:CO:CH4 = 2:1:NEAR-ZERO) AND NEGATIVE OR LOW CO2 EMISSIONS

ORGANIZATION: University of Wyoming **PRINCIPAL INVESTIGATOR**: Maohong Fan
TEAM MEMBERS: Qinxi Cao, Wenyang Lu, Bang Xu, Tiberiu Popa
PRESENTER: Maohong Fan

ABSTRACT

The overall objective of this project is to develop a catalytic gasification technology with the characteristics of zero CH_4 and negative/low CO_2 generations. Specifically, the project was designed to reduce CH_4 and CO_2 by 30% and 50%, respectively; increase H_2 in the gas from pyrolysis at least 20%; generate CO with near 0 CH4 in CO_2-char gasification and syngas with H_2: CO = 2:1 and CH_4 being less than 0.5% during char gasification with the presence of H_2O; and reduce gasification activation energies by 30-50%. Almost all the tasks have been completed. The results achieved so far include: 1) 65.90 % increase of total yield of H_2 with 3%Na+1% Fe catalyst at 800°C, which is 229.50% higher than expected target (20%); 2) increase of total CO yield by 39.06 % with 3%Na+1% Fe catalyst at 800°C; 3) decrease of total yield of CO_2 by 81.7% with 4% Na catalyst at 700°C, which is 38.80 % better than the targeted value (50%); 4) decrease of CH_4 yield to near 0 in produced syngas; 5) generation of syngas with its H_2:CO ratio being ~ 2:1 or much higher than 2:1 under almost all the operating conditions; and 6) significant acceleration of carbon conversion.

Poster 23

FE0024068 – INCREASING THE RATE AND EXTENT OF MICROBIAL COAL TO METHANE CONVERSION THROUGH OPTIMIZATION OF MICROBIAL ACTIVITY, THERMODYNAMICS, AND REACTIVE TRANSPORT

ORGANIZATION: Montana State University, Energy Research Institute
PRINCIPAL INVESTIGATOR: Matthew Fields
TEAM MEMBERS: Lee Spangler, Al Cunningham, Robin Gerlach
PRESENTER: Matthew Fields

ABSTRACT

Project Goal: Improve the rates and extent of microbially-enhanced coal bed methane (MECBM) by better understanding potential biological and physical constraints to coal-dependent methanogenesis. Ultimately, we want to mitigate environmental impacts, produce multiple value-added products (natural gas and biomass), increase the longevity of existing infrastructure, and provide essential data for resource estimations. This goal will be accomplished by determining rates of microbial processes that lead to overall methanogenesis under different conditions, including thermodynamic and reactive transport considerations. These data will be used as a design tool for moving towards a field-scale demonstration of MECBM.

- Objective 1 – Determination of the chemical and biological parameters limiting methane production from coal
- Objective 2 – Develop strategies for the optimization of the MECBM technology based on thermodynamic and reactive transport considerations
- Objective 3 - Scale up laboratory microcosms to optimize microbial coal-to-methane production in column flow reactors

Benefits: The thermodynamic and reactive transport modeling activities will significantly improve the knowledge regarding the rate limiting steps for field-scale MECBM and provide the necessary insight for this work to improve the design and performance of the planned laboratory and meso-scale studies. Furthermore, together with the scale-up activities, the project will directly serve as a design tool for a planned field scale demonstration the recipient is involved in.

Poster 24

FE0026155 – OPTIMIZATION, SCALE-UP, AND DESIGN OF COAL-DEPENDENT METHANOGENESIS IN PREPARATION FOR IN SITU FIELD DEMONSTRATION

ORGANIZATION: Montana State University, Energy Research Institute
PRINCIPAL INVESTIGATOR: Matthew Fields
TEAM MEMBERS: Lee Spangler (MSU), Robin Gerlach (MSU), Al Cunningham (MSU), Adrienne Phillips (MSU), Brian Park (MET), Randy Hiebert (MET), Bill Orem (USGS), Elliott Barnhart (USGS)
PRESENTER: Matthew Fields

ABSTRACT

Project Goal: The goal of this one-year project is to mature our bio-gasification method as we consider future field tests. Achieving this goal will transform *in situ* Microbially Enhanced Coal Bed Methane (MECBM) by enhancing Coal Bed Methane (CBM) production rates, shortening the time needed to re-generate CBM fields after production is no longer economical, mitigating environmental impacts, increasing the longevity of existing infrastructure, and providing essential data for resource estimations. The combination of microbiological and engineering approaches will identify and minimize key constraints as we prepare for MECBM field demonstration.

- Objective 1. Evaluate time-delay to methane production post-stimulation during meso-scale push-pull injections.
- Objective 2. Complete site characterization.
- Objective 3. Evaluate and design potential field demonstration and economic analysis at the USGS Birney Test Site in the Powder River Basin.

Benefits: We will specifically target unminable coal seams that will provide mechanisms for the use of existing CBM infrastructure in the field and standard oil / gas field equipment that will optimize the rate of microbial conversions and the longevity of individual wells for a commercially competitive process. Injection experiments at the meso-scale at relevant pressure and temperature will inform preparation for field demonstration, namely in determination of rates and time-delay associated with stimulation of indigenous coal communities. The data will provide valuable parameter constraints to help test the feasibility of commercially competitive coal conversion to gas and will be used to design a field scale demonstration at our Birney Test Site as well as other potential bio-gasification production locations.

Poster 25
FE0024088 – CERAMIC PROPPANT DESIGN FOR IN-SITU MICROBIALLY ENHANCED METHANE RECOVERY
ORGANIZATION: University of Utah **PRINCIPAL INVESTIGATOR**: Taylor D. Sparks
TEAM MEMBERS: Co-PI John McLennan, Kyu Bum-Han, John Fuertez
PRESENTER: Taylor D. Sparks

ABSTRACT

Coalbed methane is extracted from coal that is too deep to be economically extracted. The goal of this study is to develop new technology to enhance the economic viability of *in-situ* microbial coal to methane conversion within these otherwise unmineable fossil fuel resources. Methanogen-laden ceramic proppant is created for improving fluid transport properties. The density of proppant is reduced with adequate strength while also serving as a vehicle for delivery of microbial consortia to coal seams. Nutrient and microbial consortia optimization are performed for *in-situ* coal to methane conversion. We successfully produce kaolinite-based ultralight weight proppant (1.4 g/mL). Microbial methanogenesis is optimized at 36°C, pH 5.5, and NaCl (3.3 g/L). The highest performing nutrient and coal type are tryptic soy broth and Miller Black Thunder. The microbes in the optimized condition are encapsulated by calcium-alginate polymer which can vary the particle size and release time over acceptable ranges with simple tuning of polymerization parameters. Methanogen-laden proppant tested in benchtop reactors under pseudo *in-situ* conditions show that methane gas is produced successfully over 500 hours.

Poster 26
FE0024126 – OPTIMIZED MICROBIAL CONVERSION OF BITUMINOUS COAL TO METHANE FOR IN SITU AND EX SITU APPLICATIONS
ORGANIZATION: Southern Illinois University **PRINCIPAL INVESTIGATOR**: Yanna Liang
TEAM MEMBERS: Satya Harpalani
PRESENTER: Yanna Liang

ABSTRACT

Although production of methane from coal through biogasification has been a commercial reality in several parts of the world, little work has been done on methane production from bituminous coal. Thus, this project seeks to maximize methane productivity from bituminous coal in the Illinois basin. To achieve this goal, we aim to: 1) Simplify the composition of the nutrient solution designed for biostimulation. This simplification will reduce the cost of the developed recipes; 2) Maximize methane yield by investigating individual and interactive effects from different parameters, such as coal particle size, temperature, pH, mixing, and addition of surfactants, solvents and electron donors, in microcosm setups; 3) Investigate methane production through biogasification in a fed-batch cultivation mode; and 4) Investigate methane production using our established microbial consortium in pressurized reactors simulating in situ pressures.

Upon completion of this project, biogasification processes suitable for ex situ or in situ applications will be developed. The low-cost, efficient and highly productive processes developed from this project will: 1) address the challenges facing the current Coal Bed Methane operations in the field, which are high cost and low productivity for high rank coals; 2) contribute to our technical know-how regarding biogasification of bituminous coal; 3) provide an abundant supply of natural gas to our society; 4) enable coal to be used in an environmentally-friendly and sustainable way; and 5) develop a means to utilize coal waste, thus converting a waste to a resource.

Poster 27
SC0015895 – WAVE LIQUEFACTION™: A REMS APPROACH TO MANUFACTURE FUELS, CHEMICALS, AND MATERIALS FROM COAL
ORGANIZATION: H Quest Vanguard, Inc. **PRINCIPAL INVESTIGATOR**: George Skoptsov
TEAM MEMBERS:
PRESENTER: George Skoptsov

ABSTRACT

Wave Liquefaction™ technology is a novel approach to coal liquefaction, specifically designed to overcome the inherent environmental and economic challenges of conventional coal to liquids processes. Characterized by little to no process CO_2 emissions, high thermal efficiency, and low capital and operating costs, Wave Liquefaction™ process enables production of cost-competitive liquid and solid products directly from coal with lower direct and lifecycle greenhouse gas emissions than conventional petroleum refining, without carbon capture. Lifecycle greenhouse gas emissions can be reduced further with use of coal/biomass blends. Wave Liquefaction™ small-footprint, high-throughput, ambient pressure reactors sharply lower capital costs of coal conversion and eliminate the need for economies of scale. Preliminary estimates show feasibility of modular cashflow-positive plants at scales as low as 100 tons per day of coal feed (~200 barrels of liquid product/ day). Replication of standard, pre-assembled core reactor units and process trains allows site-specific scaling, reduces technical and financial risks associated with conventional, non-modular scaling, and increases plant availability through process redundancy.

Poster 28
FE0010482 – SMALL-SCALE PILOT PLANT FOR THE GASIFICATION OF COAL AND COAL/BIOMASS BLENDS AND CONVERSION OF DERIVED SYNGAS TO LIQUID FUELS VIA FISCHER-TROPSCH SYNTHESIS
ORGANIZATION: University of Kentucky Research Foundation
PRINCIPAL INVESTIGATOR: Rodney Andrews
TEAM MEMBERS: Andrew Placido, Kunlei Liu and Don Challman
PRESENTER: Kunlei Liu

ABSTRACT

The overarching objective of this project is to implement advanced design and construction of this modular Coal to Liquids facility at the University of Kentucky Center for Applied Energy Research (UKy-CAER). The facility design and fabrication of process units have been completed, and construction is now nearing completion. The know-how, show-how associated with the facility is the expected key benefit, which can be used as test beds for new concepts, and can be repurposed depending on development needs at a level of expenditure that is affordable. The facility consists of a coal feed to finished fuels process train including: feedstock handling and process, gasification, water-gas shift, acid gas cleanup, and Fischer-Tropsch systems. The plant complex also includes ancillary systems for power generation, utilities, effluent treatment, ash disposal, and automated control systems. In order to maximize flexibility, the facility is of a modular design with skid mounted process units – and is intended to be adaptable to change-out of equipment and capabilities.
The focus of this poster will be on the development of the modular process units including design specifications, construction/installation progress and initial testing data. This facility was purposely designed to permit maximum flexibility such that it could be a test bed for future research and development with respect to fuels, chemicals and poly-generation. Research areas the UKY-CAER intends to focus on are feed preparation, coal/biomass gasification, gas clean up, and CO2 management.

Poster 29

SC0013248 – DESIGN AND FABRICATION OF NOVEL MIXED ION-ELECTRON CONDUCTING MEMBRANES FOR OXYGEN SEPARATION

ORGANIZATION: HiFunda LLC **PRINCIPAL INVESTIGATOR**: Jiwen Wang, Ph.D.
TEAM MEMBERS: Jiwen Wang, Jesse Nachlas, Chen Jiang, Isaac Corn, Balakrishnan Nair, Meilin Liu, Seonyoung Yoo
PRESENTER: Balakrishnan Nair, PhD

ABSTRACT

For a gasification based energy system the cost of the air separation unit represents 12 – 15% of the installed capital costs and requires a significant amount of power resulting in lowered operational efficiencies. Consequently, there is a significant opportunity for lowered capital costs and improved operating efficiencies for new oxygen generation technologies that can replace existing cryogenic systems. One of the most promising new technologies under development by the DOE is advanced Ion-Electron Mixed Conductors (IEMC) for oxygen separation from air. To advance IEMC technology, the potential for significant reductions in operation cost and for improving efficiency is improved oxygen permeation rates through the IEMC membrane. The primary ways to achieve that goal are decreasing the membrane thickness, developing a new material with higher ionic conductivities than current materials, improving the surface kinetics of the electrode reactions and/or lowering the cost of manufacture for producing these complex membrane structures. In this project, HiFunda and Georgia Institute of Technology (GT) are developing a new IEMC membrane material with improved ionic conductivity and surface kinetics over state of the art materials in conjunction with improvements in the manufacturing process through advancements in plasma spray technology. In the Phase I SBIR program, HiFunda/GT successfully demonstrated that a membrane material with surface exchange characteristics and ionic conductivity superior to state of the art materials such as LSCF and LSM. The potential to fabricate thin, dense membranes using the novel plasma spray process was also demonstrated. In the ongoing Phase II program, the HiFunda/GT team are developing a robust process that can produce high quality membranes, and optimizing the membrane material compositions for improved system performance.

Rare Earth Element Project Posters

Poster 30
FE0026444 – RARE EARTH OCCURRENCE IN ACID MINE DRAINAGE PRECIPITATES: NORTHERN AND CENTRAL APPALACHIA COAL BASINS
ORGANIZATION: West Virginia University Research Corporation
PRINCIPAL INVESTIGATOR: Paul Ziemkiewicz
TEAM MEMBERS: Aaron Noble, Xingbo Liu
PRESENTER: Paul Ziemkiewicz

ABSTRACT
In the Appalachian Basin, acidic mine drainage (AMD) is produced in vast quantities at both abandoned and current coal mining and preparation facilities. AMD leaches and concentrates rare earth elements (REE) from coal and associated shales. The Clean Water Act requires treatment of AMD prior to discharge. This process involves acid neutralization, oxidation and removal of metals as hydroxide precipitates. Disposal of these precipitates is an important operating cost to the operators and is designed to minimize cost. Rare earth elements (REEs) precipitate along a pH gradient that is similar to that of iron, the major component of AMD solids. These metal hydroxides are collected in settling basins while treated water is decanted to discharge.

This project institutes an expanded sampling effort to include 60 mine sites in the northern Appalachian coal basin (NAPP) and 15 in the Central Appalachian coal basin (CAPP). These sites typically contain multiple AMD discharges and treatment units, each consisting of an alkaline treatment, oxidation system, and cells for collecting sludge. A total of 600 precipitate samples will be collected from the NAPP along with a total of 150 sludge samples from the CAPP to thoroughly identify whether REEs in AMD sludge occur in sufficient quantities and qualities to justify investment as a commercial enterprise in the Appalachian basin.

Poster 31
FE0026443 – IDENTIFICATION AND CHARACTERIZATION OF ILLINOIS BASIN COAL AND COAL-RELATED MATERIALS CONTAINING HIGH RARE EARTH ELEMENT CONTCENTRATIONS
ORGANIZATION: University of Kentucky **PRINCIPAL INVESTIGATOR**: Dr Jack Groppo
TEAM MEMBERS: Dr Rick Honaker, Dr Jim Hower, Dr Cortland Eble
PRESENTER: Dr Rick Honaker

ABSTRACT

The approach that will be used in this investigation emphasizes collaboration with coal companies actively mining the Illinois Coal Basin to develop and implement a sampling and characterization program that will be representative of both current (mine face and preparation plant) and future mining in the region. The approach identifies and characterizes coal and coal-related material in the Illinois Coal Basin that contain elevated concentrations of Rare Earth Elements (REEs) by using archived core databases, analyzing existing cores from a variety of sources, including state geological surveys and mining companies, as well as new cores extracted from areas of interest and preparations plant process streams. Sampling locations will focus primarily on economic coal beds, particularly those with current mining and/or exploration activity, as well as those with sufficient reserves to sustain commercial development for the foreseeable future. Specific coal beds of primary interest are Springfield, Herrin and Baker, although other deeper coal beds may be considered, provided core data justifies further sampling and the known reserve base is sufficient.

Poster 32

FE0026648 – RARE EARTH ELEMENT IDENTIFICATION AND CHARACTERIZATION OF COAL AND COAL BY-PRODUCTS CONTAINING HIGH RARE EARTH ELEMENT CONCENTRATIONS – APPALACHIAN BASIN

ORGANIZATION: Tetra Tech, Inc. **PRINCIPAL INVESTIGATOR**: Farley Wood
TEAM MEMBERS: Tom Gray, Katie Pugh
PRESENTER: Farley Wood

ABSTRACT

Tetra Tech, Inc. is conducting sampling and characterization of Northern and Central Appalachian Basin coal and coal-related associated materials in search of high concentrations of Rare Earth Elements (REE) (minimum concentration of 300 parts per million (ppm)). Coal and coal-related associated materials are defined as run-of-mine coal; roof rock; overburden clays; shale interlayer formations; mine seam underclays; coal preparation plant refuse; etc.; and other coal-like materials as mined.

Initial interest in the Northern and Central Appalachia study areas are the Fire Clay and Williamson coal beds. Sampling the Upper Freeport and Middle/Lower Kittanning coal beds is also planned. These coals are frequently associated with kaolinitic flint clays seatearths (underclays) formed as paleolaterites prior to peat accumulation. Depending on internal results other coal seams may be added to the plan.

Tetra Tech has partnered with West Virginia Geological and Economic Survey (WVGES) to screen and conduct sampling of coal measures expecting a high probability to contain high Rare Earth Elements (REE's) in West Virginia. The Pennsylvania Department of Environmental Protection's Bureau of Abandoned Mine Reclamation (PaBAMR) has also agreed to provide Tetra Tech with access to sample specific coal seams on their project sites in central Pennsylvania.

Tetra Tech has already conducted preliminary sampling and testing. Based on the results of the preliminary testing more detailed sampling and testing will be completed to confirm the high concentrations are prevalent and not merely a onetime anomaly. This poster will present results to date.

Poster 33

FE0026929 – RARE EARTH ELEMENT IDENTIFICATION AND CHARACTERIZATION OF COAL AND COAL BY-PRODUCTS CONTAINING HIGH RARE EARTH ELEMENT CONCENTRATIONS – ROCKY MOUNTAIN BASIN

ORGANIZATION: Tetra Tech, Inc. **PRINCIPAL INVESTIGATOR**: Farley Wood
TEAM MEMBERS: Tom Gray, Katie Pugh
PRESENTER: Farley Wood

ABSTRACT

Tetra Tech, Inc. is conducting sampling and characterization of Rocky Mountain Basin coal and coal-related associated materials in search of high concentrations of Rare Earth Elements (REE) (minimum concentration of 300 parts per million (ppm)). Coal and coal-related associated materials are defined as run-of-mine coal; roof rock; overburden clays; shale interlayer formations; mine seam underclays; coal preparation plant refuse; etc.; and other coal-like materials as mined.

Based on previous REE work elevated REE coal and coal related lithologies have been recorded in the Colorado Raton Basin as well as near Florence, CO in the Canon City Embayment. In both cases, igneous material in or adjacent to the basins also exhibited high REE content, notably in lamprophyre dikes, igneous sills, and tonsteins associated with the coals of the Raton Basin. The eastern Uinta Bain of Colorado and Utah may hold similar potential as documented quasi-commercial REE deposits are present in the Iron Hill carbonatite complex near Powderhorn, CO which is just south of the Grand Mesa in Colorado and is near many mining districts in the basin, as well as reported REE-enriched pegmatites near Montrose, CO.

Tetra Tech has conducted preliminary sampling and testing. Based on the results of the preliminary testing more detailed sampling and testing will be completed to confirm the high concentrations are prevalent and not merely a onetime anomaly. This poster will present results to date.

Poster 34

FE0026527 – REE IDENTIFICATION AND CHARACTERIZATION OF COAL AND COAL BY-PRODUCTS CONTAINING HIGH RARE EARTH ELEMENT CONCENTRATIONS

ORGANIZATION: XLight Corporation **PRINCIPAL INVESTIGATOR**: Robert Uhrin, Ph. D.
TEAM MEMBERS: David Uhrin
PRESENTER: David Uhrin

ABSTRACT

This project is intended to evaluate coal and coal-byproducts from various sites in western Pennsylvania (bituminous) and eastern Pennsylvania (anthracite) for rare-earth element (REE) content. The objective is to identify sites containing >300 ppm of REEs. In order to conduct field sampling, a field-portable x-ray fluorescence (XRF) unit will be used to survey potential samples. A Niton XL3t 500 unit will be engaged to carry out this study. XRF has never been employed for measuring REEs. This unit will be modified to identify the specific range of REEs. To obtain accurate and precise data, standard samples containing REEs of known concentration will be prepared in the laboratory, where they will be measured using the XRF unit. Comparison of the standard sample data with that of measured field samples will allow determination of the samples' REE content. A cross-correlation will be made with selected samples evaluated by chemical analysis using the induction-coupled plasma mass spectrometry (ICP-MS) technique.

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