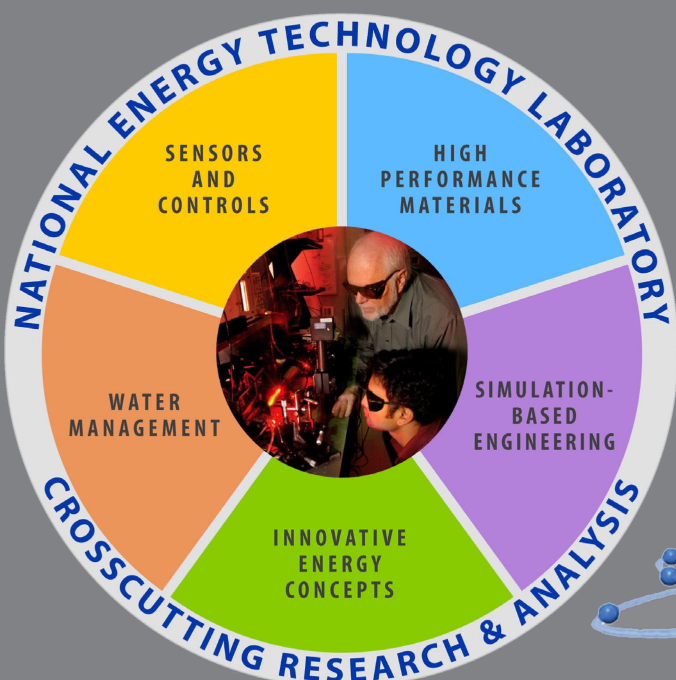
2016

CROSSCUTTING RESEARCH & RARE EARTH ELEMENTS

PORTFOLIOS REVIEW ABSTRACT

April 18–22, 2016

Sheraton Station Square Hotel
Pittsburgh, PA



REE
RARE EARTH ELEMENTS
FROM COAL AND COAL BY-PRODUCTS

U.S. DEPARTMENT OF ENERGY | NETL

REVIEW MEETING CHAIRS

Patricia Rawls
Maria Reidpath
Robert Romanosky
U.S. Department of Energy
National Energy Technology Laboratory

Meeting Coordinators

Karen Lockhart
Smart Data Solutions, LLC

Julie Jividen
Leonardo Technologies Inc.

Dale Cunningham
Sextant Technical Services

Table of Contents

MONDAY, APRIL 18, 2016 – TRACK B

Tuesday, April 19, 2016 – Track A

Tuesday, April 19, 2016 – Track B

Wednesday, April 20, 2016 – Track A

Wednesday, April 20, 2016 – Track B

THURSDAY, APRIL 21, 2016 – TRACK A

THURSDAY, APRIL 21, 2016 – TRACK B

Friday, April 22, 2016 – Track A

Friday, April 22, 2016 – Track B

POSTER SESSION – TUESDAY APRIL 19, 2016 5:00 – 6:45 PM

2016 CROSSCUTTING RESEARCH AND RARE EARTH ELEMENTS PORTFOLIOS REVIEW

MONDAY APRIL 18

Time	Session	Topic	Details
7:00 AM	**REGISTRATION** – Grand Station Foyer	**CONTINENTAL BREAKFAST** – Grand Station 3–5	
8:30 AM	**GENERAL SESSION** Grand Station 1 & 2	**Welcome and NETL Overview**	Grace M. Bochenek, Ph.D. Director National Energy Technology Laboratory
		Program Overviews	• Fossil Energy Advanced Energy Systems (FE AES) – *Regis Conrad, Division Director, FE AES* • NETL Crosscutting Research and Analysis (CCRA) – *Robert Romanosky, Acting Portfolio Manager, CCRA* • Rare Earth Elements (REE) – *Mary Anne Alvin, Portfolio Manager, REE* • Radically Engineered Modular Systems – *Jenny Tennant, Portfolio Manager, Gasification and Fuels*
		Systems Analysis	• Direct Power Extraction and Advanced Ultra-Supercritical Power Plants – *Nathan Weiland, Energy Process Analysis*
10:00 AM	**MORNING BREAK**		

TRACK A – Grand Station 1& 2

Time	Breakout Session Number	Breakout Session Title	Moderator	Organization	Presentation Title	Presenter
10:30 AM	1	Computational Materials Modeling	Charles Miller	Ames National Laboratory	The SMARTER Project – Science of Multicomponent Alloys: Roadmap for Theoretical and Experimental Research	Matthew Kramer
				Southern University and A&M College	An Integrated Study on a Novel High Temperature High Entropy Alloy	Shizhong Yang
11:30 AM	**LUNCH** (On Your Own)					
1:00 PM	2	Computational Materials Modeling	Vito Cedro	ORNL–Oak Ridge National Laboratory	Weldability of Creep Resistant Alloys for Advanced Power Plants	Xinghua Yu
				General Electric Company	Modeling Long-Term Creep Performance for Welded Nickel-Base Superalloy Structures for Power Generation Systems	Chen Shen
				ORNL–Oak Ridge National Laboratory	Corrosion Issues in Advanced Coal Fired Boilers	Bruce Pint
2:30 PM	**AFTERNOON BREAK**					
3:00 PM	3	Structural Materials	Sydni Credle	General Electric Company	A New Superalloy Enabling Heavy Duty Gas Turbine Wheels for Improved Combined Cycle Efficiency	Richard DiDomizio
				ANL – Argonne National Laboratory	Development of Nondestructive Evaluation (NDE) Methods for Structural and Functional Materials	Jiangang Sun
				Electric Power Research Institute Inc.	Predicting the Oxidation/Corrosion Performance of Structural Alloys in Supercritical CO_2	Steve Kung
				University of Illinois	Serration Behavior of High-Entropy Alloys	Karin Dahmen

TRACK B – Admiral Room

Time	Breakout Session Number	Breakout Session Title	Moderator	Organization	Presentation Title	Presenter
10:30 AM	1	Optical Sensors	Barbara Carney	University of Missouri System	Robust Ceramic Coaxial Cable Down-Hole Sensors for Long-Term In Situ Monitoring of Geologic CO_2 Injection	Runar Nygaard
				University of Florida	High-Temperature Sapphire Pressure Sensors for Harsh Environments	Justin Kiehne
11:30 AM	**LUNCH** (On Your Own)					
1:00 PM	2	Optical Sensors	Karol Schrems	University of Cincinnati	Robust Metal-Ceramic Coaxial Cable Sensors for Distributed Temperature Monitoring in Harsh Environments of Fossil Energy Power Systems	Adam Trontz
				Virginia Polytechnic Institute and State University	Reduced Mode Sapphire Optical Fiber and Sensing System	Daniel Homa
				University of Massachusetts at Lowell	Distributed Fiber Sensing Systems for 3D Combustion Temperature Field Monitoring in Coal-Fired Boilers Using Optically Generated Acoustic Waves	Jingcheng Zhou
2:30 PM	**AFTERNOON BREAK**					
3:00 PM	3	Innovative Process Technologies	Karol Schrems	NETL Research & Innovation Center	Advanced Sensor Materials and Fiber Optic Sensors	Paul Ohodnicki
				NETL Research & Innovation Center	Creep Optimization in Haynes 282 Through Gamma Prime Coarsening Control: Preliminary Results	Jeff Hawk
				NETL Research & Innovation Center	LIBS for Subterranean Measurements	Dustin McIntyre
				NETL Research & Innovation Center	NETL Advanced 9% Cr Steel: Update and Current Development Status	Jeff Hawk

2016 CROSSCUTTING RESEARCH AND RARE EARTH ELEMENTS PORTFOLIOS REVIEW

TUESDAY APRIL 19

Time	Track A – Breakout Session Number	Track A – Breakout Session Title	Track A – Moderator	Track A – Organization	Track A – Presentation Title	Track A – Presenter	Track B – Breakout Session Number	Track B – Breakout Session Title	Track B – Moderator	Track B – Organization	Track B – Presentation Title	Track B – Presenter
7:30 AM	**REGISTRATION** – Grand Station Foyer						**CONTINENTAL BREAKFAST** – Grand Station 3–5					
	TRACK A – Grand Station 1& 2						**TRACK B** – Admiral Room					
8:30 AM	4	Advanced Manufacturing	Sydni Credle	Energy Industries of Ohio Inc.	Benefits of Hot Isostatic Pressure/ Powdered Metal (HIP/PM) and Additive Manufacturing (AM) to Fabricate Advanced Energy System Components	Nancy Horton Roy Sheppard	4	Novel Sensor Concepts	Barbara Carney	New Mexico Institute of Mining and Technology	Development of a CO_2 Chemical Sensor for Downhole CO_2 Monitoring in Carbon Sequestration	Ning Liu
				Edison Welding Institute, Inc.	Additive Manufacturing of Fuel Injectors	Mahdi Jamshidinia				Palo Alto Research Center Incorporated	Heat Sensor-Harsh Environment Adaptable Thermionic Sensor	Scott Limb
				Mohawk Innovative Technology, Inc.	High Temperature Ceramic Heat Exchanger for Solid Oxide Fuel Cell	Jose Luis Cordova				West Virginia University Research Corporation	Graphene-Based Composite Sensors for Energy Applications	Charter Stinespring
10:00 AM	**MORNING BREAK**											
10:30 AM	5	Functional Materials	Jessica Mullen	Prairie View A&M University	Post Combustion Carbon Capture Using Polyethylenimine (PEI) Functionalized Titanate Nanotubes	Melisa Stewart	5	Novel Sensor Concepts	Benjamin Chorpening	University of Connecticut	Metal Oxide/Nitride Heterostructured Nanowire Arrays for Ultra-Sensitive and Selective Multi-Mode High Temperature Gas Detection	Bo Zhang
				Auburn University	Reduced Cost Bond Layers for Multi-Layer Thermal/Environmental Barrier Coatings	Jeffrey Fergus				University of Texas at El Paso	Investigation on Pyroelectric Ceramic Temperature Sensors for Energy System Applications	Ricardo Martinez
11:30 AM	**LUNCH** (On Your Own)											
1:00 PM	6	Functional Materials	Richard Dunst	North Carolina State University	Rational Design of Mixed-Metal Oxides for Chemical Looping Combustion of Coal Via Computational Experimental Studies	Fanxing Li	6	Novel Sensor Concepts	Sydni Credle	Sporian Microsystems Inc. (SBIR PROJECT)	Advanced Ceramic Materials and Packaging Technologies for Realizing Sensors Operable in Advanced Energy Generation Systems	Jason Fish
				Delaware State University	Novel Silica Nanostructured Platforms with Engineered Surface Functionality and Spherical Morphology for Low-Cost High-Efficiency Carbon Capture	Nicholas Pizzi				Tech4Imaging (SBIR PROJECT)	Adaptive Electrical Capacitance Volume Tomography for Real-Time Measurement of Solids Circulation Rate at High Temperatures	Qussai Marashdeh
				Southern Illinois University	HVOF Thermal Spray TIC/TIB2 Coatings of AUSC Boiler/Turbine Components for Enhanced Corrosion Protection	Chung-Ying Tsai				Tech4Imaging (SBIR PROJECT)	Real-Time 3-D Volume Imaging and Mass-Gauging of High Temperature Flows and Power System Components in a Fossil Fuel Reactor Using Electrical Capacitance Volume Tomography	Qussai Marashdeh
2:30 PM	**AFTERNOON BREAK**											
3:00 PM	7	Innovative Process Technologies	Karol Schrems	NETL Research & Innovation Center	Internal to External Oxidation Transition Modeling: Plasticity and Coherence Loss	Youhai Wen	7	Embedded Sensors	Maria Reidpath	United Technologies Corporation	Additive Topology Optimized Manufacturing with Embedded Sensing	Paul Attridge
				NETL Research & Innovation Center	Serrated Plastic Flow in High Entropy Alloys	Joe Licavoli				University of Missouri System	Additive Manufacture of Smart Parts with Embedded Sensors for In Situ Monitoring in Advanced Energy Systems	Hai Xiao
				NETL Research & Innovation Center	Advanced Controls and Cyber-Physical Systems	David Tucker				West Virginia University	Smart Refractory Sensor Systems for Wireless Monitoring of Temperature, Health and Degradation of Slagging Gasifiers	Edward Sabolsky
				NETL Research & Innovation Center	IPT – Direct Power Extraction	Rigel Woodside				University of Texas at El Paso	Investigation of “Smart Parts” with Embedded Sensors for Energy System Applications	Yirong Lin
5:00–6:45 PM	**POSTER SESSION** – Grand Station 3–5											

2016 CROSSCUTTING RESEARCH AND RARE EARTH ELEMENTS PORTFOLIOS REVIEW

WEDNESDAY APRIL 20

7:30 AM — **REGISTRATION** – Grand Station Foyer **CONTINENTAL BREAKFAST** – Grand Station 3–5

TRACK A – Grand Station 1& 2

Time	Breakout Session Number	Breakout Session Title	Moderator	Organization	Presentation Title	Presenter
8:30 AM	8	Multidisciplinary Computational Tools	Jason Hissam	Ames National Laboratory	Engineering of Complex Systems	Kenneth Bryden
				Process Systems Enterprise	Evaluation and Demonstration of Commercialization Potential of Carbon Capture Simulation Initiative Tools within gProms Advanced Simulation Platform	Alfredo Ramos Plasencia
10:00 AM	**MORNING BREAK**					
10:30 AM	9	Advanced Manufacturing	Richard Dunst	Ceramatec Inc.	Compact, Ceramic Microchannel Heat Exchangers	Charles Lewissohn
				PNNL – Pacific Northwest National Laboratory	Solid State Joining of Creep Enhanced Ferritic Steels	Glenn Grant
11:30 AM	**LUNCH** (On Your Own)					
1:00 PM	10	Advanced Ultrasupercritical Materials	Vito Cedro	Energy Industries of Ohio Inc.	Materials for Advance Ultrasupercritical Steam Turbines – Advanced Ultrasupercritical Component Demonstration	Horst Hack
				GE Power	Advanced Ultrasupercritical (AUSC) Materials Thick-Walled Cycling Header Development for ComTest-AUSC	Buchi (Reddy) Ganta
				GE Power	Advanced Ultrasupercritical (AUSC) Tube Membrane Panel Development	Jim Pschirer
2:30 PM	**AFTERNOON BREAK**					
3:00 PM	11	Advanced Ultrasupercritical Materials	Vito Cedro	Babcock & Wilcox Power Generation Group, Inc.	Component Test Facility (ComTest) Phase 1 Engineering for 760 °C (1400 °F) Advanced Ultrasupercritical (AUSC) Steam Generator Development	Paul Weitzel
				ORNL–Oak Ridge National Laboratory	Ultra-Supercritical Steam Cycle Turbine Materials	Phil J. Maziasz
				ORNL–Oak Ridge National Laboratory	Materials for Ultra-Supercritical Steam Power Plants	Peter Tortorelli
				ORNL–Oak Ridge National Laboratory	Creep-Fatigue-Oxidation Interactions: Predicting Alloy Lifetimes under Fossil Energy Service Conditions	Sebastien Dryepondt

TRACK B – Admiral Room

Time	Breakout Session Number	Breakout Session Title	Moderator	Organization	Presentation Title	Presenter
8:30 AM	8	Wireless Sensors	Benjamin Chorpening	University of Maine System	High-Temperature Wireless Sensor for Harsh Environment Condition Monitoring	Mauricio Pereira da Cunha
				Siemens Corporation	Novel Temperature Sensors and Wireless Telemetry for Active Condition Monitoring of Advanced Gas Turbines	Anand Kulkarni
				University of Texas at Arlington	Distributed Wireless Antenna Sensors for Boiler Condition Monitoring	Haiying Huang
10:00 AM	**MORNING BREAK**					
10:30 AM	9	Advanced Process Controls	Maria Reidpath	Ohio State University	Advanced Control Architecture and Sensor Information Development for Process Automation, Optimization, and Imaging of Chemical Looping Systems	Tien-Lin Hsie
				West Virginia University	Development of Integrated Biomimetic Framework with Intelligent Monitoring, Cognition and Decision Capabilities for Control of Advanced Energy Plants	Debangsu Bhattacharyya
11:30 AM	**LUNCH** (On Your Own)					
1:00 PM	10	Water Management	Charles Miller	Gas Technology Institute	Simultaneous Waste Heat and Water Recovery from Power Plant Flue Gases for Advanced Energy System	Dexin Wang
				Southern Company Services, Inc.	Field Demonstration Study for Heat and Water Recovery at a Coal-Fired Power Plant	Russell Noble
				SNL – Sandia National Laboratories	Exploring Energy-Water Issues in the United States	Vince Tidwell
2:30 PM	**AFTERNOON BREAK**					
3:00 PM	11	Advanced Process Controls / Sensor Placement & Networks	Sydni Credle	Oregon State University	Evolving Robust and Reconfigurable Multi-Objective Controllers for Advanced Power Systems	Kagan Tumer
				Case Western Reserve University	An Information Theoretic Framework and Self-Organizing Agent-Based Sensor Network Architecture for Power Plant Condition Monitor	Kenneth Loparo
				Ames National Laboratory	Sensors and Controls – Merged Environment for Simulation and Analysis IMESA	Paolo Pezzini
				University of Illinois	Multi-Objective Optimal Sensor Deployment under Uncertainty for Advanced Power Systems	Urmila Diwekar

2016 CROSSCUTTING RESEARCH AND RARE EARTH ELEMENTS PORTFOLIOS REVIEW

THURSDAY APRIL 21

7:30 AM — **REGISTRATION** – Grand Station Foyer **CONTINENTAL BREAKFAST** – Grand Station 3–5

TRACK A – Grand Station 1& 2

Time	Breakout Session Number	Breakout Session Title	Moderator	Organization	Presentation Title	Presenter
8:30 AM	12	Multiphase Flow	Jason Hissam	Ames National Laboratory	Kinetic Theory Modeling of Turbulent Multiphase Flow	Bo Kong
				Arizona State University	MFIX-DEM PHI: Performance and Capability Improvements Towards Industrial Grade Open-Source DEM Framework with Integrated Uncertainty Quantification	Manogna Adepu Shaohua Chen
				University of Colorado	MFIX-DEM Enhancement for Industry-Relevant Flows	Thomas Hauser
10:00 AM	**MORNING BREAK**					
10:30 AM	13	Functional Materials	Richard Dunst	Indiana University – Purdue University Indianapolis	Novel Functional-Gradient Thermal Barrier Coatings in Coal-Fired Power Plant Turbines	Jing Zhang
				West Virginia University	Ceramic High Temperature Thermoelectric Heat Exchanger and Heat Recuperators in the Power Generation Systems	Xueyan Song
11:30 AM	**LUNCH** (On Your Own)					
1:00 PM	14	Structural Materials	Vito Cedro	ORNL–Oak Ridge National Laboratory	Advanced Alloy Design Concepts for High Temperature Fossil Energy Applications	Yukinori Yamamoto
				Electric Power Research Institute Inc.	Optimization of Advanced Steels for Cyclic Operation Through an Integration of Material Testing, Modeling and Novel Component Test Validation	John Siefert
				University of Tennessee	Experimental and Computational Investigation of High Entropy Alloys for Elevated High Temperature Applications	Prof. Peter K. Liaw
2:30 PM	**AFTERNOON BREAK**					
3:00 PM	15	Computational Materials Modeling	Youhai Wen	Oregon State University	New Mechanistic Models of Long Term Evolution of Microstructure and Mechanical Properties of Nickel Based Alloys	Jamie Kruzic
				University of Tennessee	Computational Design and Performance Prediction of Creep-Resistant Ferritic Superalloys	Peter Liaw
				QuesTek Innovations LLC (SBIR PROJECT)	Computational Design of Weldable, High-Cr Ferritic Steel	David Snyder
				Tennessee State University	Large Scale Screening of Low Cost Ferritic Steels Designs for Advanced Ultra Supercritical Boiler Using First Principles Methods	Lizhi Ouyang

TRACK B – Admiral Room

Time	Breakout Session Number	Breakout Session Title	Moderator	Organization	Presentation Title	Presenter
8:30 AM	12	Water Treatment and Reuse	Barbara Carney	GE Global Research	Model-Based Extracted Water Desalination System for Carbon Sequestration	Ryan Adams
				General Electric Company	Water Desalination Using Multi-Phase Turbo-Expander	Kimberly Hammer
				Ohio University	Advanced Integrated Technologies for Treatment and Reutilization of Impaired Water in Fossil Fuel-Based Power Plant Systems	Jason Trembly
10:00 AM	**MORNING BREAK**					
10:30 AM	13	Water Treatment and Reuse	Jessica Mullen	University of Illinois	An Integrated Supercritical System for Efficient Produced Water Treatment and Power Generation	Seyed Dastgheib
				Research Triangle Institute	Fouling-Resistant Membranes for Treating Concentrated Brines for Water Reuse in Advanced Energy Systems	Zachary Hendren
11:30 AM	**LUNCH** (On Your Own)					
1:00 PM	14	Water Treatment and Reuse	Maria Reidpath	Research Triangle Institute	Low-Energy Water Recovery from Subsurface Brines	Young Chul Choi
				Southern Research Institute	Treatment of Produced Water from Carbon Sequestration Sites for Water Reuse, Mineral Recovery and Carbon Utilization	James Irvin
				University of Pittsburgh	Development of Membrane Distillation Technology Utilizing Waste Heat for Treatment of High Salinity Wastewaters	Radisav Vidic
2:30 PM	**AFTERNOON BREAK**					
3:00 PM	15	Innovative Energy Concepts	Jason Hissam	University of Nebraska	Vertically-Aligned Carbon-Nanotubes Embedded in Ceramic Matrices for Hot Electrode Applications	Yongfeng Lu
				University of Texas at El Paso	High Temperature High Velocity Direct Power Extraction Using an Open Cycle Oxy Combustion System	Manuel Hernandez
				University of Washington	Precursor-Derived Nanostructured Silicon Carbide Based Materials for Magnetohydrodynamic Electrode Applications	YiHsun Yang
				University of Idaho	Boride Based Electrode Materials with Enhanced Stability under Extreme Conditions for MHD Direct Power Extraction	Krishnan Raja

2016 CROSSCUTTING RESEARCH AND RARE EARTH ELEMENTS PORTFOLIOS REVIEW

FRIDAY APRIL 22

7:30 AM — **REGISTRATION** – Grand Station Foyer **CONTINENTAL BREAKFAST** – Grand Station 3–5

TRACK A – Grand Station 1& 2

Time	Breakout Session Number	Breakout Session Title	Moderator	Organization	Presentation Title	Presenter
8:30 AM	16	Computational Materials Modeling	Charles Miller	Purdue University	Predicting Microstructure-Creep Resistance Correlation in High Temperature Alloys Over Multiple Time Scales	Vikas Tomar
				Pennsylvania State University	Computational Design and Discovery of Ni-Based Alloys and Coatings: Thermodynamic Approaches Validated by Experiments	Bicheng Zhou
				Ames National Laboratory	Computational System Dynamics (Computational Design of Multiscale Systems)	Richard LeSar
10:00 AM	MORNING BREAK					
10:30 AM	17	Multifunctional Materials	Sydni Credle	University of Tennessee	Developing Novel Multifunctional Materials for High-Efficiency Electrical Energy Storage	Feng-Yuan Zhang
				Clark Atlanta University	Engineering Accessible Adsorption Sites in Metal Organic Frameworks for CO_2 Capture	Saki Golafale
11:30 AM	ADJOURN					

TRACK B – Admiral Room

Time	Breakout Session Number	Breakout Session Title	Moderator	Organization	Presentation Title	Presenter
8:30 AM	16	Multiphase Flow	Mehrdad Shahnam			
				Florida International University	Development of Reduced Order Model for Reacting Gas-Solids Flow Using Proper Orthogonal Decomposition	Sohail Reddy
				University of Texas at San Antonio	Use of an Accurate DNS Method to Derive, Validate and Supply Constitutive Equations for the MFIX Code	Yifei Duan
10:00 AM	MORNING BREAK					
10:30 AM	17	Process Efficiency and Heat Utilization	Jessica Mullen	Carnegie Mellon University	Evaluating the Techno-Economic Feasibility of Forward Osmosis Processes Utilizing Low Grade Heat: Applications in Power Plant Water, Wastewater, and Reclaimed Water Treatment	Meagan Mauter
				Idaho National Laboratory	The COHO – Utilizing Low-Grade Heat and Carbon Dioxide at Power Plants for Water Treatment	Aaron Wilson
11:30 AM	ADJOURN					

Track A – Monday, April 18, 2016

04-18-2016 – 10:30A
FWP-AL-14-510-075 - The SMARTER Project (Science of Multicomponent Alloys: a Roadmap for Theoretical and Experimental Research)
Ames National Laboratory Presenter: Matthew J. Kramer

ABSTRACT

Near equiatomic alloys (NEAs) have of a high degree of chemical disorder in a single high-temperature (T) phase leading to high mechanical strength. These disordered alloys have potential for fossil energy in high-T applications; however, the long-term stability in harsh combustion environments remains to be explored. We propose a new methodology to speed the discovery and optimization of these chemically complex alloys and leverage our theoretical and experimental capabilities for assessing their long-term stability. HEAs are known to form high-strength intermetallic solid solutions in transition-metal systems. We propose developing alloys with graded microstructures, with the alloy bulk comprising of an intermetallic dispersed terminal solid solution that provides strength and toughness, transitioning into a high-entropy surface, which provides excellent oxidation resistance and hardness. The alloy design and selection will precede using our hierarchical approach but with a significantly different toolset. Initial screening of potential systems will be carried out using an extended Miedema model that was developed as a part of a prior NETL funded project. For solid solutions with high configurational entropy, the standard DFT methods using large supercells has difficulty in dealing with the inherent chemical disorder and possible magnetic disorder. Hence, we will use the DFT Green's function code to address stability and electronic properties of HEA We will then test optimized alloys for phase stability and oxidation resistance. Initial studies are focused on validation of this approach using AlNiFeCrCo and ZrNbHf alloys as model materials using thermogravimetry and in-situ studies on phase stability.

04-18-2016 – 11:00A

FE0011550 - An Integrated Study on a Novel High Temperature High Entropy Alloy

Southern University and A&M College Presenter: Shizhong Yang

ABSTRACT

The high temperature high entropy alloys (HEAs), such as MoNbTaW and MoNbTaVW, show considerable promise to have higher operating temperature, good mechanical properties at high temperature, major improvement in high temperature oxidation resistance and structure stability. The recent advance on oxide dispersion strengthened (ODS) refractory alloy verified the idea that impurities within the crystal can act as pinning centers for dislocations. In this project, we investigated an ODS HEA having good low temperature mechanical property and high temperature oxidation resistance. To save time and expense, we integrate computation with experiment work to avoid trial and error.

Recently, we designed, synthesized, and characterized two senary refractory HEAs MoNbTaTiVW and HfNbTaTiVZr. Both have a BCC single phase, and the lattice constant, density, and micro-hardness are similar. The advance on HEAs MoNbTaVW, HfMoNbTaTiZr modeling and computer simulation, ODS HEA simulation, and experiment results along with the near future works will be introduced.

Graduate students Cheng Guo, Xiaoping Wang, Lokesh Chilla, Yan Yang, and a postdoc Liuxi Tan are trained to maintain, develop, and test the materials design code, sample synthesis and characterization.

Acknowledgement: This research is supported by the DOE under grant DE-FE0011550 with Jessica Mullen and Steven Markovich as the program managers. We thank Mrs. Harolynne Blackwell for her assistance. Special thanks are given to prof. S. Guo and his student B. Zhang for sample preparation and characterization and LONI Institute for HPC time allocation.

04-18-2016 – 13:00A
FEAA118 - Weldability of Creep-Resistant Alloys for Advanced Fossil Power Plants
Oak Ridge National Laboratory 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 micro-scale phenomena and finite element analysis for micro-scale to meso-scale simulation. The progress of integrated model development will be presented.

04-18-2016 – 13:30A
FE0024027 - Modeling Long-term Creep Performance for Welded Nickel-base Superalloy Structures for Power Generation Systems
GE Global Research Presenter: Chen Shen

ABSTRACT

We aim to develop physical models of heterogeneous material structures and properties for predicting long-term creep performance for nickel-base superalloy weldments in high temperature power generation systems. The methodology will be demonstrated on a gas turbine combustor liner weldment of Haynes 282 alloy. We will report the progress on: (1) microstructure-property relationships under creep conditions and microstructure characterization, (2) modeling inhomogeneous microstructure in the welded 282, (3) modeling mesoscale plastic deformation, and (4) a constitutive creep model that accounts for weld and base metal microstructure and their long term evolution. The developed modeling technology is aimed to provide a more efficient and accurate assessment of a material's long-term performance compared with current testing and extrapolation methods. This modeling technology will also accelerate development and qualification of new materials in advanced power generation systems.

04-18-2016 – 14:00A
FEAA116 - Corrosion Issues in Advanced Coal-Fired Boilers
Oak Ridge National Laboratory Presenter: Bruce A. Pint

ABSTRACT

As the ageing U.S. coal fleet is replaced with the next generation of coal-fired boilers, corrosion issues are being investigated that impact both current supercritical technology and the advanced ultra-supercritical (A-USC) concept. Three issues are being investigated: (1) To mitigate problems with steamside scale exfoliation, shot peening has been widely adopted as a technique to prevent the formation of large oxide flakes. To quantify the shot-peening benefit, specimens of commercially shot-peened 304H tube are being exposed to 1bar steam at 600°-650°C. Oxide thickness results on the first tube up to 10,000h are presented showing the benefit of shot peening compared to the thicker oxide formed on the cut faces of these specimens. Interestingly, the machined tube outer diameter showed a similar benefit as shot peening on the tube inner diameter. This observation reflects some of the difficulty in doing steam oxidation testing on austenitic steel. Specimens from a second commercially shot-peened tube also are presented. (2) Stress corrosion cracking (SCC) of creep strength enhanced ferritic steels (e.g. Grades 23, 24, 91 and 92) is being studied at 200°C for waterwall applications (2.25Cr steels for current boilers and 9Cr steels for A-USC boilers) where it has caused problems during plant startups in recent years. The next phase of testing will be done in a controlled water chemistry loop with constant oxygen levels, which is currently under construction. (3) The effect of pressure on steam oxidation at 550°C is being investigated in order to bridge the gap between laboratory and field exposures.

04-18-2016 – 15:00A
FE0026299 - A New Superalloy Enabling Heavy Duty Gas Turbine Wheels for Improved Combined Cycle Efficiency
GE Global Research Presenter: Richard DiDomizio

ABSTRACT

The drive to increase combined cycle turbine efficiency from 62% to 65% for the next-generation advanced cycle requires a new heavy duty gas turbine wheel material capable of operating at 1200°F and above. Current wheel materials are limited by the stability of their major strengthening phase (gamma double prime), which coarsens at temperatures approaching 1200°F, resulting in a substantial drop in strength. More advanced gamma prime superalloys used in jet engine turbine disks, are also not suitable due to the size requirements of gas turbine wheels. The gamma prime phase overages during the slow cooling rates inherent in processing thick-section gas turbine wheels. This program will address this need by screening two alloy design concepts. The first concept will take advantage of a gamma prime/gamma double prime coprecipitation reaction. Through manipulation of alloy chemistry, coprecipitation may be controlled such that gamma double prime is used only as a means to slow the growth of gamma prime during slow cooling, preventing over-aging, and allowing for subsequent aging to maximize strength. In parallel, phase field modeling will provide fundamental understanding of the coprecipitation reaction. The second concept will use oxide dispersion strengthening to improve on two existing alloys that exhibit excellent hold time fatigue crack growth resistance, but have too low a strength to be considered for gas turbine wheels. Mechanical milling will force the dissolution of starting oxide powders into the metal matrix allowing for the solid state precipitation of new, nanometer scale oxides that are effective at dispersion strengthening.

04-18-2016 – 15:30A
FWP49943 - Development of Nondestructive Evaluation (NDE) Methods for Structural and Functional Materials
ANL - Argonne National Laboratory Presenter: Jiangang Sun

ABSTRACT

Nondestructive evaluation (NDE) methods are being developed for thermal barrier coatings (TBCs) applied on hot-gas-path components in advanced high-efficiency and low-emission gas turbines, including syn-gas fired turbines. A TBC system consists of a thermally insulating ceramic topcoat (the TBC) typically made of yttria stabilized zirconia, a thin oxidation-resistant metallic bond coat, and a metal substrate. As TBCs become "prime reliant," it becomes important to know their conditions nondestructively to assure the reliability of these components. NDE methods may be used to assess the quality of new coatings, identify defective components that could cause unscheduled outages, monitor degradation rates during engine service, and provide data for reaching rational decisions on replace/repair/re-use of components. For these applications, the primary NDE method developed under this project is the pulsed thermal imaging – multilayer analysis (PTI-MLA) method. PTI-MLA may quantitatively measure the distributions of important TBC properties such as thermal conductivity and thickness over the entire coated component surface. While it has been extensively validated for single-layer coatings, work is underway to extend MLA for more complex coating systems including multiple coating layers and thin substrates that are common in many engine components. Besides the analytical developments, PTI-MLA has also been evaluated for experimental data generated from a low-cost, room-temperature infrared camera. This development may significantly reduce the cost of current PTI NDE systems and therefore expand the use of this technology in the industry. This presentation describes these recent developments and experimental results.

04-18-2016 – 16:00A
FE0024120 - Predicting the Oxidation/Corrosion Performance of Structural Alloys in Supercritical CO_2
Electric Power Research Institute Inc. Presenter: Steve Kung

ABSTRACT

Supercritical CO_2 (s CO_2) Brayton cycles are being considered for future fossil energy systems. These s CO_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. This objective will be accomplished through short-term, isothermal laboratory testing of structural candidate alloys at high temperatures (>700°C) and pressures (200bar and higher), and the modification of an existing mathematical model for oxide growth and exfoliation. This model was originally developed for structural alloys in service in high-temperature, high-pressure steam and has been validated against field data in utility steam generators. The formation of oxides, the potential for carburization, and propensity for oxide exfoliation in supercritical CO_2 is being examined through laboratory testing. The process of oxide growth (and exfoliation) is being modeled under realistic geometries expected in heat-exchange surfaces and used to predict long-term material performance. Based on these results, confirmatory tests will be conducted to assess the model results and provide a basis for materials selection in advanced s CO_2 power cycles.

04-18-2016 – 16:30A

FE0011194 - Experiments and Model for Serration Statistics in Low-Entropy, Medium-Entropy, and High-Entropy Alloys

University of Illinois at Urbana Champaign Presenter: Karin Dahmen and Peter Liaw

ABSTRACT

High-entropy alloys (HEAs) are new alloys that contain five or more elements in roughly-equal proportion. We present new experiments and theory on the deformation behavior of HEAs under slow stretching (straining), and observe differences, compared to conventional alloys with fewer elements. For a specific range of temperatures and strain-rates, HEAs deform in a jerky way, with sudden slips that make it difficult to precisely control the deformation. An analytic model explains these slips as avalanches of slipping weak spots and predicts the observed slip statistics, stress-strain curves, and their dependence on temperature, strain-rate, and material composition. The ratio of the weak spots' healing rate to the strain-rate is the main tuning parameter, reminiscent of the Portevin-LeChatellier effect and time-temperature superposition in polymers. Our model predictions agree with the experimental results. The proposed widely-applicable deformation mechanism is useful for deformation control and alloy design.

Track B – Monday, April 18, 2016

04-18-2016 – 10:30B
FE0009843 - Robust Ceramic Coaxial Cable Down-Hole Sensors for Long-Term In Situ Monitoring of Geologic CO_2 Injection
University of Missouri System Presenter: Runar Nygaard

ABSTRACT

Subsurface geologic formations offer a potential location for long-term storage of CO_2. However before this technology can be widely distributed, the injected CO_2 has to be accounted by advanced monitoring technology to optimize the injection processes and forecast the fate of the injected CO_2. Due to the complexity, no single data type is sufficient by itself; different monitoring and characterization approaches are deemed to be necessary. In situ down-hole monitoring of the state parameters (e.g., pressure, strain, temperature, etc.) provides critical and direct data points to validate the models, optimize the injection scheme, detect leakage and track the plume. Yet current down-hole sensors are insufficient to meet the reliability and cost requirements. This project has developed robust coaxial cable sensors (CCS) for remote measurement of temperature, pressure, and strain in a high-temperature, high-pressure down-hole harsh environment. The developed high-performance sensor and instrumentation is expected to have maintenance-free operation and dense-multiplexing capability for cost reduction. Integrate sensor data with the geological models for intelligent sensor deployment/installation, rational interpretation of the sensor outputs, and improved accuracy of plume tracking, optimized CO_2 injection, and sensor-verified model predictions. The project has characterized the performance and demonstrated the critical functions of the developed sensors and instrumentation for down-hole applications in relevance to CO_2 sequestration monitoring.

04-18-2016 – 11:00B
FE0012370 - High-Temperature Sapphire Pressure Sensors for Harsh Environments
University of Florida Presenter: Justin Kiehne

ABSTRACT

This project will demonstrate advanced manufacturing technologies for sapphire-based, high temperature pressure sensors. Picosecond laser micromachining and spark plasma sintering will be used to achieve this goal. Project objectives include identifying laser ablation process variables, the characterization (and mitigation) of thermo-mechanical damage via the manufacturing process, and the development of cost/energy efficient procedures for rapid joining of components. The final result will be a fully packaged sapphire optical sensor capable of deployment in gas turbine applications at temperatures in excess of 1000°C and pressures up to 1000 psi.

04-18-2016 – 13:00B

FE0022993 - Robust Metal-Ceramic Coaxial Cable Sensors for Distributed Temperature Monitoring in Fossil Energy Power Systems

University of Cincinnati Presenter: Adam Trontz

ABSTRACT

This project aims 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 in gases relevant to coal-based power plants. The project has concluded Phase-1 with the successful construction of the MCCC-FPI sensor using a stainless steel tube and a stainless steel wire as the outer and inner conductors, respectively, an α-alumina tube as insulator, and air gaps (or grooves) carved into the alumina tube insulator along the cable to serve as weak reflectors. The thus fabricated single point (i.e. single pair of air groove refractors) MCCC-FPI sensors have been demonstrated with desirable resolution for high temperature measurements (up to 500°C) using microwave interferometric signals in a frequency range of 2–8 GHz. Based on the demonstration of single pint FPI sensor, a three-point MCCC-FPI sensor has been constructed and demonstrated its functionality for temperature monitoring with spatial recognition. These research findings show promise for further developing multipoint FPI sensors in a single-cable to achieve in situ and continuous measurement of spatially distributed temperature in harsh environments.

04-18-2016 – 13:30B

FE0012274 - Reduced Mode Sapphire Optical Fiber and Sensing System

Virginia Polytechnic Institute and State University Presenter: Daniel Homa

ABSTRACT

The objective of this three-year project is to develop a Raman scattering based distributed temperature sensing system which utilizes a micro-structured sapphire fiber sensor with a low modal volume (LMV). The primary goals of the research include the creation of a comprehensive understanding of (1) modal propagation in single crystal sapphire fibers with novel geometries, (2) the materials and processing science of the hot wet-acid etching of single crystal sapphire fibers, (3) the Raman backscattering phenomena in sapphire fibers, and (4) the optical fiber interrogation schemes for distributed temperature sensing. To meet the goals and objectives, theoretical modeling was performed for a wide array of fiber designs and the optical transmission, numerical aperture, and waveguide intensity profiles of commercial and reduced diameter single crystal (SC) sapphire fibers were measured. Furthermore, the temperature dependence of the Raman Stokes and Anti-Stokes line intensities, frequency shifts and linewidths was characterized and a prototype sapphire fiber Raman Distributed Temperature Sensing System was successfully demonstrated in a laboratory environment. The successful completion of the project will enable the real-time, accurate and reliable monitoring of temperatures at distributed locations of sensors for harsh conditions and overcome the harsh environment challenges that severely limit the integration of mature optical fiber sensing technologies in new power plant control systems. The technologies are expected to lower operating costs by allowing more accurate measurement of the conditions inside a gasifier or boiler to better control their operation.

04-18-2016 – 14:00B
FE0023031 - Distributed fiber sensing systems for 3D combustion temperature field monitoring in coal-fired boilers using optically generated acoustic waves
University of Massachusetts at Lowell, University of Connecticut, and General Electric
Presenter: Jingcheng Zhou

ABSTRACT

This presentation presents a novel distributed optical fiber sensing system for the real-time monitoring of spatial and temporal distributions of high temperature profiles in the boiler of fossil fueled power plants. According to the principle of acoustic pyrometer system, the speed of the acoustic waves depends on the temperature of gaseous medium. Photoacoustic material coated optical fiber sidewalls will generate acoustic waves. Fiber Bragg gratings (FBG) which can be multiplexed within one optical fiber will be used to detect acoustic waves. Code division multiple access (CDMA) modulation method will be used to modulate the signal. A 3D temperature distribution profile will be reconstructed using Gaussian Radial Basis Functions (GRBF) based on the sparse measurement data.
At this point, a sidewall ultrasound generator has been fabricated and tested in the lab. FBG sensors have been characterized. This optical fiber sensing system has been used to measure the temperature in water and aluminum plate. CDMA modulation algorithm has been developed. The temperature distribution reconstruction algorithm has been improved. The field test in Alston is planning to start in April 2016.

04-18-2016 – 15:00B
Functional Material Enabled Fiber Optic Sensors for High Temperature, Harsh Environment Sensing
National Energy Technology Laboratory Research & Innovation Center
Presenter: Paul Ohodnicki

ABSTRACT

Functional material enabled fiber optic sensors and associated enabling technologies are under investigation. The goal of the effort is to develop and demonstrate sensor materials and sensor devices which are capable of providing in-situ process information in power generation systems and CO_2 sequestration applications including temperature, strain, and gas-phase chemistry. A particular emphasis is being placed on (1) functional sensor thin film materials for chemical sensing and (2) high temperature stable materials for the optical fiber device platform. Advanced interrogation approaches such as the application of optical backscattering reflectometry for distributed sensing is also being pursued to enable distributed sensing internal to power generation processes and within geological formations for CO_2 sequestration applications. Embedding of sensors through additive manufacturing techniques is also being explored in conjunction with university partners and the latest research results in this area will also be presented and discussed.

04-18-2016 – 15:30B
Creep Optimization in Haynes 282 Through Gamma Prime Coarsening Control: Preliminary Results
National Energy Technology Laboratory Research & Innovation Center
Presenter: Jeffrey Hawk

ABSTRACT

Haynes 282 has been proposed for Advanced Ultra Supercritical (A-USC) energy applications. Haynes 282 is a gamma prime strengthened nickel superalloy that also contains various carbide phases. The alloy has good high temperature strength and excellent creep resistance. However, components for use in A-USC conditions must also be microstructurally stable for long times (i.e., 100,000 hours). This presentation highlights the important strengthening features in Haynes 282 through use of TEM and ThermoCalc modeling, and then speak to its long-term stability (i.e., gamma prime and carbide coarsening) based on microstructures from various selected creep tests as well as from isothermal exposure experiments through 20,000 hours. Gamma prime coarsening in two Haynes 282 variants (designated Haynes 282B and 282C) have been determined. The main difference between these alloy variants is the Ti to Al ratio. In addition, the development of clearly identifiable phases within the microstructure is also followed from initial formation through 20,000 hours of exposure for these two variants. Also, creep tests of the two Haynes 282 variants is ongoing results are available for five test temperature/stress conditions. In general, Haynes 282B coarsens at a slower rate than does Haynes 282C. Through the creep tests to date, it appears that Haynes 282B also possesses a longer creep life than does Haynes 282C for the tests concluded to date.

04-18-2016 – 16:00B
Laser induced breakdown spectroscopy (LIBS) for subsurface measurements
National Energy Technology Laboratory Research & Innovation Center
Presenter: Dustin McIntyre

ABSTRACT

The goal of this project was to better understand the use of laser induced breakdown spectroscopy (LIBS) for underwater elemental concentration measurements. LIBS is the use of short time scale laser pulses to produce plasma emission whereby the light can be used to characterize the elemental species and their concentrations. The laboratory experimentation involved the investigation of the measurability of common elements present in subsurface fluids, how other elements affect their measurement characteristics, and how temperature, pressure, and pH all affect the use of LIBS to produce accurate measurements of elemental concentrations. Successful linear measurements were made of Li, Ca, K, Mg, and Sr over wide concentration ranges. The effect of high concentrations of Na on the measurement ability of the other elements was studied and found to produce enhancements of the atomic emission. Temperature was found to have a negligible effect over our test ranges (24-50C) however pressurization did show a significant suppression of the atomic emission. Accurate measurements were still able to be made up to 5250 psi. The final experimental investigation involved the exposure of a $CaCO_3$ wafer to varying levels of CO_2 pressurization of the fluid. Accurate measurements of the Ca concentration as a function of the CO_2 pressure (effectively pH) were made.

04-18-2016 – 16:30B
NETL Advanced 9% Cr Steel: Update and Current Development Status
National Energy Technology Laboratory Research & Innovation Center
Presenter: Jeffrey Hawk

ABSTRACT

Alloys used in fossil energy power generation must be stable for extended times with some components having expected lifetimes of up to 30 years. For steam turbines, in particular, the component life of the rotor and the rotor casing is equivalent to the expected life of the steam turbine. As such, any alloy used for these components must have a relatively stable microstructure that evolves slowly during the expected life of the steam turbine. For temperatures in excess of 600°C, advanced 9% Cr steels are used. The 9% Cr steels possess martensitic structure and are strengthened by a variety of mechanisms. Microstructural stability is provided by a 3-dimensional network of carbide that hold together the many structural sub-elements during use. As such the approach used at NETL to design and manufacture heat resistant 9% Cr steels for creep strength and microstructure stability is discussed with the results on 9% Cr steel in both wrought and cast forms presented. In particular, tensile mechanical behavior is discussed with emphasis on creep capability. In addition, the NETL 9% Cr steel's resistance to hot fireside corrosion and steam oxidation will be discussed in detail and compared against similar results from commercial and developmental 9% Cr steels. Similarities and differences between the wrought and cast versions of the alloy will be discussed. General aspects of the microstructure will be shown.

Track A – Tuesday, April 19, 2016

04-19-2016 – 08:30A
FE0024014- Benefits of HIP/PM & AM to Fabricate Advanced Energy System Components
Energy Industries of Ohio Inc. Presenter: Nancy Horton & Roy Sheppard

ABSTRACT

Advanced Energy systems require large, complex components produced from materials capable of withstanding severe operating environments. Such parts can be difficult to source, as conventional material processing technologies must be tailored to ensure a safe and cost effective approach to large-scale manufacture of quality structural advanced alloy components that meet AE performance specifications.

Hot Isostatic Pressure of Powdered Metal (HIP/PM) has shown advantages over other manufacturing methods when working with these materials, including significant savings in raw material costs, overcoming difficulties resulting from reactivity of these materials in the molten state and eliminating time and expense of post processing machining and weld repair by producing a part that is defect and porosity free.

New advances in Additive Manufacturing (AM) make it possible to further expand the benefits of HIP/PM to create an even more robust manufacturing approach. Traditional techniques for producing HIP canisters can be time consuming and costly, with limitations on the complexity of part which can be achieved. Use of AM could overcome such challenges, ultimately enabling redesign of complete energy systems.

Using Haynes 282, a high nickel alloy of interest to the Fossil Energy community, particularly for Advanced-UltraSuperCritical operating environments, and ExOne's binderjet technology, the fastest metal 3D printing technique on the market at the current time, this research is pursuing three new methods of manufacturing these advanced alloys: 1) Directly built AM parts; 2) AM cans for HIP/PM; and 3) AM cans produced in the final part material. Partners include Carpenter, ExOne and Bodycote.

04-19-2016 – 09:00A

FE0023974 - Additive Manufacturing of Fuel Injectors

Edison Welding Institute, 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.

04-19-2016 – 09:30A

FE0024090 - High Temperature Ceramic Heat Exchanger for Solid Oxide Fuel Cell

Mohawk Innovative Technology, Inc. Presenter: Jose Luis Cordova

ABSTRACT

A ceramic heat exchanger with high effectiveness and low-pressure drop is being developed for application as a cathode air preheater for a Solid Oxide Fuel Cell (SOFC). At the operating conditions of SOFCs, typical metallic alloys as those used in commercial heat exchangers may undergo chromium volatilization, which is a known cathode degradation mechanism that reduces SOFC performance and life. Use of ceramics such as alumina or alumina-silicate instead of chromium-containing metal is one approach to eliminate the effects of chromium on the SOFC cathode. This project leverages the geometric design of a heat exchanger previously prototyped and tested, and demonstrated to have a nearly constant heat transfer effectiveness of 92% with low pressure drop, to fabricate a novel heat exchanger made from a ceramic material. 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). The integration of the ceramic heat exchanger prototype is nearing completion, and it will subsequently be subjected to pressure drop and heat transfer effectiveness testing.

04-19-2016 – 10:30A
FE0023040 - Post Combustion Carbon Capture Using Polyethylenimine (PEI) Functionalized Titanate Nanotubes
Prairie View A&M University Presenter: Melisa L. Stewart

ABSTRACT

The goal of the research is to develop a solid adsorbent to capture carbon dioxide (CO_2) emitted through post-combustion flue gas from coal fired power plants. This adsorbent is anticipated to be a replacement or an addition to the current aqueous amine absorbent which is being used for CO_2 capture. This would assist in the efforts to reduce the greenhouse gas; CO_2 emitted to the atmosphere and reduce the negative impacts on the environment and climate change.
When developed, this adsorbent could bring about great cost savings such as energy and pipe replacements costs that are incurred by current amine absorption technology being used for CO_2 capture in the carbon capture and sequestration process.

Our current work had been successful with the wet impregnation of polyethyleneimine (PEI) onto synthesized titanate nanotubes. This was confirmed though X-Ray diffraction, scanning electron microscopy and transmission electron microscopy. From these analyses, it was found that the nano-tubular structures were achieved with hydrothermal synthesis, dilute acid wash and DI water wash. The nanotubes were maintained after PEI was loaded. The diameter of nanotubes is in nanometers (nm) and the length of nanotubes is in the range of several hundred nm and varied with the synthesis temperatures. The CO_2 adsorption capacity of the adsorbent was tested using our customized experimental set up. A numerical model to simulate the CO_2 adsorption from CO_2/N2 mixture in a fixed bed is being developed. The simulation was performed using ANSYS. Variation of adsorption capacity as a function of velocity, temperature and pressure is determined.

04-19-2016 – 11:00A
FE0011245 - Reduced Cost Bond Layers for Multi-Layer Thermal / Environmental Barrier Coatings
Auburn University Presenter: Jeffrey Fergus

ABSTRACT

The major goal of the project is to improve the resistance of thermal barrier / environmental barrier coating systems to calcium-magnesium-aluminum-silicon oxide (CMAS) corrosion. The project addresses this goal in two ways. One is to investigate an alternative bond coat system and the other is to investigate alternative environmental barrier coating materials. This presentation will focus on the latter objective. Specifically, results on the reaction of pyrochlore lanthanide zirconate materials with CMAS will be presented. The extent of reaction and nature of the reaction product are important to the durability of the coating under conditions in which debris is injected into gas turbine engines.

04-19-2016 – 13:00A

FE0011247 - Rational Design of Mixed-Metal Oxides for Chemical Looping Combustion of Coal Via Computational Experimental Studies

North Carolina State University Presenter: Fanxing Li

ABSTRACT

The current project seeks to rationalize oxygen carrier design strategies for the chemical looping with oxygen uncoupling (CLOU) process. In a CLOU process, lattice oxygen from a transition metal oxide based oxygen carrier is spontaneously released into the gas phase for solid fuel combustion. In a subsequent step, the oxygen-deprived metal oxide is regenerated with air, releasing heat. The ability for oxygen release during the fuel combustion steps allows improved combustion kinetics when compared to conventional chemical looping processes. Moreover, heat integration for the process can be simplified.

In this presentation, perovskite-structured oxygen carriers with a general formula of AxA'1-xMnyB1-yO3-δ (A/A' = Sr, Ca, Ba; B = Al, V, Fe, Co, Ni) are reported for CLOU applications. Results indicate $CaMnO_3$ provided satisfactory oxygen uncoupling ability; 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 reactivity. Sr doped and Fe doped $CaMnO_3$ exhibited superior stability and solid fuel combustion kinetics. Density Functional Theory (DFT) calculations were also carried out to interpret the experimental data and to guide further optimization of the mixed-oxide based oxygen carrier particles for CLOU applications.

04-19-2016 – 13:30A

FE0023541 - Novel Silica Nanostructured Platforms with Engineered Surface Functionality and Spherical Morphology for Low-Cost High-Efficiency Carbon-Capture

Delaware State University Presenter: Nicholas Pizzi

ABSTRACT

The project aims to develop a silica nanosphere platform as solid sorbent for post-combustion CO_2 capture in fossil-fired plants. The spatial arrangement prerequisite toward stable CO_2 capture demands two amine groups proximity. This will be achieved by rationally designing the amine functionalization toward spatially-controlled, high amine coverage. In addition, the project aims to enrich the capability of this platform by adding a gate-keeping polymeric layer (corona) on the surface of nanospheres toward rendering it nitrogen-phobic and thus, directing its selectivity to CO_2 capture.

Objectives are: 1. Demonstrate a nanosheets-made silica nanosphere (NSN) platform as solid sorbent with spatial control of CO_2 capture amine functionality and high amine loading at least 7 mmol N/g sorbent, with hybrid absorption–adsorption capacity of at least 5 mmol CO_2 per gram of NSN sorbent; 2. Perform parametric and long-duration tests to demonstrate performance target of CO_2 capture at >90% of simulated flue gas with 15% CO_2; 3. Engineer a gate-keeping polymeric layer on NSN surface (PolyNSN), designed to increase CO_2 capture selectivity of by excluding N2 from in the capture process; 4. Perform parametric and long-duration tests to demonstrate proof-of-concept of nitrogen exclusion in selective CO_2 capture in PolyNSN.

We aim to develop a fabrication technology for silica nanospheres with high CO_2 capture capacity at low-cost and with high recyclability, and a subsequent coated platform with enhanced nitrogen selectivity. The technology is applicable to other sectors such as operation of alkaline fuel cells. The project involves training students in materials science and carbon capture.

04-19-2016 – 14:00A

FE0008864 - HVOF Thermal Spray TiC/TiB2 Coatings of AUSC Boiler/Turbine Components for Enhanced Corrosion Protection

Southern Illinois University Presenter: Chung-Ying Tsai

ABSTRACT

Supercritical Rankine cycles facilitate the attainment of higher efficiencies and lowered emissions. The high temperatures and enhanced reactivity of supercritical water still pose significant risk of degradation and fatigue from oxidizing, corroding and eroding environment. In addition, ash particulates and unburnt carbon and pyritic sulfur can cause erosion of the surface and thus loss of material. Unburnt carbon and pyritic sulfur may also cause localized reduction sites TiC and TiB2 are suitable coating alternatives on account of the material features such as the high hardness, the high melting point, the high strength, low density and chemical stability required for long-term service. The paper presents the research endeavors to corrosion resistance performance and characteristics of TiC and TiB2 coatings on various boiler materials for applications at high temperatures (500 -750 °C) and high pressures (~350 bars) using the HVOF process and to demonstrate the feasibility of these coating to be used in AUSC boilers and turbines

04-19-2016 – 15:00A
Internal to External Oxidation Transition Modeling: Plasticity and Coherence Loss
National Energy Technology Laboratory Research & Innovation Center
Presenter: Youhai Wen

ABSTRACT

Structural alloys applied at high temperatures invariably rely on formation of a slowly growing external layer of oxide for the necessary oxidation resistance. An electrochemistry based phase-field model for external oxidation has been developed that shows capability to continuously simulate oxidation kinetics across a wide range of lengths and times. External oxidation is, however, not the only mode for alloy oxidation. In some situations oxidation may proceed predominantly by inward penetration of oxygen through the alloy matrix and new oxide is formed internally with a much faster rate. Understanding internal oxidation and its transition to external oxidation is equally important especially in design of Fe-, Ni- and Co-base structural alloys. Essential issues that may be involved during internal oxidation will be discussed, in particular dilatation caused by oxide particles, plastic deformation and coherency state of the oxide-alloy interfaces, and how they and their interplay can be modeled by phase-field approach.

04-19-2016 – 15:30A
Serrated Plastic Flow in High Entropy Alloys
National Energy Technology Laboratory Research & Innovation Center
Presenter: Joseph Licavoli

ABSTRACT

High entropy alloys are multicomponent systems in which solid solution strengthening effects are maximized. Solid solution strengthening and sluggish diffusion within the alloy impart a combination of strength and resistance to environmental effects which make high entropy alloys appealing for advanced energy systems. As a consequence of their composition, these alloys have demonstrated particular susceptibility to dynamic strain aging effects during tensile tests. The following study examines these effects in several high entropy systems including both single phase and multiphase high entropy alloys. Plausible alloying constituents responsible for dynamic strain aging are identified and discussed. The influence of strain rate and temperature on the cumulative distributions function of stress drops are also presented. Dynamic strain aging can have negative impacts on an alloy's ductility as well as the aesthetic appearance of sheet products. This study helps to identify potential remediation methods and enhance the general understanding of deformation in FCC high entropy systems.

04-19-2016 – 16:00A
Hybrid Performance Project
National Energy Technology Laboratory Research & Innovation Center
Presenter: David Tucker

ABSTRACT

The Hybrid Performance (Hyper) project facility at NETL incorporates a cyber-physical approach to characterization of novel power cycles still in preliminary development. This facilitates the discovery of new opportunities, system identification methodologies, and controls development, all of which substantially accelerate future technology adoption. The Hyper facility has been used to evaluate fuel flexibility and degradation in fuel cell turbine hybrids, and, through collaboration with Ames National Laboratory, used to develop biomimetic and multivariable control methods on hardware. Collaborations with other labs, universities, and industry have resulted in several joint publications.

04-19-2016 – 16:30A
IPT – Direct Power Extraction
National Energy Technology Laboratory Research & Innovation Center
Presenter: Rigel Woodside

ABSTRACT

Direct Power Extraction (DPE) refers to the direct conversion of the thermal or kinetic energy in a fluid to useable electrical power. A known approach for achieving DPE is through the use of a device called a magnetohydrodynamic (MHD) generator. NETL's Innovative Process Technologies (IPT) DPE task is focused on generating useful engineering data sets, simulation tools, and materials suitable for MHD generators and their application. Additionally, continued data driven analysis is applied toward assessing and pursuing the technical viability of DPE approaches. For open cycle MHD application, momentum transfer collisional cross sectional data have been collected, reviewed, and summarized for use in electrical conductivity calculations. Experimentation is underway to validate electrical conductivity predictions with a seeded oxy-methane burner and double Langmuir probe. Experimentation is also underway to assess the heat losses in a high velocity oxy-fuel combustor as well as the seed particle behavior in a supersonic flow. Developed CFD simulations are compared to the data. Additionally, 3D modeling of electrical current paths are applied toward understanding non-uniform current transfer in MHD generators. NETL's 1D+ MHD generator design code has been extended, with additional features added like consideration of boundary layer voltage drops. Candidate electrode materials have been fabricated, and are undergoing high temperature exposure testing to potassium. Lastly, novel concepts for DPE are being explored. These include use of photoionization to enhance the process, and use of a dusty plasma instead of a traditional alkali seed.

Track B – Tuesday, April 19, 2016

04-19-2016 – 08:30B
FE0009878 - Development of a CO_2 Chemical Sensor for Downhole CO_2 Monitoring in Carbon Sequestration
New Mexico Institute of Mining and Technology Presenter: Ning Liu

ABSTRACT

The objective of this project is to develop a CO_2 chemical sensor for in-situ monitoring CO_2 movement in carbon sequestration. The proposed CO_2 sensor includes a pair of electrodes, a gas-permeable membrane, a porous stainless steel cup, and a bicarbonate-based internal electrolyte solution. Iridium oxide-based electrode was prepared and used for fabrication the CO_2 sensor. To fabricate the iridium oxide electrode, iridium oxide nanoparticles were first synthesized and then electrodeposited on stainless steel substrate. It was observed that the surface of the deposited iridium oxide film exhibited porous and rough surface morphology. The iridium oxide electrode thus prepared displayed excellent pH sensitivity, obtaining super-Nernstian behavior with pH sensitivity value of -72.6 mV/pH. The CO_2 sensor prepared with the as-synthesized iridium oxide electrode was tested under different high pressures and high salinity solution. A linear correlation was obtained between the CO_2 sensor potential change and CO_2 concentration in water. CO_2/brine coreflooding tests were carried out to evaluate the performance of the CO_2 sensor in simulate CO_2 storage process. The results indicated that the sensor could detect CO_2 movement in the tests. Further studies showed that the sensor could be recovered by brine flooding after CO_2/brine flushed the core. The results of the coreflooding tests demonstrated that the sensor had potential application for CO_2 monitoring in carbon sequestration.

04-19-2016 – 09:00B
FE0013062 - Ultra-High Temperature Thermionic Sensors
Palo Alto Research Center Incorporated Presenter: Scott J. Limb

ABSTRACT

The Harsh Environment Adaptable Thermionic (HEAT) sensor is a technology platform optimized for sustained operation in extreme environments. Rather than attempting to mitigate the effects of high temperature on conventional sensing approaches, HEAT turns a 900-1600C environment into the key enabler for a new class of device that is based on control and measurement of high temperature thermionic emissions. Utilizing a basic thermionic element as a common building block, the HEAT technology can provide in situ sensing of a wide range of relevant process conditions (temperature, pressure, strain, flux, and flowrate). Designs for wireless transmission capability and energy harvesting will be presented along with experimental thermionic sensing results.

04-19-2016 – 09:30B

FE0011300 - Graphene-Based Composite Sensors for Energy Applications

West Virginia University Research Corporation Presenter: Charter D. Stinespring

ABSTRACT

The objectives of this research are to develop and demonstrate the use of graphene-nanoparticle composites as a high sensitivity, rapid response electronic nose for sensing gas species in energy applications. Graphene based device structures suitable for the temperature range of 500 °C - 1000 °C are targeted. The work includes: a) development of procedures for controllable nucleation and growth of nanoparticles on graphene surfaces, b) fabrication graphene-nanoparticle composite sensors, c) measurement of electrical properties of graphene-nanoparticle composites, and d) determination of sensor characteristics in simple mixtures. The graphene films are synthesized on 6H-SiC (0001) surfaces using a halogen based plasma etching process followed by rapid thermal annealing at atmospheric pressure in Ar. Using lithography free methods, simple sensor structures consisting of interdigitated fingers are then deposited on these films. This is followed by the nucleation of either Ag, Au, Pt, or Ir nanoparticles on the graphene surfaces using solution based techniques. The graphene and graphene-nanoparticle composites are characterized by x-ray photoelectron spectroscopy and Raman spectroscopy to establish film quality and characterize defect structures which play a key role in determining the electrical and sensor characteristics of the films. Atomic force microscopy is used to characterize the particle size distribution of the nucleated nanoparticles. Electrical properties of the graphene and graphene-nanoparticle composites are characterized using two and four point current-voltage measurements. This presentation will provide an overview of the research performed to date.

04-19-2016 – 10:30B

FE0011577 - Metal Oxide based Heterostructured Nanowire Arrays for Ultra-Sensitive and Selective Multi-Mode High Temperature Gas Detection

University of Connecticut Presenter: Bo Zhang

ABSTRACT

Using vapor phase and solution phase deposition methods, heterostrutured nanowire arrays have been successfully fabricated composed of metal oxide nanowire cores ~100-200 nm in diameter, ~1-30 nm thick shells of perovskite, metal oxide and noble metal nanoparticles on ceramic planar substrates. The microstructure features can be tuned including density, geometry, and typical dimensions of these core-shell nanowire arrays through varying the deposition temperature, concentration, pH, substrate temperature, time, etc. 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. Specifically the materials-synergy effect in Ga2O3/(La, Sr)FeO3 and ZnO-Au core-shell nanowire array sensors are 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.

04-19-2016 – 11:00B

FE0011235 - Investigation on Pyroelectric Ceramic Temperature Sensors for Energy System Applications

University of Texas at El Paso Presenter: Ricardo Martinez

ABSTRACT

The goal of this project is to develop a low cost, self-powered, temperature sensor for energy system applications. This work includes design, fabrication, and characterization of the sensor as well as testing using a torch and inside a combustor rig. The objectives of the proposed project are: 1) Fabricate and characterize pyroceramic temperature sensor materials, 2) Construct sensing system and demonstrate the wireless temperature sensing capability, and 3) Demonstrate temperature and other properties data transmission and durability at high temperatures and environmental conditions applicable to a coal based system. There exists a strong demand in developing sensors that are reliable, accurate, and yet low cost for these hostile environments. In energy system applications, wireless sensors are drawing increasing attention to overcome the issues associated with wired sensors; however, most of them require built-in electronics, power sources, of which most of them are still high cost. Therefore, this project will be focused on development of sensor system using pyroceramic and inductive coupling technique, where the current generated by pyroceramic upon temperature change will be converted to magnetic flux that is wirelessly detected using an inductance coil.

04-19-2016 – 13:00B

SC0008269 - Advanced Ceramic Materials and Packaging Technologies for Realizing Sensors Operable up to 1800 Celsius in Advanced Energy Generation Systems

Sporian Microsystems, Inc.

Presenter: Jason Fish

ABSTRACT

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

04-19-2016 – 13:30B
SC0011936 - Adaptive Electrical Capacitance Volume Tomography for Real-Time Measurement of Solids Circulation Rate at High Temperatures
Tech4Imaging Presenter: Qussai Marashdeh

ABSTRACT

In this effort, we will build a functional prototype of an AECVT system for mass-flow gauging of solids circulating at high temperatures. The intrinsic high measuring speed of capacitance measuring technology and high resolution capability of Adaptive Electrical Capacitance Volume Tomography (AECVT) technology will enable such mass flow measurements at 5% spatial resolution and 1 Hz temporal resolution. Simulation and preliminary measurement results have verified feasibility of the AECVT architecture.
Advanced power generation technologies that rely on solid circulation for combustion (e.g. chemical looping and combustors), and cracking (e.g. oil refineries and feedstock processes) demand online monitoring of mass-flow rate, flow progression, and distribution. Successful completion of project will provide a prototype of an AECVT system for hot temperature applications in harsh conditions reactors that can be extended to many energy-related applications.

04-19-2016 – 14:00B
SC0010228 - Real-Time 3-D Volume Imaging and Mass-Gauging of High Temperature Flows and Power System Components in a Fossil Fuel Reactor Using Electrical Capacitance Volume Tomography
Tech4Imaging Presenter: Qussai Marashdeh

ABSTRACT

For advanced power generation technologies that rely on solid circulation for combustion, online monitoring of mass-flow rate, flow progression, and distribution is essential. In this project, a demonstration unit of a hot flow ECVT system will be built for quantifying multi-phase flows in hot reactors using capacitance sensors. Successful completion of this project will provide a novel system ready to be deployed in industrial settings under harsh conditions. The pressing demand for such a system has been recognized through the feedback from potential users and customers of the proposed system.

Project tasks here are planned toward a full realization of an ECVT system for hot flow applications in power generation processes, whereas Phase I was focused on testing capacitance sensors at various conditions of temperatures and flow variables to assure soundness of the approach.

04-19-2016 – 15:00B

FE0012299 - Additive Topology Optimized Manufacturing with Embedded Sensing

United Technologies Corporation Presenter: Paul Attridge

ABSTRACT

Ubiquitous sensing is rapidly emerging as a means for globally optimizing systems of systems by providing both real time PHM (prognostics, diagnostics, and health monitoring), as well as expanded in-the-loop control. In closed or proprietary systems, such as in aerospace vehicles and life safety or security building systems; wireless signals and power must be supplied to a sensor network via single or multiple data concentrators in an architecture that ensures reliable/secure interconnectivity. In addition, such networks must be robust to environmental factors, including: corrosion, EMI/RFI, and thermal/mechanical variations. In this talk, we describe the use of additive manufacturing processes guided by physics based models for seamlessly embedding a sensor suite into aerospace system components; while maintaining their structural integrity and providing wireless power, sensor interrogation, and real-time diagnostics. We detail this approach as it specifically applies to industrial gas turbines for stationary land power.

04-19-2016 – 15:30B

FE0012272 - Additive Manufacturing of Smart Parts with Embedded Sensors for In-Situ Monitoring in Advanced Energy Systems

Missouri University of Science and Technology Presenter: Hai Xiao

ABSTRACT

The project aims to develop and demonstrate the novel concept of “smart parts” with embedded sensors for in situ monitoring of the critical parameters in advanced energy systems. The research focuses on solving the fundamental and engineering challenges involved in design, fabrication, integration, and application of the sensor embedded smart parts. Innovative research has been performed on novel optical carrier based microwave interferometric (OCMI) sensors and signal processing, comprehensive thermal and mechanical models of the sensor-integrated smart parts, multifunctional protective layers between the OCMI sensors and the host materials, and additive manufacturing of the smart parts with embedded sensors. The innovative and collaborative research enables a new paradigm for harsh environment sensing, and delivers novel measurement techniques that are directly applicable to equipment health monitoring and process controls in existing and future advanced fossil fuel systems. The groundbreaking technology will become an important enabling factor to achieve the challenging goals of enhanced efficiency, reduced emission, and improved reliability in energy productions.

04-19-2016 – 16:00B

FE0012383 - Smart Refractory Sensor Systems for Wireless Monitoring of Temperature, Health, and Degradation of Slagging Gasifiers

West Virginia University Presenter: Edward M. Sabolsky

ABSTRACT

The objective of the work is to develop smart refractory bricks, with embedded temperature, strain, and spallation sensors throughout volume of chromia refractory brick. The proposed work includes interconnecting sensors to the reactor exterior, where the sensor signals may be processed by low-power electronics and transmitted wirelessly to a central processing hub. The data processing and wireless transmitter are designed to be isolated and adaptable to future implementation of energy-harvesting strategies for extended life. The collected data is validated with a model to estimate refractory degradation. The long-term goal of this program is to demonstrate high-temperature, wireless sensor arrays for in situ three-dimensional refractory monitoring for slagging gasification systems. The research is in collaboration with HarbisonWalker International (HWI) Technology Center. The work completed in the previous year focused on: 1) Investigation of chemical stability, microstructure/grain growth, mixedness, electrical properties of silicide-oxide composites between 750-1450°C; 2) Fabrication of composite thermocouples and thermistors, embed them within chromia refractory bricks. The thermoelectric properties were studied up to 1350°C under slagging conditions; 3) Utilization of commercial off-the-shelf components to prototype circuits for interfacing between smart brick sensors and wireless network. The prototypes were used to design an integrated circuit for smart brick sensor interfacing; 4) Interfacing of the smart bricks with wireless motes, yielding a complete signal chain. This end-to-end data collection system was tested at 1350°C; 5) Development of a slag penetration model and a nonlinear unknown input filter for the data from embedded sensors for estimating temperature and extent of slag penetration.

04-19-2016 – 16:30B

FE0012321 - Investigation of "Smart Parts" with Embedded Sensor for Energy System Applications

University of Texas at El Paso Presenter: Yirong Lin

ABSTRACT

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. In details, 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 research is centered on fabrication and demonstration of the "smart parts" with considerations of overall material property as well as sensing functionalities. The feasibility of using additive manufacturing to fabricate energy system components with embedded piezoceramic sensor will be the foundation of the proposed project thus first initiative under this research. We successfully fabricated the "smart parts" and their pressure and temperature sensing capabilities are demonstrated in the lab scale.

Track A – Wednesday, April 20, 2016

04-20-2016 – 08:30A
FWP-AL-14-450-011 - Engineered complex systems: Development of a cloud-based modeling framework for complex advanced power systems
Ames National Laboratory Presenter: Kenneth "Mark" Bryden

ABSTRACT

To provide for future power consumption needs while meeting higher regulatory standards, low carbon fossil energy advanced power plants are needed. The current advanced power plant concepts being developed are increasingly complex, and tools that enable the holistic design, deployment, and operation of these complex systems are needed. Past integrated modeling efforts have focused on model integration based on developing a single conceptual schema and semantic framework in which the information flow and convergence of boundary conditions between the models are built on a fixed framework. In this talk a novel decentralized approach based on developing federated model sets to support the coordinated sharing and exchange of information between autonomous models will be introduced. As discussed here, a federated model set consists of self-describing information entities (e.g., models, data, and user input); a library that contains the set of available models and manages the model development community; a federation schema that defines the purpose of the federation, describes the models used in the federation, and defines the topology of the federation; and a federation management system that coordinates information transport, convergence of boundary conditions, and error. Development of the federation management system including the needed API and SDK will be discussed.

04-20-2016 – 09:00A
FE0026307 - Evaluation and Demonstration of Commercialization Potential of Carbon Capture Simulation Initiative Tools within gProms Advanced Simulation Platform
Process Systems Enterprise Presenter: Alfredo Ramos Plasencia

ABSTRACT

This project aims to identify market opportunities for the Carbon Capture Simulation Initiative (CCSI) tools combined with existing gPROMS platform capabilities and develop a clear technical plan for the proposed commercialization activities. The research will assess and rank the CCSI tools according to their commercial potential, technical feasibility and technology readiness level when integrated with gPROMS platform capabilities; develop detailed integration plans and commercialization plans for promising tools, drawing on technical expertise from PSE and the project team, as well as our client base and industrial advisory board structures; and research suitable applications across advanced energy systems and further afield (prototypes will be built during Phase 1 to evidence and publicize potential).

Commercialization of the CCSI toolkit by this consortium will contribute to the overall goals of expanding gPROMS capabilities to increase robustness of complex simulations and maintaining state-of-the-art models of promising CCS technologies. In addition, this project will provide opportunity to extend the application of the CCSI toolkit. Finally, success will contribute towards the accelerated development of advanced energy technologies and to the wider scientific community by moving forward the state-of-the-art in dynamic modelling and optimization of novel processes.

04-20-2016 – 10:30A
FE0024077 - Compact Microchannel Heat Exchangers
Ceramatec Inc. Presenter: Charles Lewinsohn

ABSTRACT

Ceramatec has developed innovative microchannel designs and manufacturing methods to produce scalable, cost- effective ceramic heat exchangers with high reliability, high heat transfer efficiency, and low pressure-drop suitable for a variety of power cycle applications. In addition to high effectiveness, excellent creep resistance, and ease of manufacturing, ceramic heat exchangers can be fabricated from materials with significantly lower cost, per kilogram, than nickel-based alloys. Ceramatec uses a modular approach to assembling ceramic heat exchangers that scales easily for both a wide variation in size, capacity and temperature. The Colorado School of Mines has analyzed specific requirements for high temperature recuperation in microturbine systems and the effect of microchannel design parameters on performance. This presentation will discuss the principles of fabrication of Ceramatec's, ceramic, compact heat exchangers, some results from heat transfer testing, and the development tasks required for application of these heat exchangers in existing and future power cycles.

04-20-2016 – 11:00A
FWP-66059 - Solid State Joining of Creep Enhanced Ferritic Steels
Pacific Northwest National Laboratory Presenter: Glenn Grant

ABSTRACT

Creep Strength Enhanced Ferritic (CSEF) Steels are an important class of materials in fossil energy power plant construction. CSEF steels show a combination of excellent creep resistance and moderate oxidation resistance, while at the same time have lower cost and improved thermal conductivity over austenitic steels and nickel alloys. The next generation of power plant design will require plant materials to be operated at higher temperature and pressure. A primary problem in the high temperature application of welded CSEF steels is the propensity of the fusion welds in these steels to display a creep life far below the parent material (Type IV cracking). This has led to inefficient up-gaging in wall thickness and low weld-strength reduction factors in design.

04-20-2016 – 13:00A

FE00025064 - Materials for Advanced Ultra-supercritical Steam Turbines - Advanced Ultra-supercritical Component Demonstration

Energy Industries of Ohio Inc. Presenter: Horst Hack, Electric Power Research Institute Inc.

ABSTRACT

Following the successful completion of a 14-year pre-competitive R&D effort to develop and test materials that would allow Advanced Ultrasupercritical (AUSC) coal-fired power plants to be operated at steam temperatures up to 760°C, a United States-based consortium has begun a project to design, engineer, manufacture, construct, and operate an AUSC component test facility (AUSC ComTest). Among the goals of the facility are to validate that components made from the advanced high-temperature alloys can perform under A-USC conditions, to accelerate the development of a U.S.-based supply chain for the full complement of AUSC components, to decrease the uncertainty for cost estimates of future commercial-scale AUSC power plants, and to minimize risks associated with ownership, operation and maintenance of future AUSC power plants.

The AUSC ComTest facility is being designed to include a superheater, thick-walled header, steam piping, steam turbine (7 MW nominal size) and valves. The facility will be constructed at a host site in Ohio. Current plans call for the components to be subjected to AUSC operating conditions for at least 8,000 hours, with testing concluding by September 2020.

The U.S. consortium, principally funded by the U.S. Department of Energy and the Ohio Coal Development Office with co-funding from Babcock & Wilcox, GE Power, and the Electric Power Research Institute, has completed the Front End Engineering Design (FEED), and is currently working on the Detailed Engineering phase of the AUSC ComTest project. This presentation will describe the project's structure and schedule, and provide details on the facility design.

04-20-2016 – 13:30A

FE0026183 - Advanced Ultrasupercritical (AUSC) Materials Thick-Walled Cycling Header Development for ComTest-AUSC

Alstom Power, Inc. Presenter: Reddy Ganta

ABSTRACT

Recently developed advanced nickel alloys such as Inconel 740H (740H) and Haynes 282 (H282) have been successfully tested for fireside corrosion and steam oxidation using steam loop tubing at AUSC temperatures of 760°C in actual operating coal fired boilers. Thick-walled super heater outlet headers to which these tubing materials are connected will also operate at high temperatures and pressures. (4250-5000 psi). Under expected severe cycling conditions, these header systems are considered one of the most critical components in the AUSC coal fired boiler. Over the design life of such plants, these components are exposed to the most severe fatigue and creep damage accumulation and need to be properly designed for reliable flexible cyclic operation. To validate design guidelines, these components need to first demonstrate that they can achieve a design life of 20 to 30 years with the creep and fatigue conditions required.

04-20-2016 – 14:00A
FE0024076 - Advanced Ultrasupercritical (AUSC) Tube Membrane Panel Development
Alstom Power, Inc. Presenter: James Pschirer

ABSTRACT

General Electric Steam Power Systems – Boilers (GE) is executing a cooperative agreement Project with the DOE/NETL for an "Advanced Ultrasupercritical (AUSC) Tube Membrane Panel Development". The AUSC Tube Membrane Panel Development is a two year Project to develop and verify the manufacturability of welded tube membrane panels made from high performance materials suitable for the AUSC steam cycles.

Use of these high performance materials for tube membrane panels pose challenges in the manufacturing process. These challenges associated with the creep strength enhanced ferritic alloys include: a) consistent control of weld penetration, b) distortion control to sufficiently insure the dimensional integrity of the panels, c) shop handling and manipulation using conventional shop equipment and practices, and d) the degree of preheating to avoid problems with hydrogen-delayed cracking at different stages of panel production. Challenges associated with panels constructed from a nickel base alloy include e) development of welding parameters necessary for welding Ni-based alloys, f) determine what dimensional tolerances can be maintained during manufacturing.
GE, through its Power Plant Laboratories (PPL) and Boiler R&D team in Windsor, CT, is executing the Project under direction of Principal Investigator Mr. James Pschirer. Other participants include GE Boiler Engineering, GE Chattanooga Manufacturing, GE Materials Technology Center, and a Technical Consultant from Electric Power Research Institute (EPRI). GE will also collect industry input through a Power Generator Technical Advisory Committee for this proposed project.

04-20-2016 – 15:00A
FE0024067 - Novel Functional Graded Thermal Barrier Coatings in Coal-fired Power Plant Turbines
Babcock & Wilcox Power Generation Group, Inc. Presenter: Paul S. Weitzel

ABSTRACT

Babcock & Wilcox has performed the preliminary front-end engineering design (Pre-FEED) of an advanced ultra-supercritical (A-USC) steam superheater for a component test program (ComTest) achieving 760C (1400F) steam temperature. The project provides the engineering data necessary to proceed to final performance design, detail engineering, manufacturing, construction and operation planning of Com Test. The ComTest Superheater would supply an A-USC intermediate pressure steam turbine. The ComTest facility site is being considered at the Youngstown Thermal heating plant facility in Youngstown, Ohio.

ComTest would operate in coordinated boiler and turbine service and introduce the plant operation and maintenance personnel to the skills required by providing a hands-on training experience. The initial exercise of the supply chain has provided more in-depth knowledge to help focus on the issues to be overcome.

ComTest would be firing natural gas in a separate steam generator and not jeopardize the host facility or suffer from conflicting requirements in the host plant's mission that could sacrifice the nickel alloy components. ComTest will use smaller quantities of the expensive nickel materials. Com Test reduces the risk for the first full demonstration A-USC plant.

04-20-2016 – 15:30A
FEAA125 - Advanced Ultra-Supercritical Steam Cycle Turbine Materials
Oak Ridge National Laboratory Presenter: Philip J. Maziasz

ABSTRACT

The U.S. is pursuing world-leading goals for advanced ultra-supercritical (A-USC) materials technology for much more efficient coal combustion with reduced emissions at steam conditions of 760°C/35 MPa. These advanced steam conditions will require Ni-based superalloys for high-temperature strength, like cast and wrought Haynes 282 alloy. Creep-rupture properties of welded specimens of cast Haynes 282 alloy were obtained previously. Creep-rupture life of as-welded specimens at 750-800°C were about half the base-metal values, but the creep-rupture life of fully heat-treated specimens was similar to the base metal. This year duplicate creep-tests were performed on the welded and heat-treated cast Haynes 282 alloy, and these tests at 750-800°C confirm even longer rupture lives that exceed the cast base metal. This year, high cycle fatigue (HCF) testing at 760°C of the large triple-melted forging of Haynes 282 alloy from GE with significantly refined grain size that showed very high strength. HCF testing at ORNL showed no effect of steam on degrading fatigue life, but did not show strength as high as the GE testing. This year, new efforts began at ORNL on long-term creep-testing at 700-800°C of the largest forged and cast Haynes 282 alloy components done by GE, in an effort to support the ComTest phase of the program being pursued by DOE and the A-USC Steam Consortium, and these will be summarized.

04-20-2016 – 16:00A
FEAA061 - Materials for Advanced Ultrasupercritical Steam Boilers
Oak Ridge National Laboratory Presenter: P.F. Tortorelli

ABSTRACT

In support of the U.S. DOE/Ohio Coal Development Office Advanced Ultrasupercritical (A-USC) Steam Boiler Consortium, this project provided application-critical mechanical properties data on nickel-based alloys needed for use at the highest temperatures and pressures in these high efficiency coal-fired boilers. The work included producing creep data in the range of 650-850°C for wrought materials as well as welded specimens, understanding microstructural stability over extended periods, and performing the necessary analyses to improve the ability to predict creep-rupture lifetimes of Ni-based alloys well past laboratory testing times.

Long-term creep-rupture data for Super 304H stainless steel, HR6W, alloy 617, Haynes alloys 230 and 282, and Inconel 740/740H were generated, compiled, and compared. Only Ni-based alloys with a significant volume fraction of ⍰⍰ (Inconel 740/740H and Haynes 282) were sufficiently strong to assure adequate A-USC boiler lifetimes at 750°C, with the Haynes 282 alloy projecting the longest lifetime at a given stress and temperature. Microstructural characterization studies showed that the ⍰⍰ coarsening kinetics for Inconel 740/740H and Haynes 282 were generally well described by the precipitation model developed by Soare and Shen (General Electric Global Research).

04-20-2016 – 16:30A
FEAA115 - Creep-Fatigue-Oxidation Interactions: Predicting Alloy Lifetimes under Fossil Energy Service Conditions
Oak Ridge National Laboratory Presenter: Sebastien Dryepondt

ABSTRACT

Fossil-fueled power plants incorporated into any future energy portfolio will be required to be capable of flexible operation. This mode of operation will involve frequent load cycling and an increased number of shutdown events, resulting in significant thermo-mechanical cycling superimposed on the expected creep loading. Creep-fatigue interaction, therefore, has the potential to become particularly damaging for critical pressure parts in such power plants, and to have a significant impact on component lifetimes. The goal of this project, focused so far on alloy Gr.91, is to generate pertinent creep-fatigue data and develop new lifetime models that will allow accurate prediction of the lifetimes of those components subjected to flexible operation. Creep tests conducted at 550-650°C with an unloading/loading sequence every 10h showed lower creep lifetimes than similar conventional creep tests without load cycling. Creep-fatigue tests with hold times varying from 10min to 10h were also conducted at 625°C, and the number of cycles to rupture decreased with increasing the hold time duration. Finally, creep-fatigue crack growth measurements were conducted at 550°C, and hold times resulted in a decrease of the crack propagation rates in comparison with the rates measured for standard fatigue tests. The impact of these results on component lifetime modeling will be discussed.

Track B – Wednesday, April 20, 2016

04-20-2016 – 08:30B
FE0007379 - Wireless Microwave Acoustic Sensor System For Condition Monitoring In Power Plant Environments
University of Maine Presenter: Mauricio Pereira da Cunha

ABSTRACT

The goals of this project have been to develop and demonstrate the performance of wireless microwave acoustic sensors positioned in arrays and embedded into equipment and structures located in fossil fuel power plant environments to monitor the condition of components, such as steam headers, re-heat lines, water walls, burner tubes, and power turbines.

The specific objectives for the current project include: (i) The advancement of novel thin film nanocomposite electrodes for wireless surface acoustic wave (SAW) sensors to achieve stable and reliable operation above 1000°C; (ii) The development of sensor interrogation methods and sensor encapsulation materials and techniques for embedding sensor arrays into power plant components; and (iii) The demonstration of the viability of prototype sensor arrays and interrogation systems through laboratory furnace and power plant field testing.

The project has successfully achieved the goals of: developing new electrode materials to extend the previous maximum operation temperature of the devices from 800°C to 1100°C; identifying and establishing packaging and interrogation methods for embedding the sensors in power plants; and finally installing and verifying the wireless SAW sensor array performance for over two years of operation in a working waste-to-energy power plant. Currently, efforts are geared towards installing sensors on the power plant superheater tubes employing a modified wireless LGS SAW sensor array. The wireless monitoring of the superheater tube temperature is important to improve the effectiveness of the soot blower operation, thus improving maintenance, reducing power plant down-time, and ultimately reducing operational costs.

04-20-2016 – 09:00B

FE0026348 - Novel Temperature Sensors and Wireless Telemetry for Active Condition Monitoring of Advanced Gas Turbines

Siemens Corporation 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 specific objectives are (1) to fabricate and install Smart Turbine Blades with thermally sprayed sensors and high temperature wireless telemetry systems in an H-Class engine, (2) to integrate the component engine test data with remaining useful life (RUL) models for Operation-Based Assessment (OBA). The main objectives of materials prognostics effort are a component-life prediction system for actual and planned operation regimes, optimization of maintenance intervals and scopes based on real-life consumption of components. Phase 1 involves 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.

04-20-2016 – 09:30B

FE0023118 - Distributed Wireless Antenna Sensors for Boiler Condition Monitoring

University of Texas at Arlington Presenter: Haiying Huang

ABSTRACT

We are developing wireless antenna sensors to provide distributed sensing of temperature, strain, and soot accumulation inside a coal-fired boiler. The benefit of this project includes distributed sensing for in-process control, real-time health assessment of structural components, and improved heat transfer efficiency of boilers. We will present 1) the wireless interrogation of an antenna sensor without electronic components up to 300 °C; 2) the preliminary results on the design, material selection, fabrication, and test of the high temperature antenna sensor; and 3) the development of an efficient antenna simulation model for multi-variant data processing. Experiments were conducted to demonstrate wireless temperature sensing inside a high temperature oven. A good linearity between the antenna resonant frequency and the temperature variation was obtained. We also designed and fabricated a microstrip antenna-sensor with alumina as high temperature dielectric and electrode materials. This sensor has been preliminary tested up to 100 °C with a good linearity between the antenna resonant frequency and the temperature variation. In addition, an efficient simulation model of the patch antenna will be presented. The simulation model will be further developed for inversely extracting multiple measurands from one single antenna measurements.

04-20-2016 – 10:30B

FE0026334 - Advanced Control Architecture and Sensor Information Development for Process Automation, Optimization, and Imaging of Chemical Looping Systems

Ohio State University Presenter: Tien-Lin Hsieh

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 H2 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. The intelligent process automation controller and optimization sensor information will be tested in OSU's existing sub-pilot SCL test unit. Additionally, 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 developed imaging sensor software will be tested and verified in an existing bench test unit test apparatus and incorporated into the sub-pilot test unit. The proposed work is scalable for larger demonstration units and will impact the fuel conversion industry as the control scheme and sensor measurements are very applicable to similar gas-solid circulating systems.

04-20-2016 – 11:00B

FE0012451 - Development of Integrated Biomimetic Framework with Intelligent Monitoring, Cognition and Decision Capabilities for Control of Advanced Energy Plants

West Virginia University Presenter: Debangsu Bhattacharyya

ABSTRACT

The objective of this project is to develop algorithms and methodologies for a novel, biomimetic control system that utilizes distributed intelligence and the power of the biological world for optimal control of advanced energy plants. Through a transformative biomimetic framework, 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, multi-agent environment.

In this project, 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 biological organisms (e.g., ants) in nature. Although this process is dynamic, often non-intuitive and nonlinear, these organisms move according to a coordinated pattern, suggesting an intelligence that transcends the ability of each group member or individual agent. A true biomimetic process should also take into account the randomness present in biological systems as well as their adaptability under unexpected disturbances. To exploit these aspects of nature, the immune system of superior organisms is being mimicked and adaptive control laws for intelligent monitoring, cognition, and decision capabilities are being developed and deployed for power plant control.

At the end of this project, algorithms and methodologies will be available for developing an integrated biomimetic control framework with intelligent monitoring, cognition, and decision capabilities that can be exploited for optimal control of highly complex and strongly interacting advanced energy plants.

04-20-2016 – 13:00B

FE0024092- Simultaneous Waste Heat and Water Recovery from Power Plant Flue Gases for Advance Energy System

Gas Technology Institute (GTI) Presenter: Dexin Wang

ABSTRACT

GTI has been developing a new technology based on a nanoporous ceramic separation membrane to extract a portion of the water vapor from flue gases, which is patented as TMC. Water vapor from flue gas condenses inside the nanoscale membrane pores and passes through by directly contacting with a low-temperature water stream on the permeate side. Contaminants and permanent gases such as CO_2, O2, NOx, and SO2 are inhibited from passing through the membrane by its high selectivity, therefore the recovered mineral-free high purity water can be directly used as boiler makeup water. GTI has successfully commercialized the TMC for industrial package boilers, and customer reported 12% fuel savings and 20% makeup water savings. Under previous support from NETL and Illinois Clean Coal Institute, the TMC has also been developed for utility boilers and field tested by a slip stream flue gas at a coal fired power plant with encouraging results. In this project, GTI will develop the TMC for greater efficiency to maximize its waste heat and water recovery. This will be done by a novel multi-stage TMC design and optimization, and membrane development work tailored for high water vapor transport flux. This version TMC will be ready for the next generation Advanced Energy System with CO_2 capture in consideration, for example, pressurized oxy-combustion, chemical looping combustion, and H2 turbine. They all have much higher moisture content flue gases than existing plants, and the CO_2 capture procedure also has a greater need for the recovered pure water.

04-20-2016 – 13:30B

FE0024085 - Field Demonstration Study for Heat and Water Recovery at a Coal-Fired Power Plant

Southern Company Services, Inc. Presenter: Russell Noble

ABSTRACT

Technology analyses and engineering assessments are being conducted to determine the best combination of a low-grade heat-recovery and use process to improve the overall energy efficiency and water usage rate for a coal-fired electrical generating unit. A prior assessment by the project team of existing commercial heat-recovery technologies will be updated to include new technology, performance, and cost data that will be compared to a survey of novel technologies. Results of this study will be evaluated against key process performance metrics to determine technologies warranting consideration for a field demonstration. A similar analysis will be conducted for a wide range of heat uses to determine the most technically and economically feasible options for installation at a coal-fired plant. Collective results from the analyses will determine the best combination of heat-recovery technology and end use based on projected performance and costs, ease of installation and operation at a coal-fired plant, and overall benefit in terms of reduced water usage rates, improved efficiency, and economics. The project will culminate in the recommendation of a selected heat-recovery/ use process for a next-step field demonstration.

04-20-2016 – 14:00B
FWP-14-017626 - Exploring Energy-Water Issues in the United States
Sandia National Laboratories Presenter: Vincent Tidwell

ABSTRACT

While long-term regional electricity transmission planning has traditionally focused on cost, infrastructure utilization, environmental impact, and reliability, the availability of water is an emerging issue. Toward this growing need, thermoelectric expansion should consider competing demands from other water use sectors balanced with fresh and non-traditional water supplies subject to climate variability. With the help of eastern water managers, water availability was mapped for over 1300 watersheds throughout 31-Eastern states. Five water sources were individually examined, including unappropriated surface water, unappropriated groundwater, appropriated water, municipal wastewater and brackish groundwater. Also mapped was projected change in consumptive water use from 2010 to 2030. Associated costs to acquire, convey and treat the water, as necessary, for each of the five sources were estimated. This work compliments prior work where similar water metrics were mapped for the 17-Western states, thus completing the conterminous United States. These metrics were developed to support regional water planning and policy analysis with application to electric transmission planning.

04-20-2016 – 15:00B
FE0012302 - Evolving Robust and Reconfigurable Multi-objective Controllers for Advanced Power Systems
Oregon State University Presenter: Kagan Tumer

ABSTRACT

With the ever increasing power requirements of our society, there is an urgent need for advanced power systems that are more efficient, reliable, and robust. However, designing such advanced power systems introduces two new challenges. First, they 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 multi-dimensional 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 a neuro-evolutionary-based time domain simulator trained (beyond backpropagation to match one step ahead) to match power plant dynamics as well as generate "novel" solutions tracks the 19 studied input to an average error of 0.39%, and a maximum error of 1.26%. In addition, using a multi-objective neuro-evolutionary controller and the Pareto Concavity Elimination Transformation (PaCcET) we develop a Pareto front of control policies which represent tradeoffs between tracking desired turbine speed profiles and minimizing transient operation of the fuel cell.

04-20-2016 – 15:30B

FE0007270 - An Information Theoretic Framework and Self-Organizing Agent-Based Sensor Network Architecture for Power Plant Condition Monitor

Case Western Reserve University Presenter: Kenneth Loparo

ABSTRACT

The focus of this research is the development of an agent-based framework for the robust and resilient collection, organization, fusion, and application of actionable information available from sensing processes and instrumentation in a coal-fired power generation plant. To that end, an information theoretic perspective is utilized wherein the disparate systems, subsystems and processes are treated as information processing systems connected in the form of a communications network. Specifically, the physical phenomena associated with their behavior (e.g., heat, vibration, pressure, chemical outputs) are viewed as "messages" communicated to other elements of the generation plant via physical transmission of these phenomena. The transmission paths between the elements of the plant, including sensors and instrumentation systems, are treated as information channels. The development of the sensor network framework can thus be cast in terms of network discovery, communication channel characterization, and network routing.

04-20-2016 – 16:00B

FWP-AL-12-470-009 - Merged Environments for Simulation and Analysis: Testing and Demonstrating a Stigmergic Control Strategy based on Distributed Construction

Ames National Laboratory Presenter: 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, based on stigmergy and distributed construction, raise several questions. These questions include optimum sensor density; overlap, duplication, and reuse of sensors; and the composition of the agents (i.e., what sensors are used to create an agent and control a particular actuator). This talk discusses the development and testing of a stigmergic multi-agent control strategy and compares the performance of this control strategy to a multivariable controller using an advanced gas turbine—fuel cell hybrid power system (i.e., the Hyper facility at NETL). Results showed that in some cases the multivariable controller provides a faster response, whereas in most cases the response of the stigmergic controller is comparable. In addition, modeling and tuning of the system is much simpler with the stigmergic controller relative to the multivariable approach. This can be important when the dynamic coupling of diverse components cannot easily be simulated (e.g., in an advanced hybrid cycle). The multivariable controller was found to provide better disturbance rejection compared to the agent based controller.

04-20-2016 – 16:30B

FE0011227 - Multi-Objective Optimal Sensor Deployment Under Uncertainty For Advanced Power Systems

University of Illinois at Chicago Presenter: Urmila Diwekar

ABSTRACT

An efficient, safe, and reliable operation of an IGCC plant requires effective strategies for monitoring and control. Sensors play a key role in the monitoring and control endeavor through the quantification of temperature, dynamic gas pressure and flow, fuel/exhaust gas composition, and structural integrity in the various components. A variety of sensor choices are available ranging in cost, accuracy, and suitability for the operating conditions encountered in an IGCC plant. This paper presents a stochastic programming approach to sensor placement using coupled virtual and actual sensors. The objectives of the proposed research is to develop a fundamental understanding of the relationships involved in the sensor placement, interaction with the process, and hierarchal interactions of the sensor intelligence, with a goal of identifying the type, number, and deployment of sensors for maximum effectiveness and efficiency of the measurement technology and the process itself. Since there are number of objectives to be satisfied in sensor placement such as maximizing observability, maximizing efficiency, and minimizing cost, we develop an efficient multi-objective framework which can consider uncertainties or errors in sensor measurement explicitly. This multi-objective framework is based on the BONUS algorithm developed in our group for stochastic programming and a new 2-tier constraint method for multi-objective optimization. A non-linear stochastic multi-objective problem has been solved to determine the non-dominated or Pareto set which contains different options for optimal sensor network locations that can simultaneously satisfy the three objective functions, (maximizing observability, minimizing cost and maximizing the IGCC power plant thermal efficiency).

Track A – Thursday, April 21, 2016

04-21-2016 – 08:30A
FWP-AL-14-330-058 - Kinetic Theory Modeling of Turbulent Multiphase Flow
Ames National Laboratory Presenter: Bo Kong

ABSTRACT

Gas-solid flows are important in energy processes such as coal and biomass gasification. In these systems, solids concentrations can vary from dilute through dense regimes manifesting in complex multi-scale phenomena that are not well understood or predicted in spite of their critical importance to engineering design and energy policy. In the kinetic theory of gas-particle flows, the transport equations for the moments contain spatial fluxes arising from (i) free transport and (ii) particle-particle collisions. The former are dominant is dilute flows (i.e., particle-phase volume fraction is less than 0.1), whereas the latter are dominating in dense flows, especially in regions where the particles are nearly close packed. When quadrature-based moment methods (QBMM) are applied to solve for the moments, the free-transport flux can be efficiently treated using explicit kinetic-based finite-volume (KBFV) methods. However, in dense regions, implicit methods are required to efficiently treat the collisional fluxes. An operator-splitting scheme is proposed to combine the KBFV and implicit flux schemes to treat gas-particle flows exhibiting both dense and dilute regions in the same flow domain. As a proof of concept, a monodisperse system is considered with velocity moments up to second order (i.e., anisotropic Gaussian velocity distribution).

04-21-2016 – 09:00A

FE0026393 - MFIX-DEM PHI: Performance and Capability Improvements Towards Industrial Grade Open-Source Framework with Integrated Uncertainty Quantification.

Arizona State University Presenter: Manogna Adepu & Shaohua Chen

ABSTRACT

Multiphase flows are ubiquitous in many industrial processes, such as granulation and fluidization. Typically, separate discrete element method (DEM) and computational fluid dynamics (CFD) software are coupled to model the governing physics in such flows. MFIX-DEM is an open-source CFD-DEM code developed and maintained by NETL, which provides a unified framework under a single user interface to simulate a diverse range of multiphase flow problems. The objective of our project is (i) to improve the performance and various capabilities of MFIX-DEM while tightly integrating these improvements with a GUI-driven uncertainty quantification framework, and (ii) to effectively pave the way to ubiquitous industrial adoption of the open-source MFIX-DEM. The anticipant benefits of project outcome success includes:

- improved time-to-solution for solving industrial size problems on high-performance computing platforms that are affordable and available to typical research and commercial organizations in the next two- to five-year horizon,
- enhanced the physical modeling capabilities of the computational models for more accurate solution of the real engineering problems encountered by the industry,
- capability for the assessment of predictive credibility of the simulation results through the integration of uncertainty quantification process as part of the routine analysis performed with the CFD software, and
- development of industrial scale test cases based on industry feedback on improvements and enhancements to demonstrate the power of MFIX-DEM Phi for simulation-based engineering.

The end goal is to create a user-friendly, powerful open-source multiphase flow simulation environment that provides an assessment of the credibility of the results and easily usable by diverse users.

04-21-2016 – 09:30A

FE0026298- MFIX DEM Enhancement for Industry-Relevant Flows

University of Colorado Presenter: Thomas Hauser

ABSTRACT

This project will improve performance of the MFIX-DEM code to enable a transformative shift for industrial use. The largest simulations performed to date using MFIX are O(107) particles. This falls short of the O(108) particle simulations that must be completed on a timescale of days (vs. months) to enable simulations with physically-relevant domain sizes to be incorporated into industrial design cycles within five years. More specifically, the proposed approach will enhance MFIX DEM by using a state-of-the-art profiling methodology developed by our team members to comprehensively and continuously identify numerical and algorithmic bottlenecks. Both serial and parallelization bottlenecks will be overcome via vectorization, cache utilization, algorithmic improvements, and implementation of hybrid MPI/OpenMP parallelization methods that synergize with current heterogeneous high performance computing (HPC) architectures and accelerators. Optimizing MFIX-DEM and implementing parallelization for accelerated HPC systems will enable simulations of industrially relevant problems and on machines that industry are likely to have in the coming years. The ultimate goal is to achieve a speedup of two orders of magnitude; a refined estimate will emanate from the profiling effort.

04-21-2016 – 10:30A
FE0008868 - Novel Functional Graded Thermal Barrier Coatings in Coal-fired Power Plant Turbines
Indiana University – Purdue University Indianapolis Presenter: Jing Zhang

ABSTRACT

The primary research goal of the project is to investigate novel lanthanum zirconate ($La_2Zr_2O_7$) based thermal barrier coating (TBC). The objective of the project is to develop a manufacturing process to produce novel multilayer and composite $La_2Zr_2O_7$ based thermal barrier coatings with improved thermal durability. Compared with current standard TBC material, yttria stabilized zirconia (YSZ), $La_2Zr_2O_7$ has demonstrated lower thermal conductivity and better thermal stability, which are crucial to high temperature applications such as gas turbines in coal-fired power plants.

$La_2Zr_2O_7$ and 8YSZ multilayer and composite thermal barrier coating systems were deposited using air plasma spray technique. Thermal and mechanical properties of the coatings were measured. Furnace heat treatment and jet-engine thermal shock tests were implemented to evaluate coating performance during thermal cycling. The results provide important information of using $La_2Zr_2O_7$ in future gas turbine applications.

04-21-2016 – 11:00A
FE0024009 - Ceramic High Temperature Thermoelectric Heat Exchanger and Heat Recuperators for Power Generation Systems
West Virginia University Presenter: Xueyan Song

ABSTRACT

The objective of this research effort is to develop all-oxide thermoelectric (TE) generators, which will be highly efficient, cheaply produced, small, lightweight, non-toxic, and highly stable in air at high temperatures, for recovering the waste heat from power systems including Solid Oxide Fuel Cells (SOFCs) at temperatures of 600-980ºC. Novel device configurations has been developed using mature, inexpensive, easily scalable manufacturing techniques. The TE generators will be incorporated into SOFC systems. With the incorporation of TE device into SOFC systems, it is expected to increase the electricity production by more than 15%, corresponding to system electrical efficiency increases of 5 percentage points. High performance CaMnO3 *n-type* semiconductor with engineered nanostructure has been developed, and integrated with the available state-of-the-art Ca3Co4O9 *p*-type material into all-oxide TE devices. Bulk scale all-oxide prototype TE generators have been fabricated, and will be tested for device operation efficiency evaluation, and integrated into SOFC power generation systems**.** The devices from this project have the following features: (a) integrated design composed of strongly textured *p*-type Ca3Co4O9 fabricated directly onto an insulating layer, buffered onto the *n*-type material, for simplicity of device fabrication, (b) micron-sized, closely-packed insulating separator for better thermal management and reduction of the overall-size and weight of the device, and (c) the novel device will be easy to fabricate in anticipation of mass production, with a high potential for use in large-scale operations.

04-21-2016 – 13:00A

FEAA114 - Advanced Alloy Design Concepts for High-Temperature Fossil Energy Applications
Oak Ridge National Laboratory 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 steel alloys should incorporate improved properties, including creep strength, environmental resistance, and weldability, intended for upper limit temperatures higher than that of the materials currently in service. A developmental effort on a new fully-ferritic Fe-30Cr-3Al base alloy has been conducted, which includes minor alloying additions with guidance from computational thermodynamic tools and process development to control microstructure for improved mechanical properties, suitable for the alloy design concepts with a target service temperature range up to 800°C. It was found that the combined additions of Al and Nb successfully improved steam oxidation resistance, coal-ash corrosion resistance, tensile properties, and creep-rupture properties. They showed superior properties to Gr.91/92 type ferritic-martensitic steels above 650°C. The “third-element” additions such as W, Mo, and Ti substituting for a part of the Nb content has also been conducted, which resulted in successfully lowering the solvus temperatures. However, it was also found that the second-phase (Fe_2Nb type Laves) precipitates exhibited either faster coarsening or coarser precipitate sizes compared to the alloy with only Nb added, indicating the need for optimization to balance these competing features. In the presentation, the effect of Y additions on microstructural stability and the characterization results of the trial e-beam welded materials will be discussed.

04-21-2016 – 13:30A

FE0026260 - Optimization of Advanced Steels for Cyclic Operation through an Integration of Material Testing, Modeling and Novel Component Test Validation

Electric Power Research Institute Inc. 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.

04-21-2016 – 14:00A

FE0008855 - Experimental and Computational Investigation of High Entropy Alloys for Elevated-Temperature Applications

University of Tennessee Presenter: Peter K. Liaw

ABSTRACT

The objective of the research is to (1) perform fundamental studies on the high-entropy alloys (HEA) system for use at temperatures up to 1,033 K and a stress of 35 MPa, and (2) develop an integrated approach, coupling theoretical (thermodynamic calculations and crystal-plasticity finite-element modeling) approaches and focused experiments, to identify HEAs that outperform conventional alloys. Thermodynamic predictions are performed to provide phase fractions, phase compositions, and phase stability as a function of temperature and composition. These calculations will help understand the stability of desired phases. Focused experiments are used to verify thermodynamic calculations and develop mechanical properties desired at elevated temperatures. Experimental techniques, such as neutron and synchrotron diffraction, are used to study the structures. In-situ testing of mechanical behavior under tension and creep loading allows for the identification of the deformation mechanisms. The tensile creep behavior of Al0.3CoCrFeNi HEA is superior to conventional fossil energy alloys at 973 K. Taking the case at 100 MPa for example, the creep rate of Al0.3CoCrFeNi is two orders slower than P92 and P122 alloys. This integrated modeling and experimental approach can streamline the alloy-development and manufacturing process and develop HEAs suitable for structural applications of boilers, steam turbines, and gas turbines.

04-21-2016 – 15:00A

FE0024065 - New Mechanistic Models of Long Term Evolution of Microstructure and Mechanical Properties of Nickel Based Alloys

Oregon State University Presenter: Jamie Kruzic

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.

04-21-2016 – 15:30A
FE0024054 - Computational Design and Performance Prediction of Creep-Resistant Ferritic Superalloys
University of Tennessee Presenter: Peter K. Liaw

ABSTRACT

Novel ferritic superalloys based on the Fe-Al-Cr-Ni-X (X = Ti, Hf, Ta, and Zr) systems has 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. In this project, the bulk thermodynamic properties (the formation and ordering energies), interfacial energies, including anisotropic effects, and elastic constants (Cij) in the system of the body-centered-cubic (bcc) iron, and relevant B2 and L21 intermetallics, is calculated and determined by first-principles calculations. Besides, advanced microstructural characterization tools (e.g., the high-resolution analytical-electron microscopy, local-electrode-atom probe, high-resolution electron microscopy, laboratory and synchrotron x-ray diffraction, neutron diffraction, and ultra-small angle X-ray scattering) and mechanical tests (e.g., compression, tension, and creep) coupled with in-situ neutron diffraction, are conducted for the validation of the calculated results. Dislocation-dynamics simulations, which incorporates the data of the first-principles calculations and experimental results, are developed to guide the alloy design with optimal microstructural parameters (e.g., the precipitate size, morphology, volume fraction, and lattice mismatch) to improve the creep resistance of ferritic superalloys for applications in FE power plants. With all these results, we are able to develop and integrate modern computational tools and algorithms to design high-temperature alloys for applications in FE power plants, and to understand the processing-microstructure-property-performance links underlying the creep behavior of novel ferritic alloys strengthened by hierarchical coherent B2/L21 precipitates.

04-21-2016 – 16:00A
SC0006222 - Computational Design of Weldable, High-Cr Ferritic Steel
QuesTek Innovations LLC Presenter: David Snyder

ABSTRACT

The goal of this SBIR program is to create a new alloy for A-USC coal-fired boilers using QuesTek's computational alloy design methodology, targeting a creep-resistant ferritic superalloy with low processing cost related to welding. QuesTek is collaborating with engineers from a boiler OEM as well as technical experts from the DOE to identify key design goals, which includes mitigation of post-weld heat treatment and increase in creep-resistance at operating temperatures in excess of baseline incumbent alloy P92. QuesTek has designed a series of prototype alloys using computational models to target critical design parameters, building on a design concept of intermetallic strengthened (L21 Ni_2TiAl and B2 NiAl) steel with a fully-ferritic microstructure for cost and welding. High temperature properties and weldability have been demonstrated in coupon-scale testing, and extended property demonstration is in process with scaled-up production of a final alloy design. A brief status update will be provided on other QuesTek SBIR programs sponsored by NETL as well.

04-21-2016 – 16:30A

FE0011549 - Large Scale Screening of Low Cost Ferritic Steels for AUSC

Tennessee State University Presenter: Lizhi Ouyang

ABSTRACT

The overall goal of this proposal is to develop large scale screening approaches based on physical properties of matrix BCC solid solution phase of 9-12Cr ferritic steel. The goal of this project is two-fold: (1) implement fast algorithms such as special quasirandom structure (SQS) method for physical properties calculation of solid solution; develop modules to calculate additional mechanical properties need to assess ductility; (2) to calculate the formation energy and elastic properties of the BCC solid solutions for given composition sampling. The result will be used to construct the database for likelihood analysis which can be used to identify composition of new ferritic steel that are likely to succeed in quest for high temperature application in AUSC.

We have implemented modules to automate the solid-solution modeling for a given composition using the SQS method and computed elastic constants of all phases in more than 10 9-12 Cr steels. We used Eshelby’s inclusion theory to estimate the steel’s mechanical properties. In addition, we have developed a method to index crystal structures in a finite searchable space. Any crystal structure can be mapped to a space group number, three integers and a binary array. Based on the Crystallography Open Database, we have implemented a web interface for searching the database using these indices.

Track B – Thursday, April 21, 2016

04-21-2016 – 08:30B
FE0026308 - Model-based Extracted Water Desalination System for Carbon Sequestration
General Electric Global Research Center Presenter: Ryan Adams

ABSTRACT

Carbon sequestration in tight, deep saline aquifers requires water extraction from the formation to safely accommodate injection of supercritical carbon dioxide. Many such formations contain highly saline brines; such brines require desalination prior to beneficial reuse or surface disposal.
The objectives of this project are to (1) define a scalable, multi-stage extracted water desalination system that yields clean water, concentrated brine, and, optionally, salt from saline brines (180 gm/L total dissolved solids, TDS), (2) validate the overall system performance with field-sourced water using GE pre-pilot facilities, and (3) design a pilot-scale desalination system.
Using commercial thermal brine concentration technology as a base case, five alternate desalination technologies were analyzed for two extracted water compositions. Water lifecycle analyses were conducted using Aspen Plus with the electrolytes package from OLI Systems. This techno-economic analysis enables realistic estimates of the cost to desalinate high-TDS extracted water and allows the processes to be ranked according to cost for various scenarios.

The anticipated benefit of this project is to identify high-TDS desalination methods that are lower cost than conventional technologies. Such methods will enable deep saline aquifers to store carbon dioxide without over pressurization, while generating a new source of clean water.

04-21-2016 – 09:00B
FE0024022 - Water Desalination Using Multi-Phase Turbo-Expander
General Electric Presenter: Kim Hammer

ABSTRACT

Project objectives are to demonstrate the technical and economic feasibility of the multi-phase turbo-expander based water desalination process. In the process, brine droplets directly injected into cold stream of propane resulting in droplets cooling and freezing. Mixture of ice and salt are then separated from propane which is re-used in the closed loop refrigeration system. Ice crystals, separated from salt crystals and the remaining brine, consist of pure water. The key component of the process is energy recovery by using propane stream to melt the ice. Project goals are to achieve at least a) 20% reduction in cost of water treatment in comparison with thermal crystallizer and b) 80% water recovery. Process model developed in Aspen Plus shows that energy requirement for 100% water recovery from 18% salinity brine is ~17 kWh/m3 of water produced. Total cost of water treatment is estimated to be 40% lower than that of thermal crystalyzer. The process is flexible and robust, allowing it to handle changes in water salinity by adjusting parameters in the refrigeration system. Because of the low process temperatures, the brine freeze method has fewer corrosion problems than conventional desalination technologies and can use cost-effective materials for construction.

04-21-2016 – 09:30B

FE0026315 - Advanced Integrated Technologies for Treatment and Reutilization of Impaired Water in Fossil Fuel-based Power Plant Systems

Ohio University Presenter: Jason Trembly

ABSTRACT

This project is a collaborative effort between Ohio University (OHIO), West Virginia University (WVU), and American Electric Power (AEP) with an overall objective to validate the technical/commercial promise of an advanced multi-stage 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, if successful. The proposed process is based upon an advanced multi-stage treatment process which utilizes commercial solids filtering and ultra violet light treatment to remediate bacteria, a low-cost natural zeolite to remove naturally occurring radioactive material (NORM) found in oil/gas-based impaired water, electrochemical stripping (E-stripping) and selective sulfation to remove minor constituents, and a supercritical water (SCW) unit design to remove major constituents and hydrocarbons.

The objective of this project is to evaluate new advanced impaired water treatment operations to further reduce treatment costs. Small scale testing efforts including evaluating the performance of a new breakthrough SCW 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 Cl- content. In addition, a techno-economic assessment will be completed to determine overall treatment cost for the process and at each treatment stage, and identify best suited power plant make-up water applications for the process water product.

04-21-2016 – 10:30B

FE0024015 - An Integrated Supercritical System for Efficient Produced Water Treatment and Power Generation

University of Illinois at Urbana-Champaign 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 high-TDS water to ~100 ppm by shock crystallization at SC conditions, and developed advanced 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, purifying water from high-TDS saline or produced water, and recovering valuable minerals that may be present in the brine, in a zero-liquid discharge system.

04-21-2016 – 11:00B

FE0024074 - Fouling-Resistant Membrane for Treating Concentrated Brines for Water Reuse in Advanced Energy Systems

Research Triangle Institute International 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.

04-21-2016 – 13:00B
FE0026212 - Low-Energy Water Recovery from Subsurface Brines
Research Triangle Institute International Presenter: Zachary Hendren

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 CO_2 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.

The design and implementation of a solvent-based water extraction system would eliminate or reduce many of the operational challenges that current technologies face during high TDS water treatment, since a water/solvent system would be simpler to operate, provide greater reliability, and reduce equipment costs. A successfully developed NAS water recovery technology could replace current thermal process for high saline water (TDS>60,000 ppm) and reduce energy cost by eliminating phase changing step (evaporation/condensation) and lower capital equipment costs. Additional potential savings from this technology include reduced pretreatment costs relative to complicated membrane or thermal processes that require several pretreatment processes.

04-21-2016 – 13:30B
FE0024084 - Treatment of Produced Water from Carbon Sequestration Sites for Reuse, Mineral Recovery, and Carbon Utilization
Southern Research Institute Presenter: James H. Irvin

ABSTRACT

Southern Research is working with multiple industrial partners to develop robust cost effective solutions to treat and reuse produced water from CO_2 sequestration sites. The water produced during the sequestration of CO_2 can contain high concentrations of total dissolved solids which may include strategic and rare earth minerals (SREMs), naturally occurring radioactive materials (NORMs), hydrocarbons and metals such as lithium, zinc and magnesium. The effective reservoir pressure management can pose a significant challenge because of the need to discharge the produced water into the environment. To address these concerns, Southern Research and our project partners will characterize four reservoirs with regards to their chemical and geologic properties then develop commercially viable methods to treat the produced/impaired waters, create useable/potable water streams, stabilize the residual solids and quantify plant operating efficiency improvements.

04-21-2016 – 14:00B

FE0024061 - Development of Membrane Distillation Technology Utilizing Waste Heat for Treatment of High Salinity Wastewaters

University of Pittsburgh Presenter: Omkar Lokare

ABSTRACT

The objective of this project 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. Technical information developed in these laboratory-scale studies will be utilized for a systems-level integration of MD process with low-grade heat sources (i.e., thermoelectric power plants and NG and CO_2 compressor stations) or NG as a fuel source. The project has the following technical objectives: (1) Examine the laboratory-scale performance of two MD schemes (Direct Contact Membrane Distillation and Vacuum Membrane Distillation), along with operating conditions, and process configurations in terms of productivity and permeate quality; (2) Conduct laboratory-scale studies with synthetic and actual wastewaters to assess capabilities and limitations of MD technology and define key design and operating parameters. High-salinity produced waters representative of several shale gas plays and geologic sequestration locations would be used to study how water composition affects MD performance; (3) This information will be utilized for a systems-level analysis to assess the feasibility of integrating MD process with low-grade heat sources (i.e., thermoelectric power plants and natural gas and CO_2 compressor stations); (4) Conduct preliminary techno-economic assessment of MD technology for saline wastewater treatment.

04-21-2016 – 15:00B

FE0023061 - Vertically Aligned Carbon Nanotubes Embedded in Ceramic Matrices for Hot Electrode Applications

University of Nebraska Presenter: Yongfeng Lu

ABSTRACT

Fossil-fuel power plants produce about 70% electricity in the United States. However, state-of-the-art fossil-fuel power plants are running at an average energy efficiency of 32%. The low energy efficiency results in excessive greenhouse gas emissions and fuel consumption. To satisfy the ever-growing electricity request and ensure national energy security, innovative solutions are in demand. It is predicted that a magnetohydrodynamics (MHD) power generator could achieve efficiency above 65% by eliminating mechanical moving parts. However, implementation of MHD generators is impossible until material challenges are satisfactorily addressed, i.e. the hot-electrodes that can survive the extreme environments and extract power from combustion fluids. The primary goal of the project is to develop carbon-nanotube-boron-nitride (CNT-BN) composite structures, in which vertically aligned CNTs (VACNTs) are embedded in BN matrices. It is anticipated that the BN matrices protect CNTs from the harsh environments and CNTs extract electricity from the combustion fluids. The following objectives will be achieved: 1) super growth of VACNTs on copper, 2) fabrication of CNT-BN composite structures, 3) stability and resistance studies of the CNT-BN composite structures, and 4) thermionic emissions properties of the CNT-BN composite structures. During the reporting period, VACNTs up to 3 mm were successfully grown with an average thermal conductivity of 1.76 W/mK. By pattering catalysts, VACNT arrays were produced. By forming a metallic carbide buffer layer between VACNTs and Cu, VACNTs were successfully bonded on Cu substrates. A laser-assisted chemical vapor deposition system was constructed for growing BN.

04-21-2016 – 15:30B

FE0024062 - AOI [7-A] High Temperature High Velocity Direct Power Extraction Using an Open-Cycle Oxy- Combustion System

University of Texas at El Paso Presenter: Manuel Hernandez

ABSTRACT

Direct power extraction (DPE) is an innovative energy concept (IEC) for advanced power generation. Supersonic flows of charged combustion products can cause electromagnetic induction when acted upon by magnetic fields. However, charged combustion gases must achieve a certain temperature threshold to permit electrical current transport. The combustion dynamics and electrical conductivities of oxy-enriched air flames have thus far limited the progression of DPE systems. Therefore, it is of critical importance to explore oxy-fuel combustion dynamics. Hydrocarbon-oxygen flames, such as CH_4/O_2, exhibit high-temperature combustion fronts and exhibit favorable combustion emissions. The research objective of this project is to investigate the design of different scale DPE combustors capable of achieving temperatures that allow electrical current transport and supersonic velocities. The first task is the development of a 60kW combustor and nozzle composed of a nickel-based superalloy. Aerospace-graded materials were selected to sustain exposure to temperatures in excess of 2500�C, which requires active cooling. Non-premixed combustion models are used to design the active cooling system, combustor geometry, and nozzle. This scale combustor serves as a proof-of-concept for flame stability and material durability. A second 1MW oxy-fuel combustor is also designed to investigate various parameters at larger scales. Scaling testing will include comparison of combustion stability phenomena and material cooling for extended burn times. These heat engines support the development and application of DPE topping cycles at the component and system level and investigations of oxy-fuel partially premixed flames in advanced power cycles.

04-21-2016 – 16:00B

FE0023142 - Precursor-Derived Nanostructured Silicon Carbide Based Materials for Magnetohydrodynamic Electrode Applications

University of Washington Presenter: YiHsun Yang

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. 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 that was previously designed and built on the UW campus. 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.

04-21-2016 – 16:30B

FE0022988 - Boride Based Electrode Materials with Enhanced Stability under Extreme Conditions for MHD Direct Power Extraction

University of Idaho Presenter: Krishnan S. Raja

ABSTRACT

The operating conditions of the magneto-hydrodynamics (MHD) ducts are expected to be very aggressive. The major objective of the work is to develop a boride based ultrahigh temperature ceramic that possesses all the desired properties to function as sustainable electrodes. Transition metal borides exhibit high melting point, high electrical and thermal conductivity, high strength even at high temperatures and enhanced chemical stability. However, the major concern is their limited resistance to oxidation in air. The ongoing work is developing materials containing ZrB2-HfB2 with varying additives including rare earth compounds via high energy ball milling followed by spark plasma sintering. Mechanical, electrical and thermal properties of the developed materials at elevated temperatures are investigated. The oxidation kinetics is studied as a function of oxygen partial pressure. Further, electrochemical anodic coating is formed on the samples via anodization to improve oxidation resistance. Extensive characterization work involving SEM, XRD etc. have also been undertaken.

The outcome of this project lead to a better understanding of charge/mass transport behavior of transition metal borides and their oxidation kinetics in presence of rare earth and other compounds. The results of the project will help develop ultrahigh temperature electrode materials for MHD direct power extraction applications with improved life-time. Two graduate students have been trained during the course of the project. One graduate student has already completed his MS thesis based on the boride processing work and another graduate student is working toward his PhD degree focusing on analytical characterization and properties evaluation of borides.

Track A – Friday, April 22, 2016

04-22-2016 – 08:30A
FE0011291 – Predicting Microstructure-Creep Resistance Correlation in High Temperature Alloys Over Multiple Time
Purdue University West Lafayette Presenter: Vikas Tomar

ABSTRACT

NETL is partnering with Purdue University to predict the creep and associated microstructure evolution, using tungsten-based refractory alloys as model systems. Researchers establish time-dependent creep resistance and associated microstructure evolution of grain-boundary controlled creep as a function of load, environment, and temperature, and relate creep behaviors with computed grain boundary diagrams, a new materials science tool. The goal is to conduct a systematic study that includes the development of a theoretical framework, multiscale modeling, and experimental validation using W-based body-centered-cubic alloys, doped/alloyed with one or two of the following elements: nickel, zirconium, cobalt, iron, and copper. Prior work has established and validated a basic theory for segregation-induced high-temperature interfacial disordering in W-based binary and ternary alloys; the study conducted under this project extends this proven work. Based on the high-temperature interfacial thermodynamic models and a related phenomenological grain-boundary diffusivity model, phase-field models are developed to predict long-term microstructural evolution. In order to validate the models, controlled W-alloy specimens are prepared and nanoindentation creep data are used to elucidate the role played by the interface properties in predicting long-term creep strength and microstructure evolution.

04-22-2016 – 09:00A

FE0024056 – Computational Design and Discovery of Ni-Based Alloys and Coatings: Thermodynamic Approaches Validated by Experiments

Pennsylvania State University Presenter: Bicheng Zhou

ABSTRACT

The collaborative project between Pennsylvania State University and University of Pittsburgh aims to understand the effects of the reactive elements Hf and Y on the phase stability and protective oxide scale formation in MCrAl-based coatings used in Ni-based turbine systems through combined computational and experimental approaches. Additions of reactive elements can play a critical role in beneficially affecting the oxide scale formation on alloys during high-temperature exposure to oxidizing environments; however, adding too much can be detrimental to protectiveness. Computation-based guidance on optimizing the levels of Y and Hf additions in multi-component Ni-based alloys will be a significant outcome of this study. An experimentally-verified thermodynamic database of the Ni-Al-Cr-Co-Hf-Y system will be developed, which will be used to determine the effects of major and minor alloying constituents on the stability and reactivity of trace Hf and Y additions in Ni-based systems. The modeling approach is based on the integration of first-principles calculations based on density functional theory (DFT) and CALPHAD (CALculations of PHAse Diagrams) method. First-principles calculations are not only capable of calculating energetics-related properties of stable structures accessible experimentally, but also be able to predict the properties of unstable structures which cannot be measured directly by experiments, which are critical to CALPHAD modeling. A further project objective is the application and further development of an automated thermodynamic modeling tool (ESPEI - self-optimizing phase equilibrium computer program) which will more efficiently arrive at accurate thermodynamic descriptions and hence, will have the potential to significantly enhance computational alloy and coating design.

04-22-2016 – 09:30A
FWP-AL-14-450-012 – Multiscale Design of Materials
Ames National Laboratory Presenter: Richard LeSar

ABSTRACT

Our primary focus is to use materials models in the design of engineered systems, with the goal of accelerating 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. As part of this project, we have developed the BMI interfaces and extensions needed to connect disparate materials models into an integrated multiscale simulation. We will review our successful implementation of two independent methods, a Lattice Boltzmann model of continuum flow and a molecular dynamics code at the atomistic scale, as well as the recent addition of a heat flow code into our library. We will discuss ongoing and future applications of these methods.

04-22-2016 – 10:30A
FE0011585 - Developing Novel Multifunctional Materials for High-Efficiency Electrical Energy Storage
University of Tennessee Presenter: Feng-Yuan Zhang

ABSTRACT

Advanced multifunctional materials with desired transport, electrical and thermal properties, and high durability are crucial for improving efficiency and performance in not only renewable energy storage devices, but also medical devices, electronic systems, and military uses. The novel thin liquid/gas diffusion layers (LGDLs) with well-tunable pore morphologies was developed by employing micro/nano-manufacturing and showed significant performance improvements in proton exchange membrane electrolyzer cells (PEMECs) for renewable energy storage and hydrogen/oxygen production. The PEMEC efficiency with developed LGDLs reached a report high of up to 88%. In addition, the LGDL thickness reduction from hundreds of µm of conventional LGDLs to 25 µm will greatly decrease the weight and volume of PEMEC stacks, which can lead to new directions for future developments of low-cost/weight/volume PEMECs with higher performance. Its well-tunable features, including pore size, pore shape, pore distribution, and thus porosity and permeability, will be very valuable for developing PEMEC models and validating simulations of PEMECs with optimal and repeatable performance. More importantly, with the nanomanufactured thin LGDLs, the rapid electrochemical reactions in both micro spatial and time scales have been revealed by developing a state-of-the-art characterization system and an innovative transparent PEMEC. Improvement to energy storage technology will promote modernization of power plant assets and result in lower capital and operating costs for long-term coal energy as well.

04-22-2016 – 11:00A
FE0022952 - Engineering Accessible Adsorption Sites in MOFs for CO_2 Capture
Clark Atlanta University Presenter: Saki T. Golafale

ABSTRACT

The goal of this project is to rationally engineer adsorption sites in 3D stable and porous metal organic frameworks (MOFs) for high capacity CO_2 uptake. To achieve this, we have embarked on 1) synthesizing diaza crown ether ligands-containing MOFs with metal ions positioned within the center of the organic linker, 2) incorporating nitrogen-containing ligands into MOFs and 3) using post-synthesis modification techniques to create accessible adsorption sites in large pore MOFs. This presentation will outline recent synthesis of two new transition metal diaza-crown ether coordination polymers with metal sites positioned within the crown moiety. Additionally, methods of post-synthesis modification and CO_2 adsorption behavior of our new, porous lanthanide metal organic frameworks based on pyrazine-2,3,5,6-tetracarboxylate and 4,4-stilbene dicarboxylate ligands respectively, will be discussed with emphasis on their structures and adsorption properties. We anticipate that the rational design of MOFs containing isolated metal sites within the center of organic linkers will increase CO_2 access to the sites. We also envisage that post-synthesis modification of MOFs with large pores can not only enhance CO_2 uptake, but also enhance thermal and chemical stability of MOFs. Our 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 to reduce CO_2 emission from fossil fuel combustion.

Track B – Friday, April 22, 2016

04-22-2016 – 09:00B
FE0023114 – Development of Reduced Order Model for Reacting Gas-Solids Flow Using Proper Orthogonal Decomposition
Florida International University Presenter: Sohail Reddy

ABSTRACT

The field of numerical analysis has dedicated much of its resources to the development of reduced order models to reduce computational time that can no longer be achieved by HPC. This work presents one such reduced order model based on proper orthogonal decomposition. The reduced order model is validated against a full order model for a lightly fluidized problem. A constrained reduced order model, utilizing the Karush-Kuhn Tucker conditions, which constrains the solution to user specified bounds, is developed and presented. The robustness and efficiency of the constrained reduced order model is validated on the transport equation. The reduced order solution and constrained reduced order solution of the transport equation is compared to the analytical solution. The use of the developed model, to constrain the gas void fraction in bubbling fluidized bed, is also investigated. The results show that the constrained reduced order model is able to satisfy the user-defined constrained for a continuous solution problem. It is however unable to constrain a problem whose discontinuous solution is represented by continuous basis functions. An alternative method, based on the concept of point modes that is able to cope with discontinuous solution is presented.

04-22-2016 – 09:30B
FE0011453 – Use of an Accurate DNS Method to Derive, Validate and Supply Constitutive Equations for the MFIX Code
University of Texas at San Antonio Presenter: Yifei Duan

ABSTRACT

A new drag model has been developed based on the resolved Direct Numerical Simulation (DNS) method. This drag model has been implemented in the MFIX code. Comparisons of different drag models have been conducted. In modeling gas-solid flows with Discrete Element Method (DEM) and Two-Fluid Model (TFM), the momentum exchange between particles and gas is attributed to the drag model. DEM and TFM simulations, with the incorporation of different closure laws, were performed using the MFIX code in order to study the hydrodynamics and bubble dynamics inside a bubbling fluidized bed. Four drag models including the Syamlal-O'Brien, Gidaspow, Koch-Hill and our recently developed model have been tested. The results of each model are then compared with the available experimental data. It was shown that regardless of drag model, the DEM simulation has a better accuracy compared to the TFM. Different drag models yielded different momentum exchanges. As a result the model will have a significant impact on the prediction of the "bubble" size in fluidized beds. The effect of a drag model on the bubble dynamics in bubbling fluidized beds will be quantitatively analyzed.

04-22-2016 – 10:30B
FE0024008 - Evaluating the Techno-Economic Feasibility of Forward Osmosis Processes Utilizing Low Grade Heat: Applications in Power Plant Water, Wastewater, and Reclaimed Water Treatment
Carnegie Mellon University Presenter: Meagan S. Mauter

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.

04-22-2016 – 11:00B
FE0024057 - COHO - Utilizing Waste Heat and Caron Dioxide at Power Plants for Water Treatment
Porifera Inc. & Idaho National Laboratory Presenter: Aaron Wilson, Idaho National Laboratory

ABSTRACT

For this project, we are developing a water treatment system, the COHO that is powered by low-grade heat and carbon dioxide at power plants. COHO combines the high-performance of a novel forward osmosis (FO) membrane with a carbon-dioxide based switchable draw. Forward osmosis technology excels in processing difficult-to-treat waters, such as blow down waters created by power plants. Porifera's novel FO membrane has higher flux and reduced reverse salt flux compared to conventional membranes. It is more chemically stable, enabling the development of a system that uses a draw solute that can capture carbon dioxide from flue gas. For this project, Porifera is collaborating with Idaho National Laboratory, the developers of a switchable draw solute that can obtain high osmotic pressure and is recyclable for reuse within the system. Porifera and Idaho National Laboratory are developing methods to achieve high water recovery with COHO in power plant feeds and optimizing the carbon capture process. COHO will reduce the volume of waste water, reduce the energy costs to treat wastewater, expand the capabilities of water treatment, and reduce the cost of carbon capture from flue gas.

2016 CROSSCUTTING RESEARCH & RARE EARTH ELEMENTS PORTFOLIOS REVIEW

GRAND STATION 3–5

POSTER PRESENTATIONS

TUESDAY, APRIL 19 — 5:00—6:45 P.M.

ADVANCED SENSORS

1 • **Passive Wireless Sensors Fabricated by Direct-Writing for Temperature and Health Monitoring of Energy Systems in Harsh-Environments** *– Ioannis Kortidis and Michael Comparetto, West Virginia University*

2 • **High Temperature Integrated Gas and Temperature Wireless Microwave Acoustic Sensor System for Fossil Energy Applications** *– Anin Maskay, University of Maine System*

3 • **Low-Cost Efficient and Durable High Temperature Wireless Sensors by Direct Write Additive Manufacturing for Application in Fossil Energy Systems** *– Rahul Panat, Washington State University*

4 • **Wireless Three Dimensional (3D) Nanorod Composite Arrays-Based High-Temperature Surface Acoustic Wave Sensors for Selective Gas Detection through Machine Learning Algorithms** *– Dongwook Kwak, University of Connecticut*

5 • **Metal Three Dimensional (3D) Printing of Low-Nitrous Oxide (NO_X) Fuel Injectors with Integrated Temperature Sensors** *– Jorge Mireles, University of Texas at El Paso*

HIGH PERFORMANCE MATERIALS

6 • **Physics-based Creep Simulation of Thick Section Welds in High Temperature and Pressure Applications** *– Thomas Lillo, Idaho National Laboratory*

7 • **Materials Qualification and Deployment for High Efficiency Coal Fired Boilers** *– Bruce Pint, Oak Ridge National Laboratory*

8 • **Microstructure and Properties of Ni-based Components Fabricated by Additive Manufacturing** *– Sebastien Dryepondt, Oak Ridge National Laboratory*

9 • **Data Science Initiative** *– Slava Romanov, NETL Research & Innovation Center*

INNOVATIVE ENERGY CONCEPTS

10 • **Combustion Synthesis of Boride-Based Electrode Materials for Magnetohydrodynamic (MHD) Direct Power Extraction** *– Sergio Cordova, University of Texas at El Paso*

SIMULATION BASED ENGINEERING

11 • **Interfacing MFIX with PETSC and HYPRE Linear Solver Libraries** *– Gautham Krishnamoorthy, University of North Dakota*

12 • **High Fidelity Computational Model for Fluidized Bed Experiments** *– Vinod Kumar, University of Texas at El Paso*

13 • **Institute for the Design of Advanced Energy Systems (IDAES)** *– John Eslick, NETL Research & Innovation Center*

14 • **Prediction of Discretization Error using the Error Transport Equation** *– Ismail Celik, NETL Research & Innovation Center*

Poster 01

FE0026171 - Passive Wireless Sensors Fabricated by Direct-Writing for Temperature and Health Monitoring of Energy Systems in Harsh-Environments

West Virginia University Presenter: Ioannis Kortidis and Michael Comparetto

ABSTRACT

The objective of the work is to develop 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 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 500-1700°C. A "peel-and-stick"-like transfer process to deposit the entire sensor circuit to various energy-system components will be developed.

The proposed work will be directed at the following areas: *1)* Investigation of phase formation, sintering/grain growth, and electrical properties of polymer-derived electroceramic composites between 500-1700°C; *2)* Definition of processes to direct-write through ink-jet and robo-casting the polymer-derived electroceramic composites onto oxide and polymer surfaces; *3)* Development of methods to form monolithic "peel-and-stick" preforms that will efficiently transfer the sensor circuit to ceramic surfaces after thermal treatment; *4)* Design of passive wireless LCR circuits and receiver (reader) antennas for communication and testing at temperature up to 1700°C.

Poster 02

FE0026217 - Integrated Harsh Environment Gas / Temperature Wireless Microwave Acoustic Sensor System for Fossil Energy Applications

The University of Maine Presenter: Anin Maskay (Student Researcher), 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 system capable of passive operation (no batteries) over the temperature range of 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 specific objectives of the project include: (i) the advancement of SAW sensor design, thin film development and integration, and device fabrication for simultaneous temperature and gas detection (H2, O2, and/or NOx) in harsh-environments between 350°C and 1000°C; (ii) implementation of a packaged sensor and interrogation system to demonstrate the acquisition of both temperature and gas information in harsh environments including laboratory test-beds, and possibly end-user sites to transition the technology into fossil energy power plant environments, such as the PERC waste-to-energy plant, the NETL Aerothermal Facility, and/or other end-user locations. The project is in its first six months of implementation, and is currently addressing: the thin film fabrication for gas sensor detection; the appropriate SAW platform design for the targeted gas sensor performance; and identification of the gas testing equipment and procedures.

The outcomes of this project are expected to enable the monitoring of gas / temperature sensor data in harsh environments up to 1000°C. The simultaneous detection of temperature and gas properties will be extremely valuable for real-time diagnostics and prognostics of fuel burning processes and equipment monitoring within advanced fossil energy power plants.

Poster 03

FE0026170 - Low-Cost, Efficient and Durable High Temperature Wireless Sensors by Direct Write Additive Manufacturing for Application in Fossil Energy Systems

Washington State University Presenter: Rahul Panat

ABSTRACT

Additively manufactured sintered 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 studying the electrical properties and microstructural changes of the metal nanoparticle films fabricated using an Aerosol Jet based micro-additive manufacturing method. High temperature in-situ impedance spectroscopy analysis was performed in ambient environment on Ag and Ni nanoparticle films at a frequency range of 20Hz-300KHz and at a temperature range of 24°C-500°C to characterize their electrical properties. X-ray diffraction, XPS, and SEM studies are performed to understand the microstructural changes and oxidation behavior of the films. 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. The real part of impedance increases as a function of temperature up to about 150°C, and then drops upon further heating before rising further. This behavior could be modulated by changing the initial film microstructure through nanoparticle sintering conditions. Unlike the Ag, the Ni films showed a high increase in impedance beyond 350°C indicating the onset of oxidation. In-situ impedance measurements of Ni films show that Ni undergoes a two stage oxidation behavior, with accelerated oxidation beyond 450°C. The work establishes the temperature range of operation for Ag and Ni films for sensor and other electronic applications.

Poster 04

FE0026219 - Wireless 3D Nanorod Composite Arrays based High Temperature Surface-Acoustic-Wave Sensors for Selective Gas Detection through Machine Learning Algorithms

University of Connecticut Presenter: Dongwook Kwak

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.

Poster 05

FE0026330 - Metal 3D Printing of Low-NOX Fuel Injectors with Integrated Temperature Sensors

The University of Texas at El Paso Presenter: Jorge Mireles

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. Low-NOx natural gas fuel injectors, commonly used in Dry Low NOx (DLN) gas turbine combustors, have complex internal cavities and passages to ensure tailored mixing of air and fuel to achieve ultra-low level of NOx emission. Since the current design methodology of these injectors is based on conventional fabrication techniques (e.g. multi-step machining and welding processes), a new paradigm of design methodology needs to be developed for their adaptation in the EBM fabrication process. A generic Low-NOx fuel injector 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.

Poster 06

FEAA090 - Physics-based Creep Simulation of Thick Section Welds in High Temperature and Pressure Applications

Idaho National Laboratory Presenter: Thomas M. Lillo

ABSTRACT

The welded microstructure of nickel-based alloys shows large variation in grain size and shape, as well as gamma-prime volume fraction, size and distribution. These heterogeneities can have a strong influence on the dislocation and/or diffusion mediated secondary creep, and, localization behavior leading to tertiary creep. Crystal plasticity based finite element method (CPFEM) has been widely used to incorporate the effect of microstructural heterogeneities on deformation at the polycrystalline scale and is being utilized in this work to model the creep behavior of the 740H welds. Current model development is focused on secondary creep considering dislocation climb, glide, and, anti-phase boundary shearing or Orowan looping. These secondary creep mechanisms have been extensively observed in base metals of nickel-based alloys at the temperature and stress levels the welds are expected to operate. A dislocation-density based CPFEM model addressing these mechanisms is currently being implemented in MOOSE software that provides the ability to solve problems involving multiple physics concurrently and implicitly. The workability of the model is being verified with available Alloy-617 base metal secondary creep data. Additionally, an experimental validation effort on ASME-qualified welds in Alloy 740 is under way and will include short term creep tests at 600-800°C of cross weld and all weld metal samples to determine input parameters for the model and long term creep tests at 760°C to validate the results of the modeling and simulation effort.

Poster 07
FEAA117 - Technical Qualification of New Materials for High Efficiency Coal-Fired Boilers and Other Advanced FE Concepts
Oak Ridge National Laboratory Presenter: Peter Tortorelli

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 and cross-weld creep and tensile testing needed for an ASME Boiler and Pressure Vessel Code Case and the associated microstructural analyses needed for assurance of boiler-relevant lifetimes. The major part of the work is the creep rupture testing from 593°-927°C (1100°-1700°F), which is over 500,000 h for three base metal heats and two different welding methods. Creep testing on the three base metal heats is in progress on 21 creep frames with over 50,000h of testing completed. The majority of the creep tests for the first heat have been started and 14 specimens have ruptured. The first 10,000 h creep tests are expected to fail in late 2016. In order to support the incorporation of this alloy into COMTEST, the component test project for the advanced ultrasupercritical concept, tensile testing at 25°-927°C will be conducted this quarter on the three base metal heats. Fabrication of the welds for the cross-weld specimens is in progress. This project includes cost share from Haynes International.

Poster 08
FEAA119 - Microstructure and Properties of Ni-based Components Fabricated by Additive Manufacturing
Oak Ridge National Laboratory Presenter: Sebastien Dryepondt

ABSTRACT

Additive manufacturing (AM) offers the possibility to fabricate complex near-net-shape components and can result in significant savings by decreasing the cost of tooling and materials. The large-scale production of high-temperature high-strength components has however not yet been achieved because of the difficulty to control the final microstructure, and, thus, properties of parts made by laser or electron beam melting. 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, Ni-22Cr-18Fe-9Mo) alloy. A collaboration between ORNL and Siemens will provide the unique opportunity of comparing results for HX alloy products made by the three main AM techniques, electron beam melting (EBM), laser metal deposition (LMD) and selective laser melting (SLM). So far, HX powder provided by Siemens was used at the ORNL manufacturing demonstration facility to fabricate test bars using EBM in order to conduct tensile, creep and fatigue testing. Microstructure characterization revealed large grains elongated along the build direction, and the presence of large precipitates along the grain boundaries.

Poster 09
Innovative Process Technologies (IPT): Data Science Initiative
NETL Research & Innovation Center Presenter: Vyacheslav Romanov

ABSTRACT

NETL data science initiative is a focused effort to support data-intensive research projects that will adapt and develop software tools so that it is possible to curate, archive and analyze large volumes of raw data, with the initial focus on fuel cell materials and advanced alloys, while they are used under extreme environments and power plant cycling conditions. Predictive materials degradation 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 experimental data are gathered as part of the ongoing domain science research at NETL as well as via literature search and collaboration with external organizations. The developed analytical tools and user interfaces will allow the FE experts and technology developers to train the system and to extract hypotheses and promising 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. Preliminary results of the alloys data analytics pilot are in line with domain knowledge expectations and suggest that cluster analysis might be a useful statistical analytics technique.

Poster 10
FE0026333 - Combustion Synthesis of Boride-Based Electrode Materials for MHD Direct Power Extraction
The University of Texas at El Paso Presenter: Sergio Cordova

ABSTRACT

NETL is partnering with the University of Texas at El Paso to develop a novel technology for an advanced, low-cost manufacturing of boride-based ultrahigh-temperature ceramics (UHTCs) for direct power extraction applications. The project will determine optimal conditions of mechanical activation, self-propagating high-temperature synthesis (SHS), and pressureless sintering for fabrication of doped zirconium diboride (ZrB_2) and hafnium diboride (HfB_2) that possess all the required properties 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 allow the production costs to be significantly less than in the case of synthesis from elements.

The combined technology will solve SHS problems, such as difficult ignition of low-exothermic mixtures and high porosity of products, and will allow for the utilization of great SHS advantages: low cost, low energy consumption, and high product purity.

Poster 11
FE0026191 - Interfacing MFIX with PETSc and HYPRE Linear Solver Libraries
University of North Dakota Presenter: Gautham Krishnamoorthy

ABSTRACT

High computational cost associated with the solution of large, sparse, poorly conditioned matrices is currently a serious impediment towards increasing the utility of computational fluid dynamic (CFD) models for resolving multiphase flows. This project will interface NETL's Multiphase 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 third-party solver libraries. The overall objective of this project is to first establish a robust well-abstracted solver interface that will present an extensible back-end that would allow 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. It is anticipated that this project could cut down the time to solution when compared to current linear solver options in MFIX, by at least 50 percent. It also could show that near linear scaling in parallel performance can be achieved to at least 1000 processors.

Poster 12
FE0026220 - High Fidelity Computational Model for Fluidized Bed Experiments
University of Texas at El Paso Center Presenter: Vinod Kumar

ABSTRACT

The objective of this work is to develop, validate and implement advanced linear solvers to replace the existing linear solvers that are used by the National Energy Technology Laboratory's (NETL) open source software package Multiphase Flow with Interphase eXchanges (MFIX). This is achieved by integrating Trilinos, a publicly available open-source linear equation solver library developed by Sandia National Laboratory, with MFIX. The work will demonstrate scalability of the Trilinos-MFIX interface on various high-performance computing facilities including the ones funded by the Department of Energy (DOE).

The objective of this work is achieved by (i) creating a framework to integrate the existing MFIX linear solver with Trilinos linear solver packages such as AztecOO, Belos, (ii) evaluate the performance of the state-of-the-art preconditions and linear solver libraries in Trilinos and perform a scalability analysis for the selected libraries on large parallel computing systems to improve computing performance of the Trilinos-MFIX interface, and (iii) compare the performance of the Trilinos-MFIX package on massively parallel high performance computers with the existing MFIX-linear solver packages for gas-solid fluidized bed problems.

The project will reduce the computational cost as well as convergence instabilities when solving gas-solid flow in large scale flow problems using MFIX. The project allows MFIX to use various preconditioner and solvers in Trilinos to solve complex flow problems on massively parallel computers.

Poster 13

The Institute for the Design of Advanced Energy Systems (IDAES)

NETL Research & Innovation Center Presenter: John Eslick

ABSTRACT

The Institute for the Design of Advanced Energy Systems (IDAES) will be the premier resource for development and analysis of innovative energy systems through advanced process systems engineering (PSE) approaches. Capabilities of IDAES will build on the groundbreaking advances developed under CCSI, such as the Framework for Optimization and Quantification of Uncertainty and Sensitivity (FOQUS) and Automated Learning of Algebraic Models for Optimization (ALAMO) tools, and will extend beyond existing capabilities. IDAES's computational capabilities will allow for development of new equipment, processes, and approaches, thus avoiding limitations associated with fitting a new material or concept to existing equipment.

The Institute will develop a 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). CCSI pushed the limits of what is possible with commercial simulation tools. Thus, IDAES will build on existing open source software to the extent possible and build new capabilities when required.

IDAES and its capabilities will be applicable to development of the full range of advanced fossil energy systems, including chemical looping and other transformational CO_2 capture technologies, as well as integration with new technologies such as supercritical CO_2. The tools and capabilities will be applicable to renewable energy development, such as biofuels, green chemistry, and Nuclear and Environmental Management, such as design of complex, integrated waste treatment facilities.

Poster 14
Prediction of Discretization Errors using Error Transport Equation
NETL Research & Innovation Center/ORISE Faculty Fellowship Program Presenter: Ismail B. Celik & Mehrdad Shahnam

ABSTRACT

Extensive application of computational fluid dynamics (CFD) in engineering design and analysis requires quantification of numerical and modeling uncertainty inherent to such calculations. A significant contributor to the overall simulation uncertainty is the discretization errors, arising from approximation of continuous derivatives by using discrete (finite) number of data points. Discretization error is function of mesh size; theoretically it should go to zero as the mesh size tend to very small (fine mesh) values. However, computational time and cost becomes exponentially higher as the mesh is refined. Hence, in practical industrial applications usually relatively coarse meshes are employed. The objective of this study is to formulate some strategies to quantify the extent of discretization error using relatively coarse meshes, and preferably using only a single mesh with the help of an error transport equation (ETE) formulated for a selected variable of interest. If this approached is successful, it will have significant consequences in uncertainty quantification (UQ) across the spectrum of all fields where computer simulations are used. This poster presents preliminary results for a classical multiphase flow problem, namely that of core-annual flow regime with a periodic, transient solution. The results presented in this poster demonstrate the potential of the approach developed so far, which is encouraging.

Poster 15
SC0013811 - Wireless Networked Sensors in Water for Heavy Metal Detection
NanoSonic, Inc. Presenter: Hang Ruan

ABSTRACT

The overall goals of this project are to develop wireless networked sensors using conformal nanomembrane-based (NM-based) chemical field effect transistors (chemFETs) for the detection of all eight Resource Conservation and Recovery Act heavy metals (the RCRA 8s) in water and to combine advanced nanotechnology thin film deposition process—Electrostatic Self-Assembly—and conformal nanomembrane chemFET technology to produce a wireless sensor network for in situ environmental monitoring.

To achieve these goals, the project will: 1) Develop an improved understanding of the operation of NM chemFET sensors through engineering analysis, modeling, and direct side-by-side experimental comparison of commercial chemical sensors, 2) Further design polymer and semiconductor chemistries to improve sensor sensitivity, selectivity, and re-usability, 3) Integrate wireless chemFET sensors on a unmanned aerial vehicle (UAV) platform (as a transceiver) to demonstrate small size, low power consumption and energy harvesting feasibility and 4) Characterize improved NM chemFET sensors using NanoSonic facilities and equipment available at Virginia Tech.

The successful completion of this project could allow for efficient monitoring of RCRA 8 heavy metals for environmental surveillance in water, locate pollution sources using analysis from concentration gradients, and detect and map chemical concentrations that are potentially harmful to people and/or destructive to industry agriculture.

Poster 16
SC0013863 - Integrated Sensors for Water Quality
Sporian Microsystems, Inc. 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 expensive, large, and difficult to install or deploy, which inhibits the ability of utilities 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, and that can relay relevant, real-time in-situ water measurements. Ideally such hardware would simultaneously monitor multiple water quality factors and contaminants at a reduced overall cost. Sporian is currently developing an integrated, inexpensive, portable, easy-to-use sensor designed to monitor a range of water quality factors (pH, turbidity, TDS, etc.) and contaminants including RCRA 8 heavy metals in near real time. Such a technology will be highly attractive for broad application within energy, industrial/agricultural, and civilian drinking water and wastewater monitoring sectors.

Poster 17
Advance Membrane Materials & Processes for Desalination of High Salinity Brines
NETL Research & Innovation Center Presenter: Nicholas Siefert

ABSTRACT

There are a number of high salt concentration waters produced during oil/gas development, during CO_2 storage, or from geothermal reservoirs. The overall goal of this research is to reduce the volume of saline water produced as a result of operations involving these high salinity waters. A NETL/CMU/LANL team is developing two distinct polymeric-membrane based approaches toward treating these high salinity brines. One approach utilizes waste heat in a hot gas sweep evaporative membrane distillation process to both further concentrate the brine and improve co-located power production opportunities and efficiencies. The second approach utilizes a multi-stage, osmotically-assisted reverse osmosis process with the goal of enabling the use of commercially-available RO membranes to treat brines with significantly higher salt concentrations than those accessible with conventional RO processes. Finally, we will be optimizing these process approaches for specific applications and conducting techno-economic analyses of both process, and comparing them against commercially-available process for treating high salinity brines.

Poster 18

FE0026927 - Recovery of REEs from Coal Mine Drainage

West Virginia University Presenter: Paul F. Ziemkiewicz

ABSTRACT

Phase 1 objectives include: 1) development of a cost-effective and environmentally benign process to treat and recover Rare Earth Elements (REEs) from acid mine drainage (AMD), which has been considered a serious long-term environmental problem associated with coal mining; and 2) preparation for Phase 2 of the project, which entails a process design for prototyping and a through techno-economic analysis (TEA). This project will take advantage of autogenous processes that occur in coal mines and associated tailings which liberate and concentrate REEs. Recent evaluations of AMD samples yielded elevated concentrations of REEs in low pH influent to AMD treatment systems that were nearly absent in the discharge water. This indicates REEs precipitate, with other largely transitional metals in the AMD treatment precipitates (sludge), most likely as hydroxides. Sparse direct measurement data exists on REEs concentrations in AMD sludge. Therefore, we developed an estimation method to assess the input/output REEs loads through AMD treatment systems and estimate the total mass of sludge. The model suggests REEs in AMD sludge are concentrated by factors ranging from 800 to 24,000 over the concentrations in untreated AMD. The same model suggests AMD sludges range from 100 mg REE/kg to 3,000 mg REE/kg.

Poster 19

FE0027012 - Recovery of Rare Earth Elements from Coal Ash with a Closed Loop Leaching Process

Battelle Memorial Institute Presenter: Rick Peterson

ABSTRACT

Battelle with support from its partners will validate the economic viability of Battelle's patented closed-loop Acid Digestion Process (ADP) for recovering REEs from coal ash. 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 for the use of the ADP in REE extraction. Three sources of coal ash will be targeted for evaluation 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) residual ash from Battelle's coal liquefaction process. Making use of residual ash from coal liquefaction processes directly leverages work currently being conducted by Battelle for DOE NETL in response to DE-FOA-0000981 entitled "Greenhouse Gas Emissions Reductions Research and Development Leading to Cost-Competitive Coal-to-Liquids Based Jet Fuel Production." The techno-economic assessment will account for regional availability of high REE concentration coal sources and the preparation of the coal sources to ensure a high concentration feedstock. The anticipated result will be an economically viable process to generate rare earth concentrates from coal byproducts, along with a commercialization plan that takes into account the needs of coal industry stakeholders and product end users.

Poster 20
FE0027102 - Plasma Arc Gasification Based Rare Earth Element Recovery from Coal Fly Ash
Southern Research Presenter: Ken Jeffers, P.E.

ABSTRACT

Southern Research will evaluate an innovative technology designed to concentrate rare earth elements (REEs) in coal fly ashes (CFAs). Plasma arc technology is utilized in the proposed process which has two technology options: (a) plasma smelting and (b) plasma smelting plus volatilization and sequential condensation. CFAs will be smelted in a reducing environment in both options utilizing plasma arc technology. The CFA will partition into an upper slag layer and a lower metal matte layer. It is expected that REEs will partition mostly to the metal matte layer. In the plasma smelting only option, the molten matte layer will be cast in a mold and allowed to cool. The layer will be fragmented and processed for REE recovery. It is also possible to process the metal matte layer through multiple passes of the plasma smelting process for enhanced REE enrichment. In the plasma smelting plus volatilization and sequential condensation option, the metal matte layer will be heated following the smelting process to temperatures up to 3,700 °C thereby volatilizing most of the components of the metal layer. The volatilized components will then undergo sequential condensation. The proposed process aims to develop an economically viable domestic source of REEs from a waste stream. Since 2002, the United States has become almost 100% dependent on foreign sources of REEs. The proposed process also develops an additional beneficial use for coal fly ash. Over 27 million metric tons of coal fly ash were landfilled in 2013.

Poster 21
FE0027155 - Economically Viable and Environmentally Benign High-Performance Technology to Recover REE from Coal By-Products
Tusaar Corporation Presenter: Dr. Dean Stull and Dr. Gary Carlson

ABSTRACT

The goal of this Phase I project is to develop a bench-scale rare earth element (REE) extraction process for coal by-product materials utilizing a proprietary technology involving leaching processes and metal sorption media with the ability to process one kilogram batches and deliver a product meeting or exceeding DOE requirements. 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. These objectives have been successfully demonstrated at laboratory scale by Tusaar using other source materials.

It is expected that successful execution of this project will lead to possible reduction in the dependence of the US and other western countries on China, 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.

Poster 22

FE0026952 - Novel Membrane and Electrodeposition-Based Separation and Recovery of Rare Earth Elements from Coal Combustion Residues

Duke University Presenter: Heileen Hsu-Kim

ABSTRACT

This project will develop and demonstrate bench-scale technology to separate and concentrate rare earth elements (REEs) from coal fly ash and other coal combustion residues (CCRs). In our previous work, developed a database of CCRs to identify trends in total and acid-extractable REE contents as a function of major element contents, the origin of feed coal, as well as other characteristics. As part of this work we will use these parameters to identify and group CCR feedstocks for REEs recovery. The general approach will involve hydrometallurgical techniques, in which REEs are leached from fly ash by acid extraction and further separated from the leachates by membrane filtration and electrochemical deposition. A variety of nanofiltration, carbon nanotube-enabled electrodeposition, and other ion separation configurations will be tested with leachates of the CCR samples. From this work we will identify the most promising system for Phase 2, which entails development and optimization of a bench-scale system. 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.

Poster 23

FE0027035 - 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

University of Kentucky Presenter: Rick Honaker

ABSTRACT

The main objective of project is to develop, design and demonstrate a pilot-scale processing system for the efficient, low-cost and environmentally benign recovery of high-value rare earth elements (REEs) from coal and coal byproducts. The proposed system integrates both physical and chemical separation processes that are commercially available and environmentally acceptable. The innovative enabling technology utilized in the proposed system includes an advanced froth flotation process and a novel hydrophobic-hydrophilic separation process. Both these enabling technologies were developed previously under DOE sponsorship by the project investigators working within the Center for Advanced Separation Technologies (CAST). The proposed pilot-scale circuit will have a dry solids feed rate of ¼-ton/hr (0.23 tonne/hr) and will be capable of producing 5 - 7 pounds (2.3 – 3.2 kg) per hour of combined concentrates with purity levels of at least 2% total REEs by weight while recovering greater than 50% of the REEs at a cost of less than $20 per feed ton. The total REE purity of the final product will be reported on a dry basis for solid material as measured by elemental analysis. The technical and economic feasibility of the proposed system will be fully evaluated with respect to separation performance, throughput capacity, capital/operating costs, and environmental acceptability.

Poster 24
FE0027006 – Investigation of Rare Earth Element Extraction from North Dakota Coal-Related Feedstocks
University of North Dakota Presenter: Steve Benson

ABSTRACT

The University of North Dakota is teaming with Barr Engineering and Pacific Northwest National Laboratory to develop a high performance, economically viable, and environmentally benign technology to recover rare earth elements from North Dakota lignite, associated sediments, and a lignite drying system reject stream. The project involves the following objectives: 1) develop sampling protocols and obtain statistically representative samples of lignite, associated roof and floor materials, and coal drying reject stream; 2) determine the abundance and forms of rare earth elements and relevant material properties; 3) determine the potential to concentrate REE through mineral processing methods that include gravity separation, fine coal cleaning technologies and novel separation technologies based on size and density of REE-bearing components in the samples; 4) identify the optimum methods to separate and concentrate the REEs to 2 percent by weight, 5) perform a technical and economic analysis of the optimum methods; 6) develop a design of a bench scale system (5 to 10 kg/hour throughput) to concentrate the REEs. Successful development of REEs recovery process from coal-related feedstocks will provide tremendous economic benefit and help ensure the supply of REEs to a multitude of high-importance end-use applications.

Poster 25
FE0027167 - High Yield and Economical Production of Rare Earth Elements from Coal Ash
Physical Sciences Inc. Presenter: Prakash B. Joshi

ABSTRACT

Physical Sciences Inc. will build on previous work to optimize the enrichment/recovery process stages and build and demonstrate the REE extraction process component in a continuous mode. In Phase I, the project team will develop a design of a pilot-scale plant to economically produce high-yield rare earth element concentrates and commercially viable co-products from coal ash using environmentally safe physical and chemical enrichment processes. The team will work to facilitate the optimization of individual process stages, unit operations, and process parameters. The team will develop a detailed techno-economic model of the continuous process, including ash feedstock and reagent inputs, REE concentrate, and co-product outputs of commercial value, taking into account capital and operating expenses. The pilot-scale circuit will be designed to process a dry ash throughput of 1-5 tons per day of rare earth mineral concentrates with purity levels of at least 2% REEs by weight (wt%), with the goal of producing dry mixtures of nitrates with REE concentrations above a 5 wt% threshold and preferably to greater than 10 wt%. The proposed work, if successful, will demonstrate an environmentally benign and economically feasible method of providing a reliable and cost-competitive domestic source of rare earth elements and reagents recovery.

Poster 26
FE0027069 - A Pollution-Prevention and Economically-Viable Technology for Separation of Rare Earth Elements from Powder River Basin (PRB) Coal Ashes
University of Wyoming Presenter: Hanjing Tian

ABSTRACT

The overall performance goals of the new technology are to generate near-zero pollution and achieve at least 90% REEs recovery from coal ash at 50% lower energy consumption and 30% lower total cost compared to conventional commercialized REE recovery technologies. The technical objective of this project is to develop a new pollution-avoiding and cost-effective technology with enhanced performance and easy scalability for recovering high-value Rare Earth Elements (REEs) from Powder River Basin (PRB) coal ashes that have at least 300 ppm REEs and enriching the concentration of REEs from 300 ppm (weight concentration) to at least 2.0 weight % total REE content on an elemental basis and measured on a dry basis for solid material. The expected results of the project will be that the innovative REEs separation technology will be ready for large lab or pilot scale testing based on the analysis of the bench-scale test data and the techno-economic analysis performed in this project.

Poster 27
Characterization and Recovery of Rare Earths from Coal and By-Products
NETL Research & Innovation Center Presenter: Evan J. Granite

ABSTRACT

Everything that is in the earth's crust is also present within coal to some extent, and the challenge is always to utilize abundant domestic coal in clean and environmentally friendly manners. In the case of the rare earths, these valuable and extraordinarily useful elements are present within the abundant coal and coal by-products produced domestically and world-wide. These materials include the coals, as well as the combustion by-products such as ashes, coal preparation wastes, gasification slags, and mining by-products. All of these materials can be viewed as potential sources of rare earth elements.

Much of the recent research on coal utilization in the United States has focused upon the capture of pollutants such as acid gases, particulates, and mercury, and the greenhouse gas carbon dioxide. The possible recovery of rare earth and other critical elements from abundant coal and by-products is an exciting new research area, representing a dramatic paradigm shift for coal. Additional data is needed on the rare earth contents of coals and by-products in order to determine the most promising potential feed materials for extraction processes. Future work will focus on identification of promising by-products, characterization of coals and by-products, and separation/partitioning methods for rare earth recovery. Some of the early and exciting results for characterization, recovery, and the geochemistry of the rare earths and other critical elements will be briefly described.

National Energy
Technology Laboratory

1450 Queen Avenue SW
Albany, OR 97321-2198
541-967-5892

420 L Street, Suite 305
Anchorage, AK 99501
907-271-3618

3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26507-0880
304-285-4764

626 Cochrans Mill Road
P.O. Box 10940
Pittsburgh, PA 15236-0940
412-386-4687

13131 Dairy Ashford Road, Suite 225
Sugar Land, TX 77478
281-494-2516

WEBSITE: www.netl.doe.gov

CUSTOMER SERVICE: 1-800-553-7681

U.S. DEPARTMENT OF
ENERGY

National Energy
Technology Laboratory

1450 Queen Avenue SW
Albany, OR 97321-2198
541-967-5892

420 L Street, Suite 305
Anchorage, AK 99501
907-271-3618

3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26507-0880
304-285-4764

626 Cochrans Mill Road
P.O. Box 10940
Pittsburgh, PA 15236-0940
412-386-4687

13131 Dairy Ashford Road, Suite 225
Sugar Land, TX 77478
281-494-2516

WEBSITE: www.netl.doe.gov

CUSTOMER SERVICE: 1-800-553-7681

U.S. DEPARTMENT OF
ENERGY