



Virtual

Thirty-Eighth Annual COAL CONFERENCE

University of Pittsburgh · Swanson School of Engineering

ABSTRACTS BOOKLET

**Clean Coal-based Energy/Fuels
and the Environment**

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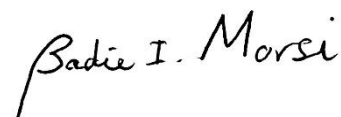
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On behalf of the Thirty-Eighth Annual International Pittsburgh Coal Conference, I wish to express my sincere appreciation and gratitude to Ms. Kristen Harper for her meticulous leadership and guidance of the entire conference till her leave on August 8, 2021. Great thanks and appreciations go to Ms. Nicole Drebsky for keeping the conference on track and controlling its final operation. My profound gratefulness goes to Mr. Rui Wang for his crucial assistance and dedication in preparing this Abstracts Booklet.

Thank you,



Badie I. Morsi, Editor
Professor and Executive Director of the Conference

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SESSION 1 (8:00 – 9:45)
GASIFICATION TECHNOLOGIES – 1
Alberto Pettinau and David Lyons

1.1 (8:05-8:25) The Influence of Interactions Among Calcium, Silicon and Aluminum on Coal Gasification

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Ningxia University, CHINA

The aim of this work is to find out the influence of other inert minerals on the catalytic activity of Ca in coal gasification. Four coal samples, demineralized coal (Dem-coal), coal loaded Ca (Ca + Dem-coal), coal containing Si and Al ((Si, Al)-coal), and coal loaded Ca, Si, and Al (Ca +(Si, Al)-coal), were prepared and the gasification activity was evaluated by a thermal gravimetric analyzer (TGA) with CO₂ agent at 900 °C. To timely record the morphology evolution of coal particles during the entire gasification process, an in-situ heating stage microscope was used. Also, nitrogen adsorption data and scanning electron microscopy (SEM) images were collected to investigate the evolution of physical structure of coal char. Additionally, FactSage thermodynamic calculation in collaboration with insitu X-ray diffraction (XRD) was applied to clarify the interactions among Ca, Si, and Al. It is found that Ca existing in the form of CaO shows an excellent catalytic performance. Si and Al, in the form of SiO₂ crystals and amorphous structure respectively, inhibit the reaction to a large degree. Remarkably, the interactions among Si, Al, and Ca accelerate coal gasification to some extent, though the gasification reactivity of Ca+(Si, Al)-coal is a bit lower than that of Ca + Dem-coal. In-situ XRD patterns demonstrate the formation of CaSiO₃, Ca₂SiO₄, and Ca₂Al₂SiO₇, suggesting that these Ca complexes are catalytically active, but the catalytic performance of them is inferior to that of CaO. The evidence proved powerfully that it is not the reactions among Ca, Si, and Al, which caused the deactivation of Ca catalyst.

1.2 (8:25-8:45) Neutron-Scattering Diagnostics for Improved Gasifier Modeling

Charles E.A. Finney, Costas Tsouris, James E. Parks II,
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Gasification involves complex processes, and theoretical simulations are critical for the design of next-generation advanced reactors. Models used for such simulations, including MFIX, rely on validation data for tuning and accuracy. Nonintrusive measurements within an operating reactor are difficult, but neutrons can traverse reactor vessel walls and interact with light elements such as hydrogen in the coal as it thermally degrades. We have been conducting neutron-based studies of coal under pyrolysis conditions to understand the dynamic behavior of a coal gasifier bed as coal particles undergo thermal degradation and release gas mixtures during pyrolysis. We are contributing to a comprehensive, multi-pronged approach to improve computational models of coal and biomass pyrolysis and gasification.

We will present progress in our development of the methodology and results of these experiments to produce nonintrusive visualization data and validation information that enable accurate simulations of coal gasification beds. Our strategy involves using neutron radiography to map reaction levels in the reactor bed with spatial and temporal variations, supplemented by additional measurements such as physical and chemical characterization of the coal particles at different stages of pyrolysis. Some of these supplemental techniques involve complementary neutron and X-ray measurements. We will present results from experiments at the Center for Neutron Research at NIST, the High Flux Isotope Reactor and the Spallation Neutron Source at Oak Ridge National Laboratory. With this study, we seek to produce a map of coal pyrolysis and associated physical-chemical changes within the vessel to improve the bed-scale modeling component of the overall system CFD model.

1.3 (8:45-9:05) Effect of Gasifying Agent During Microwave-Assisted Coal Gasification

Candice Ellison and Mark Smith,
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Application of microwave heating to coal gasification is a compelling process intensification strategy and has been shown to lower gasification temperatures, increase conversion efficiencies, and reduce tar production compared to conventionally heated gasification. Microwave gasification can offer greater energy and process efficiencies

through direct, volumetric heating and lends itself well to modular scale applications. The choice of gasifying agent (air, steam, CO₂, or mixtures thereof) has a major impact on conversion and yields of gasification products, which affects the overall process performance and efficiency. The effect of the gasifying agent during a microwave-assisted gasification process is not well understood and is the focus of this study. Microwave gasification of a sub-bituminous coal (Wyodak) was experimentally tested under CO₂, steam, and a mixture of the two (50/50 vol% CO₂/H₂O) at 700 °C. Baseline tests were carried out by conventional gasification under the same conditions. Product gases were analyzed by online mass spectrometry and micro-gas chromatography. The gasifying agent was found to significantly impact the composition of syngas with a H₂/CO stoichiometric ratio of 0.19, 0.98, and 0.63 corresponding to CO₂, steam, and CO₂/steam, respectively, under microwave gasification. Comparative gasification tests under conventional heating and CO₂/steam yielded syngas with H₂/CO ratio of 1.92, albeit with considerably less syngas yield overall compared to microwave gasification under the same conditions. By comparison of carbon conversion and product gas yields under microwave and conventional gasification, a better understanding of the role of microwaves and the gasifying agent(s) on the gasification process will be realized. Results from microwave gasification testing under different oxidant conditions will help inform process design decisions for future implementation of a microwave moving bed gasifier.

1.4 (9:05-9:25) Real-Time Measurement of Cavity Growth in Lab-Scale Underground Coal Gasification by Electrical Capacitance Tomography

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Zuzhou, CHINA

Underground coal gasification (UCG) is a promising technology for direct utilization of coal seam which is difficult to mine. Even there are lots of lab-scale UCG experiments reported in literatures, it remains a problem to monitor the growth of gasification cavity, leading to a limitation for understanding the gas-solid reaction behaviors in UCG processes. In this paper, electrical capacitance tomography (ECT) was applied to measure the transient structure of the gasification cavity, based on the difference of dielectric constants between coal and air. Given the requirements of high accuracy and fast response, both the hardware and the software of the traditional ECT needs to be modified for the measurements in the UCG experiments. The actual structure of the cavity was studied in detail with a 3-D laser scanner after the lab-scale UCG experiment, and the results were further used to validate the ECT measurements. We analyzed the performance of different settings of ECT hardware, and finally recommended a number of 18 for the electrodes and 153 for capacitance data sets. Besides, 2-D and 3-D matrix of sensitivity from COMSOL Multiphysics software was compared, and it was shown that 3-D matrix was a better choice to use in ECT processing. Moreover, different image reconstruction algorithm methods of ECT were adopted, and the Landweber method proved a good agreement with the laser-scanning results. The self-developed ECT method was further used in the real-time measurements of the gasification cavity in lab-scale UCG experiments. The error of measured characteristic length of gasification cavity by ECT is smaller than 23%.

1.5 (9:25-9:45) Overview of DOE/FE Gasification Program R&D

Jai-woh Kim, U.S. Department of Energy, Washington DC, USA
David Lyons, U.S. DOE, National Energy Technology, Morgantown, WV, USA

The Gasification Systems Program, conducted under the U.S. Department of Energy's Office of Fossil Energy (FE), is focusing on development of advanced technologies that reduce the cost of gasification of mixed feedstocks (waste coal, waste plastics and biomass) enabling high efficiency and excellence environmental performance of net zero carbon emissions with the integration of pre-combustion carbon capture (CCS) to produce decarbonized fuels like hydrogen.

Due to high capital investments required for large conventional coal gasification plants, the FE Gasification Systems Program is focusing on modularization, process intensification and solutions for process issues arising when wider feedstock combinations are deployed for hydrogen production with improvement of the efficiency and cost of small-scale gasification-based plants to make them more attractive in the marketplace.

This talk will highlight a broad overview and progress that the DOE's FE Gasification Systems Program has made on small-scale, modular gasification systems and cost reduction of each component of the overall gasification system along with a detailed discussion of future co-gasification technology advances of mixed feedstocks for high purity hydrogen production.

2.1 (8:05-8:25) Thermal Behavior of Crystalline Minerals in Argonne Premium Coals Under Air and Argon Atmospheres-Comparison Between Bituminous, Subbituminous and Brown Coals

Hung Nguyen, Tadanori Hashimoto, Yu Tsuchimori, and Atsushi Ishihara

Kurima Machiya-Cho, Tsu City, Mie, JAPAN

Masakatsu Nomura, Osaka University, Osaka, JAPAN

It is important to know the behavior of ash components with changing the processing temperature and atmosphere. Therefore, we have investigated the changes of ash components in coal with changes in atmosphere and treatment temperature. The results showed that the needle-like crystals appeared from the different heat treatments between Upper Freeport (UF) and Illinois#6 (IL) coals (ACS Omega, 2021, 6, 2, 1197–1204). In this study, we investigated the change in the behavior of ash components of Wyodak-Anderson (WD) and Beulah-Zap (BZ) Argonne Premium coals with changes in atmosphere and treatment temperature. As the coal samples, brown coal BZ, subbituminous coal WD and bituminous coal UF were used. Thermogravimetric analysis (TG) and differential thermal analysis (DTA) were carried out in an atmosphere of air at a gas flow rate of 100 ml/min, temperatures 1200 °C and a heating rate of 10 °C/min. X-ray diffraction and TEM measurements were performed to investigate the crystal structures of ash components in coal samples treated under air or argon atmosphere. Among the coals used in this study, the ash content decreased in the order UF > BZ > WD. The fixed carbon and the content of C decreased in the order UF > WD > BZ.

Initially WD was treated at various temperatures in an air atmosphere. From the XRD results, quartz and kaolinite were found in the WD before calcination. Quartz SiO₂ was found at all temperatures after calcination, but kaolinite disappeared. Lime CaO was observed at 800 °C and 1000 °C, but not at higher temperatures. Anhydrite CaSO₄ and hematite Fe₂O₃ were found at all temperatures after calcination. In addition, the strength in signals of quartz decreased with increasing temperature, indicating that quartz changed at the higher temperature by reacting with other components. Although anhydrite was observed at all temperatures, the strength decreased at 1200 °C and that of gehlenite increased instead, indicating that anhydrite partially changed to gehlenite. The similar observation was found in BZ. When XRD patterns for various coals treated at 1000 °C in an air atmosphere were compared, anhydrite was found in all coals. Hematite was confirmed in coals other than BZ, and it is considered that hematite changed from pyrite under air conditions. WD coal showed a similar tendency to UF coal. However, the peak of anhydrite was strong at all temperatures, which can be attributed to the difference in the SO₃ content in the ash.

When TG-DTA up to 1200 °C in air atmosphere was compared, bituminous coal UF showed a gradual increase in the range 200-300 °C, suggesting that this would come from the adsorption of oxygen by metal species. In addition, the sample showed a large weight loss in the range 500-600 °C and then gradually increased in weight. On the other hand, no oxygen adsorption was observed in the brown coal BZ sample, and a large weight loss was observed in the range 400-500 °C, which was lower than the cases for UF coal. WD coal had the highest weight loss compared to other coals, which was observed at lower temperature.

TEM images of UF and BZ samples treated at 1000 °C under argon were compared, small black crystals surrounded by somewhat transparent amorphous phase of coke formed large masses in all coals. Troilite formed by the reduction of pyrite was observed under argon treatment for all coals in XRD measurement, suggesting that significant parts of observed small black particles would be troilite.

2.2 (8:25-8:45) Thermal Desorption of Mercury Compounds from Coal in the Conical Spouted Bed Reactor

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Lehigh University Energy Research Center, Bethlehem, PA, USA

Quang Truong, Advanced Cooling Technologies, Inc., Lancaster, PA, USA

Huazhi Chen, Zhanjiang University of Science and Technology, Zhanjiang,

Guangdong, China

Coal combustion is currently the major source of mercury emission to the environment, which gradually becomes a worldwide concern due to its increasingly harmful effect on human health. This study focused on investigating the mercury removal efficiency of the conical spouted bed reactor (CSBR), as a pre-combustion mercury removal treatment, for three coal ranks (anthracite, bituminous, and lignite) based on the concept of thermal desorption of mercury compounds. A baseline and improved CSBR were designed by Advanced Cooling Technologies (ACT), Inc. to improve heat transfer and mixing, with

an inner diameter of 12 inches. A thermal scanning test was developed to assess static mercury removal efficiencies at different temperatures. Based on the test results, the inlet air temperatures of the CSBR were determined at 250, 300, and 250 °C for anthracite, bituminous, and lignite coal, respectively. To identify the hydrodynamic behavior of coal particles in the CSBR, two-dimensional modeling consisting of dispersed solid particles (coal) and a carrier phase (air) was performed based on the geometry of the baseline CSBR. An optimal combination of 4 mm particle size and 27.5 m/s reactor inlet airflow velocity was identified. In this combination, coal particles were spouting smoothly inside the reactor but not entrained by the airflow. Bituminous coal was firstly tested by both CSBRs. Improved CSBR removed 65% mercury from coal, which was 85.7% more mercury removal than the baseline CSBR. Therefore, anthracite and lignite coals were only tested by the improved CSBR, and their mercury removal efficiency achieved 48 and 88%, respectively. The results indicated that the CSBR is a promising pre-combustion treatment for mercury removal from coal. The research work discussed here was performed as a part of Small Business Innovation Research (SBIR) Phase I & Phase II grants, supported by the Department of Energy, under Award no. DE-SC0017232.

2.3 (8:45-9:05) Prediction of Maceral Content Based on Physical and Chemical Properties

Kai Zhao, Zhen Li, Jing Chang, and Huaqing Zhang,

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Knowing the macerals content in ultra-fine coal is of significant importance to coal gasification, liquidation and pyrolysis, however, the current methods are very complex and time-consuming. In order to predict the content of organic coal macerals in raw coal, the relationship between organic coal macerals content and its physical and chemical structure was investigated using the low-rank raw coal with high inertinite obtained from Jurassic coalfield Dabaodang coal mine. The raw coal was first crushed and ground, then separated using the float-and-sink centrifugal separation method to get 7 coal samples with different macerals contents. To provide the data demanded by the following regression fitting, the physical and chemical structures of the coal samples were characterized using Fourier transform infrared spectroscopy (FTIR), X-ray diffraction test (XRD), X-ray photoelectron spectroscopy (XPS) and nuclear magnetic resonance imaging test (NMR) technology. The hydrogen-enrichment parameters Q_{1a} and Q_{1b} calculated based on the full spectrum of FTIR showed a gradual increasing trend; the XRD analysis revealed that the aromaticity fa-XRD of the 7 samples gradually increased with the vitrinite content; the XPS carbon spectrum showed that the sum of C-C and C-H content (Q₄) gradually increased with the vitrinite content; the 13C-NMR analysis exhibited that the total aromatic carbon mass fraction fa, the mass fraction of alkyl-substituted aromatic carbon and aromatic bridging carbon f_a^{B,H}, the mass fraction of aromatic carbon f_a⁻ have a negative correlation with the vitrinite content. The total mass fraction of aliphatic carbon f_a⁺ have a positive correlation with the vitrinite content. These physical and chemical properties of macerals were used to establish a regression model of macerals with Q_{1b} (X₁), f_a-XRD (X₂), Q₄ (X₃), f_a^{B,H} (X₄) being independent variables, and vitrinite content (Y) being the dependent variable, the optimal linear regression equation obtained was: Y=298.22+5.48X₁-38.23X₂+0.28X₃-6.88X₄. This equation was verified using a set of experimental data, and the deviation between the predicted value and the test value is 0.2%. This research proves that there is a linear correlation between the content of maceral composition in low-rank coal and its physical and chemical structure, which can be used to predict the content of organic coal macerals.

2.4 (9:05-9:25) Judging the geological origin of Cretaceous coals from the Wulantuga coal-hosted Ge deposit, Shengli coalfield, northeastern China: Insights from coal petrology and geochemistry

Xiaoshuai Wang, Yifan Chen, Yuegang Tang, Tengda Ma, Guoying Yan,

College of Geoscience and Surveying Engineering,

China University of Mining & Technology (Beijing), Beijing, China

In order to provide a reference for the geological origin of the Wulantuga coals, maceral compositions of 77 coal bench samples were systematically investigated from sample collection to data analysis, regarding to which their depositional environment was discussed with the incorporation of coal geochemistry indicators. The achieved results and understandings are as follows. From top to bottom of the section of the #6 coal seam, the contents of the vitrinite increase gradually while that of the inertinite decrease by degrees. The variation of maceral compositions on the vertical profile indicates the instabilities of the peat depositional environments and the changes of coal-formation mires. As a whole, these trace elements (Sr, Ba, Th, U, and REY) are depleted or normal in Wulantuga coals and other elements, such as Ge, As, Hg, Sb are unusually enriched in them. And the concentrations of REY in the two partings are higher than their corresponding concentrations in the bench coal samples, which supports that they have inorganic affinities and indicates a major detrital source of the REY in the Wulantuga coals. Based on the maceral index analyses, the #6 coal seam in the Wulantuga mine was speculated to be formed in a limnic and rheotropic marsh with a low participation of forest vegetation. With the accumulation of the #6 coal seam, the gelification and moist of the ecosystem environment are from strong to weak and its redox condition is from

reduction to weak oxidation, which is consistent with the variation of the maceral composition from top to bottom of the #6 seam section. In regarding to these geochemical indicators, the #6 coal seam was thought to have been hardly affected by brackish or saline water. The REY anomalies (Ce, Eu, and Y) and REY distribution patterns were speculated to be dominantly depended on the detrital compositions in the sediment source region and to be affected by the reductive environment and by the hydrothermal solution inputs. According to the geological origin analysis and its weakly organic affinities, germanium unusually enriched in Wulantuga coals is closely related to the hydrothermal fluids during the diagenetic stages. Given the above, based on these indicators, the reference for the geological origin of Wulantuga coals was provided, which is of theoretical and scientific significance. In the future, coal-formation environments (Ge-rich coals) should be comprehensively studied from more aspects, such as stratigraphy, sedimentology, and palynology.

2.5 (9:25-9:45) Overview on Mercury Control Options for Coal-Burning Power Plants

Evan J. Granite,
US-DOE, NETL, Pittsburgh, PA, USA

With the USEPA issuing a national regulation requiring high levels of mercury capture, the need exists for low-cost removal techniques that can be applied to coal-burning power plants. The injection of powdered activated carbon into the ductwork upstream of the particulate control device is the most developed technology for mercury capture. Alternative techniques for mercury capture also play a major role because of the numerous configurations of air pollution control devices present within the power plants, as well as the many different coals and coal-blends being burned. These methods employ sorbents, catalysts, scrubber liquors, flue gas or coal additives, combustion modification, flue gas cooling, barrier discharges, and ultraviolet radiation for the removal of mercury from flue gas streams. The DOE Mercury Program was an enormous success, spurring continuing development, demonstration, and commercialization of many technologies for the capture of mercury. An overview of current and alternative technologies for mercury capture from coal-derived flue gas will be provided. In addition, six methods for mercury control within coal-derived flue and fuel gases have been recently developed at NETL and will be discussed. The on-going research needs for mercury control include improved sorbent-flue gas contact, development of poison-resistant sorbents and catalysts, novel sorbent promoters, new scrubber additives for retention of mercury within wet FGD systems, concrete-friendly activated carbons, new continuous measurement methods, benign coal additives, byproducts research, and exploration of international markets.

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SESSION 3a (9:55-11:15) GASIFICATION TECHNOLOGIES – 2 *Alberto Pettinau and David Lyons*

3a.1 (9:55-10:15) Integrating Biomass and Waste into High Pressure Partial Oxidation Processes: A Thermo-Economic Multi-Objective Optimization Using Flowsheet Modelling

Philip Rößger, Ludwig Seidl, Fred Compart, Bernd Meyer, and Andreas Richter,
Process Engineering, TU Bergakademie, Freiberg, GERMANY

Thermochemical conversion of biomass and waste provides an environmentally friendly alternative to fossil-based production of chemicals and even gives the opportunity to a closed carbon cycle. With high-pressure partial oxidation various feedstocks can be efficiently utilized to syngas, which can be further upgraded to e.g. Fischer-Tropsch products, hydrogen or olefins. In this context, methanol is often referred as flexible base chemical product. In this work, biomass and waste integration into the high-pressure partial oxidation process is obtained using their respective pyrolysis oils as feedstocks for methanol production. To investigate the transformation from fossil to renewable feedstocks, different blends of heavy oil, light oil, biomass pyrolysis oil and waste pyrolysis oil are considered. Thermo-economical optimization techniques using flowsheet modelling are applied to show the effect of blend variations and reactor operation conditions on gasification performance and overall production costs. Results

reveal the economic potential for biomass and waste integration with increasing carbon taxes and electricity price.

3a.2 (10:15-10:35) A Detailed Study of the Co-Gasification Behavior of Sewage Sludge and Coal in an Entrained-Flow Gasifier

Johannes Scherer, and Andreas Richter
TU Bergakademie Freiberg, Germany
Tobias Ginsberg, and Christian Wolfersdorf
RWE Power AG, Werkstraße, Bergheim, Germany

The present work numerically evaluates the co-gasification of dried sewage sludge and coal in a top-fired entrained-flow gasifier. Numerical calculations enable a spatially resolved analysis of sub-processes of the gasification behavior in the reactor, such as release of pyrolysis gas, syngas distribution and char conversion. For this purpose, fuel mixtures with 40% and 60% of sewage sludge are investigated in a pilot-scale test gasifier and are compared with the gasification of pure coal and pure sewage sludge. Using a Euler-Lagrange approach and particle conversion sub models, a particular focus lies on the difference of the conversion of sewage sludge and coal particles. For three different particle groups, 50, 150 and 250 µm mean diameter, the overall conversion rate as well as pyrolysis and residence time is analyzed in detail. The numerical calculations show that the low heating value of the pure sewage sludge has a negative impact on the gasification while the co-gasification of sewage sludge and coal is a promising approach overcoming this problem.

3a.3 (10:35-10:55) Expanded Transient Multi-Fuel Modeling of the HMI Updraft Moving-bed Gasifier Performance for Industrial Scale CHP Applications

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Sotacarbo – Società Tecnologie Avanzate Low Carbon S.p.A., Carbonia, ITALY

Ultra-high efficiency (85 to 90+%) coal and biomass gasification systems for industrial-scale (2 to 150 MWe) combined heat and power (CHP) systems can benefit from the use of computational fluid dynamics (CFD) modeling to guide and optimize reactor design and operation. The US DOE National Energy Technology Laboratory (NETL) has developed a family of multiphase fluid dynamics codes called the MFiX Software Suite. NETL is working in collaboration with Hamilton Maurer International, Inc. (HMI) and Sotacarbo to use MFiX software tools to simulate detailed physics and chemistry in prospective designs of a novel updraft moving-bed gasifier that will operate over a range of feedstocks and operating conditions. The purpose of the work reported here is to demonstrate the ability of multiphase CFD tools to accurately model gasifier performance and to serve as a design and operator training tool to accelerate and reduce the risk inherent in the design and operation of complex gasification reactors. This novel simulation-based engineering approach is being used to support the design of commercial-scale gasifiers for use at the city of North Pole, Alaska, Nebraska Power, Lincoln, NB, and will be considered for a laboratory-scale gasifier for processing advanced tri-fuel (coal, biomass, & waste plastics) pellets at Sotacarbo, Carbonia, Italy. The HMI updraft moving-bed gasifier contains discrete spatial regions where the key component reactions of the gasification process occur. From top to bottom, these zones include drying, devolatilization, gasification, and char combustion zones – all critical to efficient gasifier performance. The MFiX model has demonstrated the ability to capture all these reaction zones for the case of Alaskan subbituminous Usibelli coal. The chemical reaction mechanisms for devolatilization, gasification, and char combustion were validated using experimental data produced using Usibelli sub-bituminous coal in a 1-ft ID refractory lined lab-scale gasifier at the Sotacarbo Sustainable Energy Research Center plus similar sub-bituminous coals and lignites gasification performance data from the 4+ year USDOE and USBOM sponsored Mining and Industrial Fuel Gas Project (MIFGa). The model includes the effects of heat transfer to a water-cooled shell and complex particle and gas flow patterns in the lower grate region. The grate contains annular gaps where ash flows exit the gasifier, and inlet air and steam flows enter the ash bed and move upward to the char combustion zone. The impact of small transient fluctuations of inlet air and steam flow on char combustion zone temperatures can be seen in the simulations. The impact of ash layer depth and gasifier transients on performance is explored with the model. The level of detail exhibited by these results is extremely useful for performance optimization. The MIFGa data provides key operational data, including pyrolysis liquid yields of 99.99% recovery efficiency, for gasification systems of a similar scale to the proposed UAF design. The MIFGa data will help confirm the model's ability to accurately predict product yield and flow patterns of the pyrolysis vapor and reactive syngas through the gasifier bed along with the particulates (char and coke particles) entrained with the raw syngas. This information is

important to guide the design and operation of downstream components. For example, removal of particulates in the raw gas stream exiting the gasifier is necessary before cooling the syngas to condense and recover the pyrolysis tar fog using wet electrostatics to obtain the 99.99% removal efficiency. Throughout the 4+ year MIFGa coal/biomass gasification project, pyrolysis liquids were recovered from the raw syngas stream with 99.99% efficiency. This success resulted in the gasification efficiency of all 18 coals gasified to be quantified in the range of 92 to 93 percent efficiency including the pyrolysis liquids. The measured pyrolysis liquids (tar) produced within and recovered from the gasification process for all 18 coals gasified during the MIFGa project agreed extremely well with Fisher Schrader assay data which enables the NETL updraft moving bed gasifier to model the devolatilization process and pyrolysis liquid yield with high accuracy for all coals. This work includes a historical overview of technology development and presents a description of the multiphase flow model and the most relevant results that are being used for the design of the commercial-scale gasification unit to be installed in North Pole, AK at a commercial site with an electrical interface with GVEA for local grid control. The commercial site in North Pole will also include multi-acreage (10-20 ac.) greenhouses for CHP and CO₂ capture/utilization from syngas firing Jenbacher engine exhaust (capture) for enhanced plant and vegetable growing. Most recent gasifier modeling results include start-up transients using near zero volatile coke and/or anthracite, gasifier banking, and shut-down transients. Many coal and biomass feedstocks possess volatiles that are released within the devolatilization zone of the reactor. Devolatilization of the feedstock can be accurately predicted using the MFiX model employing both empirical and analytical devolatilization data and models. Modeling the multiphase flow of the pyrolysis vapor and reactive syngas through the gasifier bed with particulate (char and coke particles) entrained with the raw syngas and pyrolysis vapors must be removed before condensing the pyrolysis vapors. Removal of particulate in the raw gas stream exiting the gasifier before cooling the syngas is achieved using hot cyclonic separation before condensing the pyrolysis vapor and removing/recovering the pyrolysis tar fog using wet electrostatics with a 99.99% efficiency. The gasification process modeling presented addresses the effect of heat transfer to a water-cooled shell and the reaction of the ash bed to ash chemical composition to the counter flow air/steam and between the blast and the ash bed.

Acknowledgements: This work is funded by the U.S. Department of Energy, National Energy Technology Laboratory's (NETL) Research and Innovation Center under the Advanced Reaction Systems program and NETL under DOE Award Number: DE-FE0031601, with cost share by UAF, HMI, Sotacarbo (within the "Centre of Excellence on Clean Energy" project, D49J21001310002), Golden Valley Electric Association, Aurora Energy LLC, and Hobbs Industries, Inc.

3a.4 (10:55-11:15) Comprehensive Optical Investigation of Different Flame Types in a Multi-Feed Test Facility

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In the present work, a multi-feed test facility with applicable optical system was used and tested. The system is designed to use different burners for gaseous, liquid and solid feedstocks. Flame images were captured with a high-speed camera and then extensively analyzed using in-house optical data analysis software. Unlike most previous research, the current work focused on two main aspects: flame image segmentation and flame feature extraction. Regarding the flame segmentation, it was found that the contrast between the flame and the reactor walls was extremely low in the case of natural gas and diesel, which made the segmentation task impossible using the conventional methods. Therefore, a new method based on optical flow algorithms was developed to overcome this shortcoming. After determining the best segmentation approach for each flame type, the flame characteristics, such as flame dimensions, flame flicker, and velocity field, were estimated using various image processing and computer vision algorithms. This work helps to design a modeling approach for optical analysis of the flame that can be used to optimize the gasification process, monitor the flame, or validate numerical results.

SESSION 3b (11:15-11:55) RARE EARTH ELEMENTS –1 *Evan Granite and Allan Kolker*

3b.1 (11:15-11:35) Datamining Analysis of Rare Earth Element Recovery Research Trends – A Path Forward with Functionalized Silica Sorbents

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The U.S. Geological Society (USGS) showed that global rare earth elements (REEs)

production in 2019 reached an estimated 210,000 tons, a 10.5% increase from 2018. While the U.S. reached about 26,000 tons produced, China continued to show dominance in this area with $\geq 120,000$ tons produced. The growing utilization of REEs for modern technology and the need to establish reliable domestic sources for the United States' and other countries' national security or economic progress largely drive the rise in REE-related research across the world. Our work here focuses on datamining the Web of Science library for publications related to REEs retrieval methods then subsequently performing key word frequency analysis via Python v3.5 software programming to examine shifts in the research interest/foci, and on successful REE-Oselective silica-based sorbents. We found that key research topics since 1947 concentrating on rare earth element recovery, separation, extraction, or pre-concentration key words involved both the conventional mineral processing route – precipitation, stripping, leaching, flotation, etc.– and the growing solid-based separation route that largely employs different membranes and a vast collection of sorbents –ion exchange resins, activated carbons/chars/nanotubes, zeolites, and functionalized silica– to capture the valuable REEs. Data showed that interest in REE recovery utilizing these solid-based materials experienced sharp growth over the past 10 years. This was largely due to the recognized deleterious impact of conventional mining practices on the surrounding environment, which can be mitigated by recovering/recycling REEs already present in liquid sources like coal-based acid mine drainage (unintentionally extracted) and waste electronic leachate (intentionally extracted). Interest in functionalized silica sorbents represented a significant portion, ~22%, of that for solid-based materials studied for REE recovery. Excluding membranes, this category of materials had the highest interest among the solid sorbent materials examined. We expect this can be attributed to the following factors: the commercially available and low-cost SiO₂ support; easily modified SiO₂ surface chemistry and high REE capacity offered by exposed hydroxyl groups within a high pore volume; and well-developed existing reactor systems (fixed beds, etc.). Analysis of REE-selective functionalized silica sorbents pointed toward further studying size-selective ligand synthesis; commercial liquid extractant immobilization; active site saturation; pore size control; and selective elution. A multi-bed adsorption approach for selective REE extraction is presented.

3b.2 (11:35-11:55) Rare Earth Elements (REE) Distribution on Commercial Coal and Respective Combustion Ashes from a Portuguese Thermoelectric Power Plant

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Due to their unique properties rare earth elements (REE) are crucial in several industries such electronics and clean energy technologies, and these have seen substantial growth in recent years. Their substitution is quite challenging, and its recycling is generally residual compared to the current needs. Efforts have been made on finding secondary sources of REE and coal combustion ash has been pointed has having a good potential for REE recovery. All over the world, several studies have been made to assess the REE-potential of coal ash from, but few have combined an integrated study including their provenance within the power plant and seasonal variations.

Samples of coal, fly ash (FA) and bottom ash (BA) were collected, every three months from December 2016 to December 2017, at Pego thermoelectric power plant (Portugal). The FA was collected from several sampling sites inside the power plant, which included economizer (ECO) and electrostatic precipitator (ESP) hoppers and silos. The global coal and ash samples were characterized via proximate analysis – ISO standard (moisture, ashes, and volatile matter), X-ray fluorescence (XRF; major oxides), Inductively Coupled Plasma Mass Spectrometry (ICP-MS; sample fusion in LiBO₂/Li₂B₄O₇ to REE determination) and Scanning Electron Microscopy with Energy Dispersive Spectroscopy (SEM-EDS; detailed imaging of REE-bearing morphotypes and semiquantitative chemical characterization). Selected FA and BA samples were physically separated according to particle size (dry mechanical sieving) and magnetic properties (wet magnetic separation with ferrite magnet) and characterized by ICP-MS to assess the REE distribution and find the most promising fractions.

The feed coal samples studied present low contents of ash (<10 wt. % d) and sulfur (0.9 wt. % daf) and are depleted in REE relatively to World Clarke Coal (concentration coefficient < 0.5). The ash samples collected presented in average 16 times more Σ REE than the respective feed coals and the highest enrichments (>20 times) were found on the samples collected in December 2016. Concerning the sampling locations, the lowest REE content was found in the economizer FA whereas the highest in the ESP FA. In general, it is observed an increase in the REE content into the last ESP rows although in some cases the highest concentration occurs in the ESP middle row.

SEM-EDS experiments in selected coal and ash samples revealed discrete REE-bearing particles (<10 μ m), and the assessment of the REE potential through the projection of Coult vs. critical REE percentage classifies the analyzed ash as promising raw-REE materials. However, the REE content as oxide (REO) is far below the cut-off established for being economically recovered (REO = 1000 ppm).

The FA sized-fraction samples show an increase of the REE content with decrease of the particle size, with exception of the fraction >150 μ m from ECO which has REE contents similar to the 45-25 μ m size-fraction. Regarding BA, the REE are found in larger concentrations at the 1-4 mm fractions. The highest Enrichment Factor (EF) value (up to 1.4) is found at ECO < 25 μ m fraction, which contains approx. 20% of the total

REE. On the other hand, the ESP FA < 25 μm fraction, which represents approx. 50 wt.% of the FA global sample, contains more than 50% of the total REE. After magnetic separation, both magnetic and non-magnetic fraction show no particular REE enrichment or depletion relatively to the global samples, which indicates that REE are not associated to iron-rich phases.

Low REE concentrations are expectable in power plants burning highly beneficiated coals, but the huge amounts of coal combustion ash generated ready to the used and future market variations may foster REE recovery from low grade rocks and secondary raw materials. The results contribute to highlight the REE partitioning from the feed coals to the combustion ashes, especially that the characteristics of the ashes and their REE concentration, which can be an advantage when looking for separation solutions aiming at concentrating REE. However, the present study shows that currently neither the commercial coals studied, nor the respective global ashes and their fractions have potential to be economically exploited for REE. Most probably, a larger concentration of REE remained in the tailings of coals beneficiation process since these elements are related to the coals mineral matter, which should be addressed in further investigations. Acknowledgments: PhD scholarship financed by FCT – Fundação para a Ciência e Tecnologia, Portugal, (SFRH/BD/131713/2017); 3rd ERA-MIN Joint Call (2015), project CHARPHITE: FCT, Portugal (ERA-MIN/0005/2015); Institute of Earth Sciences (ICT) through the project COMPETE 2020 (UIDB/04683/2020), POCI-01-0145-FEDER-007690, Pego Power plant (Portugal).

SESSION 4 (9:55-11:35)

COAL SCIENCE – 2

Leslie Ruppert and Brian Shafer

4.1 (9:55-10:15) Acid-Leached USY Zeolites Catalysts for Catalytic Cracking of Coal Tar

Zhuozhuo Wu, Zhiyuan Yang, Xiaoqian Ju, Yinyan Li, and Xinbo Duan, University of Science and Technology, Xi'an, P. R. China.

A wealth of heavy aromatics in tar produced by coal pyrolysis can generate light aromatics through catalytic cracking which can be widely used as chemical raw materials. In this work, USY zeolites leached by different inorganic acids were used as catalysts for cracking coal tar. The optimal concentration for the selection of different inorganic acids leached with USY, that is, dealumination, were explored. The results showed that different acids had different optimal concentrations for impregnation, which meant that the ability to remove extra-framework Al of USY was different. XRD performed on USY zeolite confirmed that the critical concentration of framework remains intact after acidic leaching. It was found that the HCl concentration of leaching USY exceeded 0.6 mol/L will cause skeleton collapse, whereas H₂SO₄ concentration could not over 0.3 mol/L. Finally, the best ones were selected and subsequently evaluated in a tubular furnace.

4.2 (10:15-10:35) Preparation of Sludge Semi-Coke Water Slurry by Low Temperature Thermo-Alkali Modified Sludge and its Slurry Property

Yaqian Yao, Zhiyuan Yang, Hanbo Zhu, Zhuoyue Meng, and Qi Zhang, University of Science and Technology, Xi'an, P. R. China.

With the continuous increase of urban sewage production in China, the output of urban sewage sludge increases sharply. It is of great significance to find a cost-effective and environmentally friendly way to treat sludge. A new method for sludge treatment is to add sludge to the semi-coke water slurry (SCWS) to prepare sludge water coke slurry. The mechanism of modified sludge semi-coke water slurry (MS-SCWS) was studied in this paper. The oxygen-containing functional groups in sludge form a polar bond with water, which limits the drying performance and reduces the adsorption of additives on the semi-coke surface. The flocculent structure of sludge fixes water in slurry, which is not conducive to the fluidity of S-SCWS. After the sludge was modified by low-temperature hot alkali method, the flocculent structure and polar functional groups were destroyed, resulting in dense surface structure, and thus the polar bond released water molecules. In the MS-SCWS, the sludge covered the polar groups and pores on the semi-coke surface, and formed a unique three-dimensional network structure between particles, which improved the stability of the slurry. After sludge modification, the maximum solid concentration of SCWS added with 10 wt % MS increased from 66.7 % to 68.1 %. The average apparent viscosity η₁₀₀ decreased from 711.2 Pa·s to 434.2 Pa·s. The rheological index n increased from 0.7977 to 0.9320, and the consistency coefficient K decreased from 1.6789 to 0.3542. The precipitation rate decreased from 6.09 % to 0 %. The results showed that the fluidity of MS-SCWS was improved, the stability was significantly improved, and the maximum solid concentration was also increased. This meets the needs of sustainable development, makes full use of the moisture and heat value in the sludge, eliminates harmful microorganisms in the sludge, and solidifies heavy metals, so as to achieve the goal of energy and resource utilization of the sludge.

4.3 (10:35-10:55) Survey of Research on Direct Carbon Fuel Cells

Evan J. Granite,
US-DOE, Pittsburgh, Pennsylvania, USA

The electrochemical oxidation of carbon provides the potential for portable, highly efficient, and clean power generation. The direct carbon fuel cell is a concept for efficient utilization of carbon for production of electric power. A carbon electrode is consumed in a fuel cell, with the concomitant formation of carbon dioxide and electricity. The formation of a concentrated carbon dioxide stream is advantageous for facile greenhouse gas mitigation. The direct carbon fuel cell also presents an opportunity for the use of abundant US coal reserves for power generation in a clean and efficient manner. The overall reaction for the direct carbon fuel cell is: C + O₂ → CO₂ + E (1) A battery has a limited supply of reagent, whereas a fuel cell typically has a continuous feed of reagent. Since the carbon electrode is consumed, the carbon fuel cell is somewhat akin to a battery, and fuel cell is somewhat of a misnomer. However, oxygen or air is continuously supplied for the direct carbon fuel cell. From the free energy of reaction (1), one can calculate the theoretical EMF, Etherm developed, viz: ΔG = -nF·Etherm (2) The EMF calculated from thermodynamics is 1.02 volts at room temperature. Electrochemical cells allow for high energy efficiencies, typically much higher than from combustion systems. However, a potential of 1.02 volts will not be developed by the direct carbon fuel cell. In order to pass current, the following resistances must be overcome: 1.) adsorption, electron transfer, and desorption on the electrode surfaces (kinetics); 2.) diffusion of reactants and products through the boundary layer of the electrodes (mass transfer); and 3) the iR drop across the electrolyte. Therefore, the overpotential, o.p., which is the sum of all these resistances, is defined as: o.p. = Etherm - E developed (3) There are many potential forms of a direct carbon fuel cell. Researchers have previously employed oxygen, carbonate, or hydroxide ion conducting electrolytes. Various forms of carbon such as graphite, activated carbon, or petroleum coke have been examined for the consumable electrode. Areas for future research and possible optimization of the direct carbon fuel cell will be examined in this review. Strategies for minimizing the various overpotentials will be discussed, and the exciting potential opportunities for coal will be outlined.

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4.4 (10:55-11:15) Simulation of Oxygen and Moisture Adsorption of Lignite and Its Active Groups in Low-Temperature Oxidation Environment

Jianqiao Zhao, Lulu Fan, Xianliang Meng, Ruizhi Chu,
Jiaxin Wu, Yang Zhou, and Peng Liu,
China University of Mining and Technology, Xuzhou, Jiangsu, CHINA

Lignite has a high tendency to spontaneous combustion, which limits its application. In this work, molecular simulation and density functional theory (DFT) were conducted to investigate adsorption and reaction mechanisms among oxygen, moisture, lignite and its active groups. The adsorption amount of oxygen and moisture on lignite at 278.15-318.15 K were compared. The results revealed that moisture will impede the physical adsorption of oxygen and make its adsorption capacity decrease, but it will increase the isosteric heat of oxygen adsorption. Meanwhile, adsorption characteristics of oxygen and moisture by hydroxyl and carboxyl groups on the surface were studied by DFT method. The optimal adsorption energies of oxygen on hydroxyl and carboxyl groups are 17.03 kJ/mol and 16.68 kJ/mol respectively, while the optimal adsorption energies of moisture are 47.83 kJ/mol and 57.48 kJ/mol. It was demonstrated that moisture can promote the adsorption of oxygen on the hydroxyl and carboxyl groups in a particular case, so that optimal adsorption energy of oxygen increases. The initial paths of low-temperature oxidation reactions of hydroxyl and carboxyl groups with influences of moisture were speculated on the basis of free radicals mechanism. The reaction paths is a dynamic cycle mechanism that promotes and transforms each other, involving the promotion, reaction and generation of moisture molecules.

Acknowledgement:

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4.5 (11:15-11:35) Research on Construction of Macromolecular Structure Model of Shenfu Coal

Huaiqing Zhang, Anning Zhou, Zhen Li, Kai Zhao, and YongAn Chen,
Xi'an University of Science and Technology,
Xi'an, P. R. China

Shenfu coal are generally of low ash, low sulfur, and high pyrolysis oil yield. The low and medium temperature pyrolysis is an important way for high-efficiency and low-carbon utilization of the coal. The study of the macromolecular structure of Shenfu coal has significant theoretical guiding significance for elucidating the pyrolysis mechanism and improving the quality of pyrolysis oil and gas products. This paper takes Bulianta coal (BLT) and Dabaodang coal (DBD) in the Shenfu mining area as the research objects. Firstly, industrial analysis, elemental analysis, X-ray photoelectron spectroscopy (XPS), solid ¹³C nuclear magnetic resonance (¹³C-NMR) and other analytical methods were used to analyze and characterize the structure of the two coals. On this basis, combined with the calculation of structural parameters, the two-dimensional macromolecular structure models of coals were established. The structure optimization and annealing dynamics simulation were used to optimize the above structures, and the 3D structure model with the lowest energy was obtained. Finally, the simulated FTIR spectra and ¹³C-NMR spectra of the structure models were compared with the corresponding experimental analysis results. The results show that the FTIR and ¹³C-NMR simulated spectra of the macromolecular structures are consistent with the experimental results; The molecular formulas of BLT coal and DBD coal are C₁₉₆H₁₅₉N₃O₁₅ and C₂₀₇H₁₈₈N₄O₁₅S respectively; In the 3D structures of coal, the regular and parallel arrangement of aromatic carbon layers and the non-covalent bonding potential are the main factors for the stability of the structures; BLT coal and DBD coal have similar macromolecular structure characteristics, the aromatic structural unit is mainly naphthalene ring, and the aliphatic carbon in the form of methylene, methine, aliphatic side chain and cycloalkane; The main forms of nitrogen are pyridine and pyrrole; The oxygen-containing functional groups are mainly phenolic hydroxyl, etheroxy and carbonyl groups. However, the degree of metamorphism, aromaticity, and condensation of DBD coal is slightly higher than that of BLT coal, and contains a small amount of sulfoxide groups. The carboxyl content of BLT coal is much greater than that of DBD coal. The construction of the macromolecular structure models of Shenfu coal in this study lays a model basis for studying low and medium temperature pyrolysis of coal at the molecular scale, and provides theoretical support for the clean and efficient utilization of low-rank bituminous coal.

SESSION 5 (12:35 – 14:15) RARE EARTH ELEMENTS – 2 *Evan Granite and Allan Kalker*

5.1 (12:35-12:55) Transforming Coal Resources Into Rare Earth Elements, Critical Minerals, and Other Nonfuel Products

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Landon Allen, Madison, AL, USA

Coal resources often have elements and compounds that can be transformed into a variety of nonfuel products we use every day. Careful processing of coal resources can maximize product yields while minimizing waste and environmental issues. This presentation will show results from testing to extract and recover rare elements and critical materials from coal waste by utilizing pyrite in the coal waste to generate acid for leaching, while simultaneously eliminating future acid mine drainage. Additional information will be discussed regarding the production of other nonfuel products such as carbon fiber, graphene, polymers, and resin from coal resources.

5.2 (12:55-13:15) Evaluating Rare Earth Element Speciation and Fractionalization in Appalachian Abandoned Mine Lands

Brianna O'Neil-Hankle, John J. Lenhart, Chin-Min Cheng and Tarunjit Butalia,
Department of Civil Environmental and Geodetic Engineering,
The Ohio State University, Columbus Ohio, USA

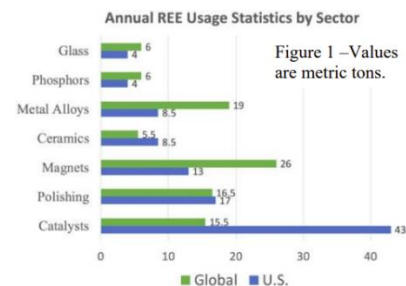
Abandoned mine lands (AMLs) and the associated discharge of acid mine drainage (AMD) impair water resources throughout the world by negatively impacting groundwater and aquatic ecosystems. Acid mine drainage and the associated AML sediments are a valuable source of rare earth elements (REEs) and critical metals. The concentrations of REEs can be orders of magnitude higher in AMD compared to average river water and seawater. REEs tend to remain in solution in acidic conditions and to precipitate or adsorb onto clays and metal oxyhydroxides under alkaline conditions. Cleaning up AMLs globally has been estimated to cost in the tens to hundreds of billions of dollars. Recovering REEs from AMD and the associated AML sediments provides the potential to offset the cost of AML reclamation and mine drainage treatment.

Abandoned mine lands are complex biogeochemical systems where the interactions of AMD and microbial communities lead to processes which control the geochemical and mineralogical characteristics of sediments. Since certain trace elements and REEs show predictable behavior such as sensitivity to pH changes and redox conditions, studies of these elements in the sediment systems are useful for determining the biogeochemical processes. The study site, 'Flint Run', is seriously affected by AMD with multiple past remediation attempts. This 240-acre site in Ohio is located between the Middleton Run and Flint Run Watersheds and the drainage exhibits high REE concentrations up to 1.7 mg/L. Previous studies have looked at the fractionalization of REE in sediments from saltwater and brackish systems. This study details sampling and analysis on AML sediments to determine the behavioral distribution patterns of REEs in freshwater systems. The aim of this present work is to describe the content, fractionalization and mineralization pattern of the REE in freshwater sediments affected by AMD. Five loose sediment cores were collected from 'Flint Run' using an auger and split-spoon sampler. Samples were collected at five-foot increments and trace element and REE concentrations were analyzed using inductively coupled plasma atomic emission spectroscopy. The quantitative mineralogy associated with the sediments were analyzed with the Rietveld method using a high-resolution X-Ray diffractometer. The amorphous iron and aluminum phases were removed from the samples using an extraction method to aid in X-Ray diffraction analysis. A known mass of rutile was added to each sample for internal standardization to determine the amount of amorphous content in the samples. Preliminary results show that the sediments which represent the composition of the coal underlay layers have higher REE concentrations in comparison to the other compositional layers studied. The authors expect to find the REEs associated with phosphate and carbonate minerals. This study will help to further the understanding of mechanisms and phases responsible for binding REEs in AML sediments.

5.3 (13:15-13:35) Current Uses and Future Opportunities for US Industry in Rare Earth Elements and Critical Materials Technologies and Markets: Knowledge-Base Tool Development

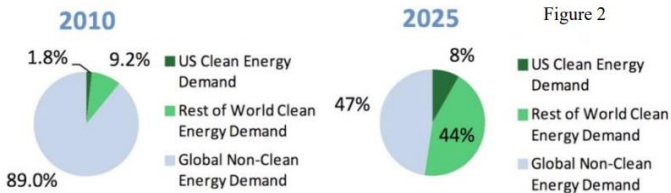
Justin Richter, and Randy Vander Wal
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Critical minerals, and the standalone subset, rare earth elements (REEs) have become important materials in a broad range of technologies significant to national security, energy, medical, and consumer products. In 2017, the United States had no primary production of 22 minerals and was limited to byproduct production of 5 minerals on the critical minerals list. In particular China has been the dominant supplier of REEs since 1988, providing 95% of the global market in 2011. In response this project seeks to address the present and future industry and market opportunities for domestically produced REEs and critical minerals. Our approach is to link REE and CM supply from novel sources to domestic demand markets. Material flows through the supply chain for rare-earth elements and critical minerals will be assessed to identify industrial opportunities with domestic consumption. Additionally, market forecasts will be used to estimate growth potential and infrastructure requirements. This work aligns with DOE-NETL's near-term goals (2020-2021) to validate the technical and economic feasibility for the operation of small-scale, domestic, prototype systems to produce high purity (90-99%), salable rare earth compounds from coal-based materials and more broadly support increased domestic supplies of critical minerals. As illustration of the approach, mature markets (such as catalysts, glassmaking, lighting, and metallurgy, q.v. Fig. 1) account for 59 percent of the total worldwide consumption of rare earth elements while newer, high-growth markets (such as battery alloys, ceramics, and permanent magnets) account for 41 percent of the total worldwide consumption of rare earth elements [1]. In mature market segments, lanthanum and cerium constitute about 80% of rare earth elements used and in new market segments, dysprosium, neodymium, and praseodymium account for about 85% of rare earth elements used [1-4].



The estimated domestic use of rare earths in 2015 was primarily in catalysts (60%), with the remainder in metallurgical applications and alloys, polishing, ceramics and glass, and other uses (10% each). The United States primarily consumed LREEs (light REEs). Because the United States has limited capabilities to produce battery alloys, magnet alloys, and phosphors, most LREE consumption is in the form of cerium and lanthanum compounds used to produce catalysts, ceramics, glass, and polishing compounds. Most HREE (heavy REE) consumption is in the form of yttrium compounds [4]. Together, the remaining HREEs (Tb, Dy, Ho, Er, Tm, Yb, and Lu) were estimated to contribute less

than 2% of domestic consumption [4]. Increasing domestic electrification, renewable energy installation, and electric vehicle consumption will drive the short term demand for CMs and REEs. The annual global installation of wind power is expected to increase from 63,360 MW in 2015 to 107,488 MW in 2030 at a moderate scenario, with offshore wind turbines contributing an increasingly larger share [5]. The electric vehicle (EV) market share is projected to increase to 30% by 2033 [6]. Oppositely the market share of NiMH batteries in hybrid electric vehicle (HEV) is projected to decrease from 85% in 2016 to 65% in 2020 and to 10% in 2025 [7]. Meanwhile demand for Nd and Dy oxides for the magnets in wind turbines and electric vehicles is expected to increase to 200% and 268% of 2016 levels [8]. Overall, Nd and Dy will be the critical REE elements in short supply for clean technologies during the next decades based on present production levels. The following sector diagrams in Fig. 2 [excerpted from ref. 9] illustrate the projected domestic versus global demand increase for Dy, based on clean energy demand Figure 1 –Values are metric tons. [10-12]. The comparative market scales gauge U.S. industry opportunity while also assessing domestic use/retention versus global (export) consumption, a key project task. Globally as well as domestically, clean energy technology will drive demand for selected critical minerals. With the current fast growth in battery production for electric vehicles and energy storage, it is predicted that lithium-ion batteries could reach 54% of cobalt end-use and 63% of lithium end-use by 2020. Lithium, cobalt and graphite production will need to scale accordingly. Limited domestic production for these and many other CMs creates a significant national security risk. This work supports DOE and NETL efforts to validate the technical and economic feasibility for the operation of small-scale, domestic, prototype systems to produce high purity (90-99%), salable rare earth compounds (oxides, and/or metals, carbonates, and the like) from coal-based materials. The scalability of domestic REE and CM production from coal-based resources requires identification of current and future supply chains, current and anticipated industrial sector consumption patterns, and final product REE and CM tracing. This work will develop a domestic supply chain strategy critical to bolstering the strength and resilience of U.S. production, manufacturing, and circularity of REEs and CMs. Some discussion of global resources and production, both new and existing, including import potential will be presented. In summary, assessment of REE and CM resources is vital to national security and economic well-being. In order to mitigate supply risks, stimulate industrial capabilities, and support supply chain infrastructure, changing domestic CM and REE demand markets that take advantage of defense-driven and commercial technology advances must be described.



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5.4 (13:35-13:55) Characterization and Recovery of REE and Transition Metals from Acid Mine Drainage Treatment Solids

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Acid mine drainage (AMD), generated from oxidative weathering of coalfields, contains elevated acidity and dissolved Al, Fe, and Mn, along with enriched levels of trace metals, such as rare earth elements (REE) and transition metals (Co, Ni, Zn). It has been estimated that AMD from the Appalachian basin alone generates between 500 and 3,400 metric tons of REE annually, representing 7% to 41% of the annual US REE consumption in 2018 (Vass et al., 2019). AMD treatment systems, designed to precipitate dissolved metals, can also sequester > 90% of the dissolved REE, and transition metals (e.g. Co, Ni, Zn) into these precipitates (treatment solids). These treatment solids (AMD solids), which are usually disposed of in landfills or on-site storage ponds, may be a promising REE and transition metal mining source. Our study aims to: (1) characterize different hosting phases for REE and transition metals in different AMD solids (Fe-rich, Mn-rich and Al-rich ones) and (2) develop extraction processes with small environmental footprint for REE and transition metal recovery based on characterization. This information can be used to guide REE and transition metal recovery efforts from AMD solids and to inform the design of new treatment systems engineered to concentrate REE and transition metals.

Selected treatment solids underwent elemental composition analysis, XRD for mineralogical analysis, and seven-step sequential extractions to quantify REE and transition metal distribution in different solid fractions. Our results demonstrated that selected solids contain up to 1,900 ppm REE, 6,026 ppm Co, 8889 ppm Ni and 13,585 ppm Zn. While REE enrichment can be associated either with high Al, Fe or Mn content, transition metal enrichments are predominantly dependent on the Mn content in AMD solids. Furthermore, the extractability of REEs and transition metals depends on the mineralogy of different AMD solids. Sequential extraction results show 70-90% REEs could be extracted from all solids via seven-step sequential extractions, whereas total extractabilities of transition metals are solid-dependent. Less than 20% Co, Ni and Zn were extracted from a high-Mn solid, while 30-60% Co, Ni and Zn were extractable in the Fe/Mn/Al-rich solids. Thin sections of representative AMD solids were further analyzed via synchrotron micro-X-ray-fluorescence (μ -XRF) for mapping elemental associations. Synchrotron micro-X-ray absorption near-edge spectroscopy (XANES) was performed to evaluate Ce oxidation states. Elemental map results revealed that REE co-localize with various elements (Fe, Mn and Al); whereas Co, Ni and Zn exclusively co-localize with Mn. Interestingly, Co, Ni and Zn often distribute in different zones within one Mn-rich area in multiple samples, indicating there might be different Mn phases with different affinity to Co, Ni and Zn in one sample. In addition, the oxidation states of Ce will influence the extractability of Ce, as we observed the Ce extractability is lower in samples with high Ce(IV) content compared to those samples with mostly Ce(III).

AMD solids went through large-scale step leaching based on advanced characterization. Direct oxalic precipitations were conducted for REE purification and production without solvent extraction. Preliminary results showed effective 80% REE extraction from AMD solids, and final oxalic products have more than 60% purity of critical materials including REY, Co, Ni and Zn.

Ref: Vass, C.R., Noble, A., Ziemkiewicz, P. F., 2019. Mining, Metallurgy & Exploration 36, 903-916. in a decrease in the exponential acceleration rates as long as $\beta < 80\%$.

5.5 (13:55-14:15) Environmentally Responsible and Efficient Extraction of Rare Earth Elements from Powder River Basin Fly Ash

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Christina Lopano, U.S. DOE-NETL, Pittsburgh, PA, USA

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Coal byproducts contain high-value materials that can be extracted, purified, and used for other applications, such as high technology devices, including computers and smart phones, clean energy systems, and defense technologies. Rare earth elements (REEs) are found in coal ash and concentrations vary by coal basins. Powder River Basin coal ash contained relatively lower REE contents, but higher Ca content compared to Appalachian Coal ash (Taggart et al., 2016). Previous studies have shown that high Ca ash samples generally contain more extractable REEs compared to low Ca ash samples, because the ash particles are irregular shaped aluminosilicate phases that are susceptible for chemical reactions (Stuckman et al., 2019). Extraction methods can be optimized for ash samples from Powder River basin to efficiently extract REEs with lower cost. In addition, our novel REE extraction from coal ash is environmentally friendly using mild acids under ambient conditions, which is more attractive to be applied in the U.S. with environmental regulations for associated production wastes Determining maximum REE

extraction efficiency for samples from the Powder River Basin (PRB) will inform scale-up methods in the field.

Fly ash, landfill ash, and bottom ash samples from the combustion of coal were obtained from two field sites in the Powder River Basin in Wyoming, in collaboration with the University of Wyoming Center for Economic Geology Research (CEGR). Fly ash and bottom ash were obtained from the Wyodak Power Plant and fly ash, landfill ash, and bottom ash were obtained from the Dry Fork Power Plant. The samples contained 0.026 - 0.029% REEs by dry weight, according to elemental analysis via LiBO₂ digestion and ICP-MS.

Acid titration experiments using mild HCl (0.4 - 2.2M) under ambient conditions were performed to carry out efficient extraction and separation from abundant metals. Calcium and REEs followed similar extraction curves in all samples tested, complicating the use of sequential extractions to separate REEs from abundant metals. We compared large-scale leaching experiments to initial titration tests to account for sample heterogeneity and found maximum REE extraction efficiency at hydrochloric acid concentrations of less than 2.0 M. Extraction efficiency using hydrochloric acid at ambient temperatures yielded greater than 50% REE recovery under pH 2.0.

Acid extraction efficiency was compared to extraction using biolixivants, a suite of low-carbon organic acids (e.g., acetate, butyrate) generated from fuel cells for carbon dioxide utilization and capture. The results of REE extraction using biolixivants will demonstrate the potential to conduct cross cutting research to achieve both carbon capture and REE extraction in future scale-up operations.

SESSION 6 (12:35 – 14:15) COAL BED METHANE AND SHALE GAS

Leslie Ruppert and Brian Shafer

6.1 (12:35-12:55) Coal Structure: Visualizing Micro- and Mesopore Distributions Through Hierarchical 3D Pore Modeling for a Bituminous Coal

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Justin K. Watson, Department of Material Science and Engineering, Nuclear Engineering Program, University of Florida, Gainesville, Florida, USA

The pore structure of coal impacts methane storage and extraction. While the macropore structure can be directly visualized with a variety of techniques, the microporous structure remain elusive. Here 3D porous structures were generated using the molecular modeling program Pymol. The coal was represented by a 100 x 100 x 100 Å atomic cubic array of carbon atoms. A hierarchical (and fractal) pore size distribution was created with control over the pore size, frequency, and interconnectivity. The pore data (specific surface area and volumes of micro-, meso-, and macropores) was obtained for a bituminous coal. Structures were generated by controlling pore placement and size using an in-house Python script to execute the sequence of Pymol commands. Visual representations of a complex, hierarchical, fractal, micro- and meso-pore structure was generated, macropores are not yet included due to initial scale constraints. Structures such as this can be used to explore the pore structures role on methane behavior.

6.2 (12:55-13:15) Pilot Scale Testing and Economic Analysis of Thermal Desorption of Mercury from Bituminous Coal

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Zheng Yao, Carlos Romero, Lehigh University Energy Research Center,
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Mercury, and other chemical compounds such as Sulphur, Lead and Arsenic, released during the combustion of coal in coal-fired boilers is of major environmental concerns. This research aims to develop a mean to remove coal contaminants using a suitable thermal desorption processes that provides an economical option for small modular plants. In previous work, thermal desorption of Mercury from coal using air at 600 K demonstrated a removal efficiency of more than 48% using lab-scale spouted bed reactor. In this study, a pilot scale spouted bed reactor was manufactured and in stainless steel, with an overall height of 14 feet, width of 8 feet, and length of 10 feet. The pilot-scale reactor is capable of thermal desorption of bituminous coal at a throughput of 200 kg/hr, and demonstrated a Mercury removal efficiency of more than 45.7%. A thermal desorption system of 150 spouted bed reactors was then designed for an implementation into a Fossil Energy Plant, Case B12A (NETL, 2015) using Aspen Plus. The spouted

bed system was integrated in the flue gas stream between the economizer and the air preheater. The parameters considered for the integration in the power plant and its modeling were 300 °C flue gas inlet temperature, 210 °C flue gas outlet temperature. As a result, the thermal desorption system will cost an additional 10.46 MWe from the Power Plant, lowering the nominal net power from 550 MWe to 539.54 MWe. However, thermal desorption of contaminant from coal would lead to a reduction in coal price due to utilization of high Mercury coal. If coal price can be reduced by 20% or more, the total leveled cost of electricity would reduce by 3 \$/MWh.

The research work discussed here was performed as a part of Small Business Innovation Research (SBIR) Phase I & Phase II grants, supported by Department of Energy, under Award no. DE-SC0017232.

6.3 (13:15-13:35) Prediction of Gas Content in the Qinglong Coal Mine in Guizhou Province, China, by Artificial Neural Network

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Thin coal seams in mines are well developed in the coalfield of Northern Guizhou and usually lack gas data. Thus, preventing and controlling gas outbursts of thin coal seams are difficult. In this study, the coal seam of No. 2 with an average thickness of only 0.80 m is the research object. Due to the thin coal seam, the coal seam of No. 2 lacks measured gas data. In accordance with the contour line of the floor of the coal seam, structural curvature was calculated to express the complexity of the coal seam structure quantitatively. The apparent resistivity of coal in logging data was used to describe the integrity of coal. Subsequently, the burial depth, thickness of coal, the structural curvature and the apparent resistivity of coal are regarded as the main factors affecting the coal seam gas content. Through Python language programming, the BP artificial neural network (BP-ANN) model was established by using machine learning library of TensorFlow. The coal seam of No. 16 with an average thickness of 3.08 m is the main minable coal seam, and there are enough measured gas data. Therefore, taking the coal seam buried depth, coal seam thickness, structural curvature value, apparent resistivity value and gas content as training set samples, 82 groups of actual data of the coal seam of No. 16 were used to train the BP-ANN model. The trained model has good accuracy and the deviation rate was 6.5%–9.2%, with an average of 7.85%. Afterwards, the gas content of the thin coal seam of No. 2 was predicted by using the model. Results show that the prediction accuracy of the aforementioned method is acceptable and has practical value in the prediction of gas content in thin coal seams without measured data. The results in the gas content prediction provide a basis for evaluating the risk of gas outbursts in thin coal seams.

6.4 (13:35-13:55) Research on Fracture Connection and Economic and Efficient Fracturing Technology in Shale Gas Reservoir

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The shale gas reservoir has poor ability to supply gas for the fissure due to the low-porosity and low-permeability. The effectiveness of fissures (i.e. whether the fissures are open or not) is of great significance in fracturing and well location optimization of shale gas reservoir. Based on the study of natural fissure feature, crustal stress and rock physical mechanics in the Ordos Basin, this paper established a mechanical model of stress controlling fissure validity, identified the mechanical condition of natural fissure slipping and faulting, researched the condition of natural fissure opening and interconnecting in different natural fissure distribution patterns. By making full use of natural fractures, a network fracture system with artificial fractures and natural fractures is formed, so as to achieve the purpose of increasing single well production. Combining with the main economic problems existing in the exploration and development of shale gas in China that a single well would have to produce about 60 to 80 million cubic meters of shale gas to make a profit., suggestions for cost reduction and efficiency increase are put forward from the fracturing technology, which is conducive to the realization of low cost and high efficiency development of shale gas.

6.5 (13:55-14:15) Application of Long-Rich Directional Drilling for Gas Drainage of Adjacent Seams in Coal Mines with Severe Geological Conditions

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Coal mine methane (CMM) released during mining operations is a severe safety hazard worldwide, being one of the leading causes of mine gas explosions and gas outburst incidents with many fatalities each year. In order to reduce gas content in gassy and tight coal seams a special drainage strategy is required.

The study aimed to demonstrate the application of long reach underground directional boreholes (LRDD) for gas drainage of adjacent seams before and during the longwall face operations. The technology was applied to low permeability-high gas content coals of Staszic-Wujek hard coal mine (Upper Silesia Coal Basin – Poland), and the obtained results were confronted with conventional cross-measure boreholes.

Five LRDD boreholes (TM1-TM5) with a length of 300 and 400 m were located over coal seam #501 in the fracture zone (mainly composed of sandstones) and monitored over five months of longwall face operations. The LRDD was drilled parallel to the longwall face what was forced by the mining plans and operation movement. The drilling operation was performed using Epiroc® Diamec PHC 8 underground core drilling rig with the nonmagnetic DeviFlex type inclinometer, which provided boreholes of a diameter of 95 mm. The results from the drainage were supported by the laboratory measurements of coals and barren rocks (sandstones and mudstones) and detailed information about key features controlling methane content, which were also used for calibration of developed geological and geomechanical numerical models.

The results from petrophysical measurements revealed low porosity-permeability features with complicated pore structure of coal samples and two types of sandstones of moderate and good filtration and reservoir properties. The efficiency of CH₄ intake of directional boreholes was on the ca. 70% level, while conventional boreholes only 30%. The drainage efficiency significantly increased in the distressed zone around the advancing longwall face due to the developed fractures and stress relief. The average concentration of methane in the directional wells was ca. 89% while average methane intake was in the range of 5-4 m³/min. Moreover, post-exploitation drainage was observed from some boreholes with a cumulative flow rate of 3.0 m³/min from TM2 and TM4 boreholes and 0.2 m³/min from TM2 boreholes. The methane concentration was in the range of 50% for TM2 borehole to 74% for TM4 borehole. The total methane intake from the boreholes drilled on part I-C was nearly 1.8 million m³CH₄.

The obtained results proved the efficiency of LRDD boreholes as a feasible technology for gas control in coal mines characterized by severe geological conditions, what bring valuable environmental benefits and assure the effectiveness of the coal production process.

SESSION 7 (14:25-16:25)
RARE EARTH ELEMENTS – 3
Evan Granite and Richard Bajura

7.1 (14:25-14:45) A Geo-Data Science Method for Assessing Rare Earth Element Occurrences in Coal and Other Sedimentary Systems

Andrew Bean, C. Gabe Creason, Scott Montross, R. Burt Thomas,
Devin Justman, MacKenzie Mark-Moser, and Patrick Wingo,
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and Kelly Rose,
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At present, no systematic method or approach exists to predict and identify REE resource potential and occurrence from coal and associated sedimentary systems. The lack of a systematic assessment method inhibits our ability to predict where REE occurrences are likely to be found and quantified for in-place or economically accessible volumes of unconventional REE in domestic coal and sedimentary systems. Thus, to quantify and establish a domestic supply of unconventional REE requires a systematic, data-driven, science-based assessment method and approach.

The National Energy Technology Laboratory (NETL) has developed an REE sedimentary assessment method (REE-SED) to characterize and predict REE enrichment in coal and sedimentary systems. The approach leverages geospatial datasets informed and guided by knowledge of REE accumulation mechanisms to systematically assess and identify areas of predicted higher REE prospectivity. Ultimately, the REE-SED method will provide users with a novel, knowledge- and big data-driven assessment tool to predict the occurrence of promising REE-bearing deposits associated with coal-bearing sedimentary strata, and quantify predicted REE resource volumes for areas with sufficient data. The effort is aimed at supporting the development of technologies that lead to the commercialization of domestic REE deposits by (1) guiding determinations of in-place resource estimates and (2) assessing whether REE are likely to occur in sufficient concentrations and recoverable volumes to support commercial extraction from domestic sedimentary basins.

7.2 (14:45-15:05) High Yield and Economical Production of Rare Earth Elements from Coal Ash

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James C. Hower, John G. Groppo, Jr., and Robert B. Jewell,
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Todd Beers, Mike Schrock, and Brad Perrine,
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Coal and coal byproducts are a potential source of REEs, particularly heavy rare earth elements (HREEs). Demonstration of technologies to recover rare earth elements including yttrium and scandium (REYSc) from these feedstocks will enable utilization of coal mining/coal combustion waste product(s) in environmentally benign ways to produce REEs of strategic importance for the United States while generating jobs and economic growth in economically-depressed regions of this country.

Under sponsorship from the Department of Energy, the team of Physical Sciences Inc., University of Kentucky/Center for Applied Energy Research, and Winner Water Services is developing and demonstrating a pilot scale plant to economically produce salable REY-rich concentrates, critical minerals such as scandium and aluminum as well as commercially viable co-products from coal ash feedstock using environmentally safe and high-yield physical and chemical enrichment/recovery processes. The pilot plants operate at the scale of approximately 0.4 tons per day (tpd) ash throughput for physical processing and about 0.5 tpd for chemical processing, producing rare earth elements and yttrium (REY) concentrates with greater than 85% content on elemental basis. The ash feedstock contains at least 500 ppm of REYSc content. The data obtained from the pilot plant operations will be used to enhance and validate the techno-economic analysis used to design a commercial scale plant (1200 tpd).

This paper will describe the approach and the key results with regard to process optimization, scale up and pilot plant implementation. The paper will provide a comprehensive overview of the overall process that provides economical production of REY concentrates and selected critical minerals. The production of valuable coproducts will also be discussed. Development and demonstration of modular, transportable pilot scale physical and chemical plants for REY recovery from coal ash, including enhancement and validation of a techno-economic model of a pilot plant operations data, will enable the design of a commercial scale plant.

7.3 (15:05-15:25) Rare Earth Elements from Coal and Related Materials: An Overview of Research at the National Energy Technology Laboratory

Thomas J. Tarka
NETL, Pittsburgh, PA, USA

The National Energy Technology Laboratory (NETL)'s Research and Innovation Center (RIC) conducts research to support the creation of a domestic supply of Rare Earth Elements (REE) and Critical Minerals (CM) from unconventional sources, such as coal, coal-related materials, and water from fossil energy-related systems. The RIC Minerals Sustainability (MS) research portfolio is focused on identifying novel and low-cost pathways to reduce the cost of REE-CM extraction/concentration, identifying and characterizing promising coal-related materials and deposits, and reducing risk to deployment through analysis, modeling, and technology maturation in partnership with industry. The presentation will provide an overview of the portfolio, an update on recent accomplishments and field deployments, and a look at the program moving forward, including potential opportunities for partner on NETL RIC-related efforts.

7.4 (15:25-15:45) Investigation of Life Cycle Assessment of Utilizing Waste Coal-based Feedstocks

Fateme Karbalaieisaleh and Raj Kiran,
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Rare Earth Elements (REEs) are one of the most important–albeit critical–commodities for our green technologies. However, there is a general perception that REEs are produced using mining and processing techniques that are unsustainable. Life Cycle Assessment (LCA) is the most widely accepted methodology to evaluate the environmental impacts of rare earth oxide (REO) production. This article aims to provide a synthesis of the currently existing LCA studies on REEs using two strategies. Firstly, an overview of published LCA results of REO production. Secondly, a detailed LCA using the best available life cycle inventories (LCIs) in order to: i). evaluate the state-of-the-art LCI for this sector ii). Understand better the impacts related to each of the three main production routes and iii). Contribute to the development of a preliminary benchmark for the sector. The analysis of the published LCA results reveal that the three main methodological issues with published LCAs are data gaps, allocation, and waste management.

7.5 (15:45-16:05) Critical Minerals Sustainability

Mary Anne Alvin,
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DOE's Office of Fossil Energy Carbon Management (FECM) and the National Energy Technology Laboratory (NETL) continue to address the potential for onshore production of rare earth elements (REEs) and critical minerals (CMs) from unconventional resources through conduct of the Critical Minerals Sustainability Program. Major thrust areas in this research development, demonstration and deployment (RDD&D) program include: (1) Addressing the upstream and midstream REE and CM supply chain and downstream manufacturing of high-value, nonfuel, carbon-based products, to accelerate the realization of the full potential for carbon ores and REE-CM within regional U.S. basins; (2) Development of advanced, reduced cost, environmentally benign, midstream, REE and CM separation, purification and reduction to metal processes; and (3) Conduct of concept and feasibility studies focused on the design, construction and operation of an engineering-scale prototype facility that uses unconventional feedstock materials in conventional separation and recovery processes to produce 1-3 ton/day mixed rare earth oxides or salts (MREO/MRES) with capabilities for production of high purity, individual or binary, rare earth metals (REMs) and CMs. Program accomplishments that have been made during the past year will be presented

7.6 (16:05-16:25) Rare Earth Elements in Coal and Coal By-products: Research and Development in Wyoming, USA

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Charles Nye, and Scott Quillinan,

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Research and development addressing rare earth elements (REE) in coal and coal by-products are important in the fossil fuel rich state of Wyoming and surrounding regions because of the potential to utilize existing infrastructure and the highly trained workforce to stimulate new development and create jobs. Multiple projects are in progress to characterize the occurrence and distribution of REE in coals and coal by-products, investigate REE extraction techniques, assess all parts of the REE supply chain, and examine the broader impacts of a REE based industry.

Geochemical assessment of coal sediment systems of the Powder River and Greater Green River Basins of Wyoming is yielding clues to the occurrences of REE enrichments in these coals. Findings include higher total REE concentrations in specific layers of coal seams relative to the composition exhibited by the majority of coal within the same system. Investigations into the minerals associated with REE enrichments are also being conducted. Likewise, analysis of coal derived ash from Wyoming power stations reveals the potential for REE extraction from Wyoming derived coal by-products. The University of Wyoming School of Energy Resources (UW SER) is partnered with the National Energy Technology Laboratory and county and city government entities under the Department of Energy (DOE) Technology Commercialization Fund (TCF) to utilize a diversity of assessed coal by-products for REE extraction technology testing and optimization. Regional stakeholders continue to support these projects by providing materials for REE extraction testing and access to coal core from across the state.

Efforts are also underway to establish strategic plans that address all aspects of the REE and critical mineral (CM) supply chain in coal producing basins. UW SER is leading two projects under the DOE funded Carbon Ore, Rare Earth, and Critical Minerals (CORE-CM) Initiative for U.S. Basins. One project focuses on the Powder River Basin of Wyoming and Montana and the other focuses on the Greater Green River and Wind River Basins of Wyoming and Colorado. The objective of the CORE-CM Initiative is to catalyze basin wide economic growth and job creation using coal and coal-based resources to generate REE, other CM, and carbon-based products. The UW SER CORE-CM projects will focus on basin wide resource assessments, develop strategies for all parts of the CORE-CM value chain, and bring together a committed network of stakeholders. Project partners from academia, industry, statewide agencies, non-profit organizations, national laboratories, state geologic surveys, and city and county governments are involved in the projects. Although the CORE-CM projects are focused on coal and coal-based resources, other potential REE and CM sources will be assessed as appropriate for each basin. The overarching goal of the UW SER CORE-CM projects is to maximize development potential while leveraging the highly trained workforce, existing coal technologies, energy infrastructure, and wide public acceptance of energy technology in Wyoming and surrounding regions.

SESSION 8 (14:25-16:25)

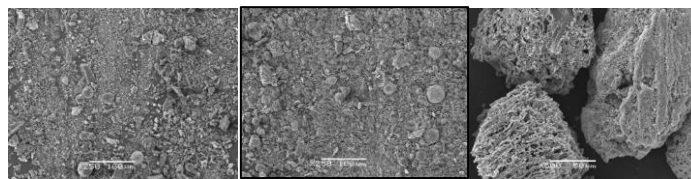
VALUE-ADDED PRODUCTS FROM COAL – 1

Tarunjit Butalia and Thomas Tarka

8.1 (14:25-14:45) Research on Characteristics and Utilization of Residual Carbon in Dry Separation of Coal Gasification Fine Slag

Ying Gao, An-Ning Zhou, Zhen Li, Wei Zhao,
Xi'an University of Science and Technology, CHINA

Coal gasification slag is a by-product of the coal gasification process. In recent years, with the rapid development of the coal chemical industry, the amount of coal gasification slag has increased at a huge rate. The higher residual carbon content in the coal gasification slag seriously restricts the recovery and utilization of the coal gasification slag. How to cleanly and efficiently use the coal gasification slag is a hot spot in today's society. In this paper, the gasification fine slag produced by coal water slurry to methanol and dry coal to oil gasification processes in Ningdong coal gasification base is studied. The residual carbon components in coal gasification fine slag were effectively separated by pre-grinding and ultra-fine classification process. The composition, structure and properties of fine slag and carbon residue were characterized by ignition subtraction (LOL), non-isothermal thermogravimetric analysis (TGA), X-ray fluorescence spectrometry (XRF) and scanning electron microscopy (SEM)(Fig1), and the composition and structure characteristics of carbon rich components under different particle sizes were explored. It is found that the grinding time has a great influence on the dissociation degree of carbon residue. After classification, the carbon residue is obviously enriched with the change of particle size, and the carbon content increases with the increase of particle size. The content of carbon in the maximum particle size is as high as 80%, the carbon content in the minimum size fraction is less than 10%. According to the characterization results, the best utilization scheme includes production of carbon silica mesoporous composites, polymers filler and adsorbent. The relatively complete porous structure of carbon residue makes the performance of adsorption materials higher than that of commercial products. The rough surface structure of carbon residue is conducive to the compatibility with polymer matrix.



(a) (b) (c)
Fig. 1: SEM of gasification fine slag

- (a) Coal water slurry gasification fine slag
- (b) dry pulverized coal gasification fine slag
- (c) residual carbon

8.2 (14:45-15:05) A Novel Process for Converting Coal to High-Value Polyurethane Products

Satya P. Chauhan, Dan Garbark, Jeff Cafmeyer, and Russ K Smit,
Battelle Memorial Institute, Columbus, OH, USA

Battelle has developed a (patent applied for) novel process for making high-value, polyurethane (PU) foam from coal, based on preparing liquefied coal via direct liquefaction, converting it to polyols as an intermediate via ozonation, and then making PU foams from these polyols. The process represents a breakthrough in innovative utilization of U.S. coals, does not require any advanced preparation of coal, and is applicable to bituminous as well as sub-bituminous coals. The resulting PU foam products are projected to have an extremely high value (over \$5,000/ton), with up to 90% of carbon being coal-based. The target products represent an extremely large (over \$80 billion/year), existing (PU foam) market, which could expand into making coatings and adhesives. The process can help reduce petroleum imports, while improving the economics of PU foam production. Battelle, with funding from National Energy Technology Laboratories (NETL), with cost share from the Ohio Development Services Agency (ODSA) and others, has advanced the process to technology readiness level (TRL) 5.

This paper will provide the details of the novel process, results of batch and continuous testing, preliminary data on PU foam properties, and present the process economic analysis. Battelle's process begins with coal liquids. These liquids were obtained by two processes: coal pyrolysis or coking to produce coal volatiles/tar and Battelle's bio-based coal-to-liquids (CTL) process to produce heavy syncrude after liquifying >85% coal. Various operating conditions for ozonolysis of the coal liquids were explored to create oxygenated intermediates of the polyaromatic coal structure, which was then converted

to the final polyester polyol. The polyols were converted to PU foam using conventional technology. The final foam rigidity benefits from the rigid polyaromatic structure contained in the polyol component. Suitable properties have been obtained for 2 lb/ft³ rigid foams, including compression strength and strain, density, and dimensional stability. The target applications for these foams will be insulation, packaging, and energy absorbing foams. The initial process economics are promising and will be presented during this presentation.

8.3 (15:05-15:25) Manufacture of Carbon Foam in Continuous Process at Atmospheric Pressure

Rudolph Olson III, CFOAM LLC, Triadelphia, WV, USA
Dan Connell, CONSOL Energy, Canonsburg, PA, USA

CFOAM LLC has been manufacturing vitreous carbon foam from coal in panel form for several years. The process is currently set up in batch mode as two steps, where the first step is conducted at very high pressure. In order to reduce cost and increase capacity, a new process for making carbon foam is being developed that can be performed at atmospheric pressure. This advance in turn would enable the development of a continuous manufacturing process, which is also being pursued. Both carbon foam panels and light weight aggregates are being investigated. Progress on the evolution of the pilot scale manufacturing plant and initial results of processing, microstructure, properties and performance of carbon foam products made using this new process will be discussed. This project is being supported by a cooperative agreement with the Department of Energy – National Energy Technology Laboratory (DE-FOA-0002185, Area of Interest 4: Coal-Derived Carbon Foam Produced via a Continuous Process, award number DE-FE-0031992).

8.4 (15:25-15:45) Status of NETL's Carbon Ore to Products Program

Joseph Stoffa
NETL, Morgantown, WV, USA

The Carbon Ore to Products Program is conducted under the U.S. Department of Energy's Office of Fossil Energy (FE) and the National Energy Technology Laboratory (NETL). The program supports R&D of technologies that utilize coal and coal wastes to produce a spectrum of products ranging from high-volume to high-value. Recent developments in the program include support for a variety of coal and coal-waste derived building products, which have the potential to reduce building costs, maintain state of the art performance, and consume significant quantities of coal and coal wastes. The performance of these coal-derived building materials will be validated through research supporting the design, testing, and fabrication of prototype building shells. In addition to high-volume applications, the Carbon Ore to Products Program continues to support R&D of moderate volume applications, most notably in the area of carbon fibers from coal. Understanding coal chemistry and processing will allow researchers to tailor precursors for the production of a range of fiber types, from commodity grade chopped fibers to aerospace grade graphitizable fibers. The Carbon Ore to Products Program also supports R&D on high-value carbon products including graphite/graphene for battery anodes and cement additives, carbon materials for integrated circuits, and conductive inks and filaments/resins for additive manufacturing applications. This talk will highlight how the Carbon Ore to Products Program supports technology across these areas in the context of larger DOE NETL goals.

8.5 (15:45-16:05) High Yield of Carbon Fiber Precursor Pitch from Low Severity Direct Coal Liquefaction of Powder River Basin Coal

Charles S. Hill, Christopher Yurchick, and Charles Atkins,
Ramaco Carbon, Sheridan, WY, USA
John Duddy, Sukesh Parasher, and Paul Sadelski,
HTI, Lawrenceville, NJ, USA

There is a vast untapped market for carbon fiber that may only be accessed through the efficient utilization of a low-cost feedstock such as PRB coal. Pitch-based carbon fibers have always demonstrated excellent properties, but the consistency of traditional source materials has plagued manufacturers. Through application of proven coal liquefaction processes at low severity conditions (lower temperatures and pressures) a spinnable isotropic pitch precursor was generated directly from PRB coal at a yield of approximately 40 W% MAF coal. Further thermal processing also demonstrated conversion of the pitch to liquid crystal mesophase in significant quantities and with acceptable spinnability. Fibers were spun under a variety of conditions, oxygen stabilized and carbonized, examined by microscopy, and tensile properties were determined. Economic analysis indicates the final carbon fiber costs to be far less than other precursors. This could help enable widespread adoption of carbon fiber and composite materials in transportation and wind energy markets, potentially increasing worldwide demand and displacing existing PAN-based fiber as a lower cost and higher performance alternative. This project is supported by a cooperative agreement with the Department of Energy – National Energy Technology Laboratory (DE-FOA-0001992,

FOA Area of Interest 2B - Producing High-Value Solid Products from Domestic U.S. Coal, award number DE-FE-0031801)

8.6 (16:05-16:25) Advanced Coal Upgrading to Produce Improved Feedstocks for Coal-Derived Value-Added Product

Alexander Azenkeng, Nicholas E. Stanislawski, and Jason D. Laumb,
University of North Dakota Energy & Environmental Research
Center Grand, Forks, ND, USA

Advanced coal-upgrading methods have been investigated on four U.S. coal ranks- lignite, subbituminous, bituminous, and anthracite-with the aim to improve the quality of the resultant coal residue as a feedstock for value-added carbon products. Preliminary results have demonstrated a residual ash content of < 1 wt% for lignite, <3 wt% for subbituminous and bituminous, and < 7 wt% for anthracite coals. The coals were cleaned by a combination of specific gravity techniques to remove coal-borne inorganic minerals and chemical cleaning using strong acids. Additional refinements are ongoing to further improve the ash reductions and obtain ultraclean coals with residual ash content of <0.5 wt%, which will significantly improve the coal residue as a feedstock for high-value carbon products such as graphene and graphite. Initial characterization of the graphene quantum dots (GQDs) produced from raw and clean coals has been done using UV (ultraviolet)-vis and UV fluorescence spectroscopy techniques. Higher absorption intensities were observed from GQDs obtained from clean coal samples compared to those obtained from raw coal samples. The emission maxima showed an increasing redshift from lowest to highest coal rank, i.e., lignite, subbituminous, bituminous, and anthracite. It was also observed that excitation of anthracite-derived GQDs in the UV region produces little to no fluorescence signal, but a maximum emission signal was observed when excitation was performed in the visible region. These results are relevant in tailoring specific optical applications of GQDs derived from different coal ranks.

SESSION 9 (8:00 – 9:45)

COMBUSTION TECHNOLOGY – 1

Evan Granite and Eric Grol

9.1 (8:05-8:25) Numerical Study on the Dispersion of Non-Spherical Particles in a Turbulent Round Jet

Wenshi Huang, Yang Zhang, Yuxin Wu, and Jingyu Wang,
Tsinghua University, Beijing, China
and Minmin Zhou
University of Utah, Utah, U.S.A.

Moderate or intense low-oxygen dilution (MILD) combustion of pulverized coal is regarded as a new combustion technology with great potential due to its advantages of reducing NO_x emission and improving the uniformity of heat flux in the furnace. In a high-speed jet with strong shear which is mostly necessary for MILD combustion of coal, the motions of particles may be significantly affected by particle shape especially for pulverized coal with irregular shape. In this work, in order to predict the translational and rotational motions of non-spherical particles more accurately in a turbulent jet, a model of non-spherical particles considering particle drag correction, lift, and rotation was established based on the Eulerian-Lagrangian method, employing the Ansys Fluent commercial platform. The dispersion characteristics of spherical and non-spherical particles with different Stokes numbers in high-speed jets were numerically analyzed and compared. The results reveal that the dispersion and radial velocity fluctuation of non-spherical particles in the turbulent jet are stronger than that of spherical particles, especially when Stokes number is large. The change of the Magnus force caused by the increase in the angular velocity of non-spherical particles plays a dominant role in the differences of particle dispersion, while the impacts of drag force and lift force are relatively small. It is concluded that the correction for Magnus force caused by the rotation enhancement of non-spherical particles cannot be neglected in the simulation of a particle-laden turbulent jet, which is important for the accurate prediction of MILD combustion of coal.

9.2 (8:25-8:45) Twice Ignition and Volatile Combustion of Isolated Coal Particles Under Low Oxygen Concentrations at Microgravity

Wantao Yang, Yang Zhang, Yuxin Wu, Junfu Lyu, and Hai Zhang*
Key Laboratory for Thermal Science and Power Engineering of Ministry Education,
Department of Energy and Power Engineering, Tsinghua University, Beijing, China

Experiments were carried out at microgravity on ignition and combustion for isolated bituminous coal particles under different oxygen concentrations, particle sizes and furnace temperature using a Chinese SJ-10 satellite. The phenomenon that twice ignition of coal particles was observed under low oxygen concentrations (XO₂ = 10%) during the volatile combustion process for the first time. When twice ignition occurs, both the ignition delay time and volatile flame duration decrease. As oxygen concentration

increases, the time interval between the twice ignition decreases, until the second ignition disappears. In addition, when particle size increases to 3.5 mm or furnace temperature decreases to 913 K, the twice ignition cannot be observed. Counterpart experiments were conducted at normal gravity to further reveal the dominant mechanisms of twice ignition of coal particles. The competition between volatile release rate and oxygen transfer rate can well interpret the occurrence of twice ignition. The first extinction of volatile flame is dominant by insufficient oxygen replenishment response and twice ignition occurs with the process of oxygen accumulation. The second extinction of volatile flame is caused by the low particle temperature and reduced devolatilization rate, which is consistent with the phenomenon of universal once ignition observed on the ground. Combining with Da number and Fo number, a diagram is established to assess the condition of whether twice ignition occurs or not under microgravity and normal gravity.

9.3 (8:45-9:05) Direct Combustion of Fine Coal From Coal Waste

Fei Yi, Jeannine Elliott, Jeff Lind, Justin Feis, Bradley Spatafore
TDA Research, Inc., Golden, CO, USA

Fine coal is a coal waste generated by grinding and washing coal at the mines. Because of its high water content, the dewatering process is very energy intensive. Therefore, coal producers often choose to discard it. To date, U.S. coal mines have discarded about 4 billion tons of fine coal waste and will continue to dispose another 70~90 million tons per year. This work presents a process to direct combust the fine coal to harness the energy from the traditional waste. Pumpable slurries were prepared from real fine coal sampled from a U.S. mine. Combustion tests in a bench-scale apparatus demonstrated the feasibility of the direct combustion concept. A swirl burner was utilized in the apparatus. Both tangential swirler and vane swirler were tested in the experiments. Temperature and flue gas composition were measured at multiple locations to characterize the flame. Experimental results showed good atomization was very critical for the stability and burnout of the flame.

9.4 (9:05-9:25) Parametric Analysis of SO_x and NO_x Removal in a Direct Contact Cooler for Pressurized Oxy-Combustion

Piyush Verma, Swarali Ghodkhande, Zachariah Wargel, Sebastian Klein, Zhiwei Yang, Washington University in Saint Louis, Saint Louis, MO, USA
and Richard L. Axelbaum
Washington University in Saint Louis, Saint Louis, MO, USA
Consortium for Clean Coal Utilization

The removal of SO_x and NO_x from the flue gas of pressurized oxy-coal combustion is required to prepare the CO₂ stream for transportation and sequestration. Elevated pressure enhances NO oxidization to NO₂, which is more soluble in water. Moreover, the liquid phase interaction between absorbed NO₂ and SO₂ enhances the removal of SO₂ from the flue gas. As a result, a direct contact cooler (DCC), which is a counter-current reactive-absorption column, can be employed to accomplish integrated pollutant removal at high pressure. This process is potentially much more economical than conventional SO_x and NO_x removal technologies. However, the understanding of the impact of operational parameters on the removal efficiency of SO_x and NO_x in a DCC is limited. In this work, we perform a parametric analysis of the impact of temperature, pressure, and inlet water pH to understand and optimize SO_x and NO_x removal. The experiments were performed in a small pilot, counter-current packed bed, DCC, with an 0.2 m inside diameter and 2.3 m long. Synthetic flue gas was created by mixing NO, SO₂ and O₂ in a balance gas of CO₂, and the gas was heated to the required temperature in a gas heater before being fed to the column. The pH of the inlet water was varied using recycled flow from the sump. The pressure, inlet gas temperature, and inlet pH were varied between 5 – 15 bar, 24 – 250 °C, and 3 – 8, respectively. To ascertain the extent of liquid phase interaction, different S/N ratios were considered in the experiment.

We found that the removal efficiency of NO increases sharply with pressure for the same residence time and O₂ concentration. However, SO₂ removal remains high at all pressure. Moreover, the overall removal of NO decreases with temperature, with a marginal reduction in SO₂ removal. Additionally, SO₂ removal depends on the amount of inlet NO, while NO removal is not a function of inlet SO₂. The experiment analysis increases our understanding of the removal process for SO_x and NO_x and aids in the design of DCCs.

9.5 (9:25-9:45) Effects of Turbulence-Radiation Coupling in Pressurized Oxy-Combustion

Lei Li, Samuel Ogunfuye, V'yacheslav Akkerman,
West Virginia University, Morgantown, WV, USA
Richard L. Axelbaum, and Zhiwei Yang,
Washington University in Saint Louis, Saint Louis, MO, USA

Concerns over climate change have led to numerous efforts in developing low-carbon energy technologies. Pressurized oxy-combustion (POC) is a promising candidate to reduce carbon emission in power generation. Due to the strong impact of pressure on thermal radiation, heat transfer in POC differs significantly from the situation of

conventional atmospheric pressure combustion. Thus thermal radiation in POC needs to be investigated to aid new combustor development. The present computational work is a step in this direction, initiating a systematic analysis of thermal radiation and heat transfer in a pilot-scale POC combustor, which has been developed at Washington University in St. Louis (WUSTL). In a POC process, pulverized coal is burned under elevated pressure and O₂-CO₂ environment. While most previous computational works on flame radiation focused on atmospheric pressure condition, this work considered a pressurized flame. Specifically, a 15-bar POC combustor of power 50 kW is modeled employing the Ansys FLUENT commercial platform, using both Reynolds-averaged Navier-Stokes (RANS) modeling and large-eddy simulation (LES).

A recently published and validated global radiation model is used to predict the radiative property of the flue gas. The discrete ordinates (DO) radiation model is chosen to solve the radiative transport equation. Incident radiation on the walls of the combustor is identified and investigated. It is revealed that for this pilot-scale, pressurized combustor, thermal radiation exhibits similar patterns in the RANS and LES models. However, the magnitudes of radiation are different in both models, presumably because interactions between radiation and turbulence are embedded in the LES model but not in the RANS model. This difference thereby underlines the major goal of this research: investigating the impact of such turbulence-to-radiation coupling on thermal radiation in a pilot-scale POC setting.

Most previous studies on turbulence-to-radiation interactions focused on bench-scale, atmospheric pressure flames. This work is the first effort to extend this study to a pilot-scale, pressurized flame.

SESSION 10 (8:00 – 9:45)

COAL MINING, PREPARATION AND HANDLING

Richard Bajura and Richard Winschel

10.1 (8:05-8:25) Hydrothermal Synthesis of NiMoS/SBA-15 Catalysts for the Hydrodesulfurization of Dibenzothiophene

Antony Rajendran, Tian-You Cui, and Wen-Ying Li,
State Key Laboratory of Clean and Efficient Coal Utilization,
Taiyuan University of Technology, Taiyuan, CHINA

The dwindling crude oil reserves emphasize the urgency to look for the alternative feedstocks to produce liquid fuels. Coal tar, being rich in aromatics, can be a suitable alternative feedstock however its sulfur content should be reduced below 10 ppm to meet the standards set by environmental protection agencies. Though hydrodesulfurization is industrially employed for the sulfur removal, its traditional Ni(Co)MoS/γ-Al₂O₃ catalysts are inadequate to produce the fuels with < 10 ppm. This is due to the strong metal-support interaction, i.e., Mo-O-Al, that suppresses the generation of highly efficient Type II NiMoS active phase possessing more edge active sites but promotes the formation of less-efficient Type I NiMoS active phase having fewer edge active sites. In this presentation, we have used SBA-15, that circumvents the metal-support interaction, in order to prepare the NiMoS/SBA-15 catalysts with more edge sites. Especially, the facile one-pot method has been chosen instead of the traditional preparation method consisting of separate sulfidation process. The prepared catalysts have been characterized by powder X-ray diffraction, Raman spectroscopy, X-ray photoelectron spectroscopy, N₂ adsorption-desorption study, and high-resolution transmission electron microscopy. The optimized catalyst can be effectively reused as it accomplishes ~100% efficiency during the hydrodesulfurization of dibenzothiophene even after 4th successive catalytic run under batch reactor conditions (T= 320 °C, P = 6 MPa (H₂) and CS = 500 ppm (w).

10.2 (8:25-8:45) CFD Simulations to Characterize Coal Dust Explosions Severity Parameters in the Standard 20L-Vessel

Andrés Rodríguez Fernández, Alain Islas Montero, María Covadonga Betegón Biempica, Adrián Pandal Blanco,
University of Oviedo, Gijón, Asturias, Spain
Emilio Martínez Pañeda,
Imperial College London, London, UK

Dust explosions are the combustion of fine dust particles in a rapid reaction regime. They are of relatively common occurrence in underground mines and processing industries, causing accidents that could seriously damage facilities and workers. To fairly describe the dust explosion hazard of any material sample, its maximum explosion pressure and deflagration index should be reported. Nowadays, the assessment of these values still relies on experimental scale tests, defined by international standards like the ASTM E1226 or UNE 14034. In them, a pressurized airflow carries the dust sample through a nozzle, allowing its injection into a closed volume. Pyrotechnical ignitors are activated after a delay time for dust cloud settling, so subsequently, the dust explodes. Since both

dust particle size and concentration can vary broadly, and turbulence plays a key role in these tests, computational fluid dynamics (CFD) technics are a useful tool to simulate these processes and reduce costs. In the present investigation, the open-source code OpenFOAM is used to assess explosion severity parameters of a coal dust sample, which has previously undergone experimental testing. The compressible multiphase flow (gas-solid) simulation is solved using the three-dimensional (3D) unsteady Reynolds averaged Navier Stokes (URANS) equations, employing a standard k- ϵ turbulence model and a Eulerian-Lagrangian (EL) description in a two-way coupling regime. Partially Stirred Reactor model accounts for the combustion of coal volatile matter, which is represented by chemical reactions that characterize the combinations of devolatilized methane and hydrogen with ambient oxygen.

Keywords: CFD, coal dust, OpenFOAM, Eulerian-Lagrangian, URAN

10.3 (8:45-9:05) A Study on Self-Heating Characteristics of Coals

Tai-Cheng Li, Pai-Yi Wang, Research Engineer, Taiwan Power Company, NEW TAIPEI CITY, TAIWAN

After long-term storage, the temperature of coal will gradually increase, which is called self-heating. The reason is that the contact between coal and air will produce oxidation reaction and release heat. When the accumulated heat of self-heating makes the temperature of coal exceed the ignition point, spontaneous combustion will occur. It will not only cause economic loss, but may also cause serious fires. Therefore, the management of coal storage is an important technology.

The purpose of this research is to establish an evaluation method for the self-heating characteristics of coals. The combination of functional group structure analysis and low-temperature oxidation experiment is helpful to understand the difference in the structure of coals and the mechanism of low-temperature oxidation, and to evaluate the self-heating characteristics of coals. In the future, the coal with a high self-heating potential can be reduced the probability of spontaneous combustion by shortening storage time and strengthening monitoring, and it can be used as a reference for coal storage management methods.

10.4 (9:05-9:25) An Overview on Air Dense Medium Fluidized Bed for Coal Beneficiation in China

Chenyang Zhou, Yumin Zhao, Liang Dong, Chenlong Duan, Yanjiao Li
Key Laboratory of Coal Processing and Efficient Utilization, School of Chemical Engineering & Technology, China University of Mining & Technology, CHINA

Air dense medium fluidized bed is a representative dry coal beneficiation technology. The technology is especially useful to solve the difficulties of coal cleaning in arid region. The paper gives an overview on the development of air dense medium fluidized bed in China. The relevant theory and technology have been highlighted and summarized. The challenging issues that need special attention are suggested for further improvement of this process.

Keywords: Fluidized bed; Dry Coal beneficiation; Dense medium; Coal Preparation.

10.5 (9:25-9:45) CFD Simulations of Coal Dust Dispersion in a 20L Spherical Vessel: An Assessment to Dust Explosion Tests

Alain Islas Montero, Andrés Rodríguez Fernández, University of Oviedo, María Covadonga Betegón Biempica, Adrián Pandal Blanco,
University of Oviedo, Gijón, Asturias, Spain
Emilio Martínez Pañeda,
Imperial College London, London, UK

Coal dust explosions in underground coal mines are among the deadliest mining disasters. Accumulations of combustible dust in coal mines create the risk of large-scale explosions that can result in multiple deaths and traumatic injuries. Among the methods to reduce the explosion potential of coal dust generated during mining, rock dusting is probably the preferred practice. The explosiveness of these air-coal-limestone mixtures is commonly determined following the ASTM E1226 or UNE 14034 standards, in which a dust sample is injected into a 20L spherical vessel by means of a pressurized flow and that is dispersed by a rebound nozzle. In these tests, an ignition delay time t_d of 60ms is assumed to cause sufficient mixing to produce a homogeneous dust cloud inside the test chamber. In the present investigation, computational fluid dynamics (CFD) techniques are used to simulate the dust dispersion process in a 20L spherical vessel by employing an open-source CFD code. The compressible multiphase flow (gas-solid) simulation is solved by means of the three-dimensional (3-D) unsteady Reynolds averaged Navier Stokes (URANS) equations, employing a standard k- ϵ turbulence model and a Eulerian-Lagrangian (EL) description in a two-way coupling regime. First, the temporal trends of the pressure and root-mean-square velocity fluctuations show good agreement with respect to the experimental measurements of the literature, suggesting that the model is capable to appropriately capture the relevant features of the transient flow. Second, the formation of two vortex structures within the sphere prevails as a mechanism of non-

homogeneous particle mixing. This condition imposes a high dust concentration in the near-wall region, thereafter, diminishing the number of available particles close to the ignition zone. Third, the particle Reynolds and Stokes numbers suggest that the dust particles do not follow the changes of the flow field, exhibiting large drifts from the flow streamlines due to a high inertial force.

Keywords: CFD, coal dust, dispersion, OpenFOAM, Eulerian-Lagrangian, URANS

SESSION 11a (9:55-10:55) COMBUSTION TECHNOLOGIES – 2 Evan Granite and Eric Grol

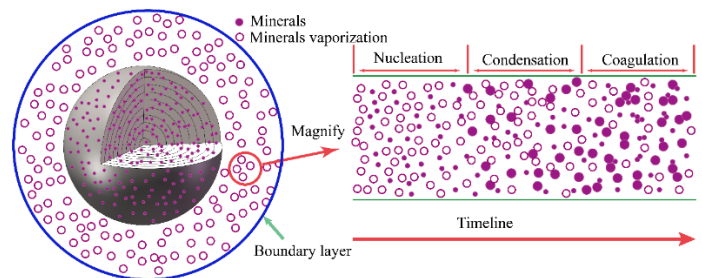
11a.1 (9:55-10:15) Impact of Pressure on the PM₁ Formation from Char Combustion via Simulation

Zhengang Zhou¹, Yueming Wang¹, Huimin Liu², Xiaolong Li³, Lin Li¹, Jost Wendt³, Lunbo Duan¹

1. Key Laboratory of Energy Thermal Conversion and Control, Ministry of Education, School of Energy and Environment, Southeast University, Nanjing, China
2. State Key Laboratory of Coal Combustion, Huazhong University of Science and Technology, Wuhan, China
3. Department of Chemical Engineering, University of Utah, 50 South Central Campus Drive, Salt Lake City, UT, USA

Pressurized oxy-fuel combustion technology has several advantages over oxy-fuel combustion technology at atmospheric pressure, such as higher combustion efficiency and economics. Sub-micron particulate matter (PM₁) has a considerable influence on the human body and the environment. However, to the best of the authors' knowledge, there are only a few studies which has investigated the mechanism of pressure in PM₁ formation during coal combustion. Therefore, it is essential to explore the PM₁ formation mechanism under pressurized conditions. In this study, a PM₁ formation model was built, which could help us investigate pressure on PM₁ formation during char combustion. In the char combustion process, minerals (SiO₂, Al₂O₃, MgO, FeO) will be reduced to highly volatile suboxides (SiO and Al₂O) and metals (Mg and Fe). The mineral vapor molecules experienced radial diffusion, transported them outwards by the difference of concentration. Afterwards, nucleation, condensation and coagulation will occur. The PM₁ formation process needs a short time (<1s). These reactions concentrate in a smaller range around the char particle called the boundary layer. According to the formation mechanisms of PM₁, we can divide the model into four sub-models. By using these models, some physical quantities can be calculated, such as char burning temperature, carbon conversion and proportion of mineral gasification, the particle size distribution of PM₁. The char particle temperature increases with increasing pressure in the study, and the carbon conversion rate increases. The mineral vaporization proportion decreases dramatically as the pressure increases. When the pressure rises from 0.1MPa to 1.5MPa, the intensity of the sub-micron peak decrease about an order of magnitude, which has a good fitting with experimental results. At the same time, with the boundary layer thickness decrease, the probability of PM collision increases, there is more large PMs formation during a short time.

Graphical abstract



Fine Particulate matter formation model

11a.2 (10:15-10:35) Pilot Study on Removal of Mercury, Sulfur and Nitrate from Coal-Flue Gas by Pulse Plasma

Jun Zhang, Chunbao Zhao, and Ri Li,
Nanjing Vocational College of Information Technology, Nanjing, Jiangsu Province,
CHINA
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Mercury emission from coal combustion has become the fourth biggest pollutants following SO₂, NO_x and dusts. The non-thermal plasma has been the potential to serve as a low cost combined removal technology of multiple pollutants. In this paper, the removal of mercury, sulfur and nitrate from coal-fired flue gas of YangChen plant after desulfurization was studied through pulse plasma and additive. The flow was controlled to 20,000 Nm³/h, the temperature and water vapor content in the flue gas were 50 ± 2 °C and 12% (volume fraction), respectively and the O₂ content was about 5%. The results shown that the average concentration of Hg⁰ and Hg²⁺ in flue gas mercury emission were 2.364 µg/Nm³ and 0.406 µg/Nm³, respectively, which could meet the national emission standards of mercury. Ammonia and NaCl had no effect on mercury removal. The mercury removal of hydrogen peroxide and NaClO was enhanced by pulse plasma treatment, which could reach 46.86% and 33.42% by pulse plasma treatment when the concentration of H₂O₂ and NaClO were 0.4 and 0.1 mol/L, respectively. Moreover, the oxidation efficiency of mercury increased with the increase of additive concentration. The concentration of NO and SO₂ in flue gas was decreased obviously after pulsed discharge plasma. Water spraying had no obvious influence on the removal of NO under plasma treatment, but the removal efficiency of SO₂ was increased obviously when spraying water.

11a.3 (10:35-10:55) Advanced Tools for Assessment of Direct-Fired sCO₂ Power Cycles

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Reaction Engineering International, Midvale, UT, USA
Frederick Dryer, Sang Hee Won, and Tanvir Farouk
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The predominant thermodynamic cycle in use today for power generation is the Rankine cycle using steam as the working fluid. In recent years, significant academic and industrial focus has been placed upon alternative thermodynamic cycles, especially those utilizing supercritical carbon dioxide (sCO₂) as the working fluid. The potential benefits of this fluid selection are well-documented, with the primary advantage being higher cycle thermal efficiency than steam Rankine cycles, as well as smaller equipment footprints. In a direct-fired sCO₂ cycle, fuel is combusted with oxygen in a highly dilute sCO₂ environment. Nearly 100% of the CO₂ present in the process is available for utilization, making the technology a near-zero emission form of power generation. Current estimates of efficiency are near 50%, while producing a near-sequestration-ready CO₂ stream. The growth and maturity of this technology depends upon defining presently unquantified constraints as the characteristics of sCO₂ oxy-combustion have not been fully established.

Reaction Engineering International (REI) has led a DOE-funded program focused on developing high-fidelity tools for characterization of the combustion environment in direct-fired sCO₂ power systems. The objective is to produce verified chemical mechanisms and real gas thermodynamic and transport properties that will be implemented into an industrially applied CFD model developed by REI. Code modifications include real gas thermodynamic and transport properties appropriate for supercritical mixtures of CO₂, and finite rate limitations associated with oxidation and emissions kinetics. This paper will provide an overview of the technical approach for developing and verifying the real gas properties; as well as the chemical kinetic mechanism for the high pressure, highly CO₂ diluted sCO₂ oxy-combustion environment. Comparisons of model results and empirical data will be provided that demonstrate the model's predictive capability with respect to global parameters (e.g. ignition delay times) as well as speciation for syngas and natural gas combustion under supercritical CO₂ conditions relevant to oxy-combustion applications.

SESSION 11b (10:55-11:55) CARBON MANAGEMENT – 1 Nicholas Siefert and Bingyun Li

11b.1 (10:55-11:15) Evaluation of Nanoparticles in the Performance of CO₂ Desorption from Monoethanolamine (MEA) in a Randomly Packed Tower

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In this study, different kinds of nanoparticles (i.e. TiO₂, SiO₂ and Al₂O₃) were used to investigate their effects on CO₂ desorption from monoethanolamine (MEA) solution in a randomly packed tower. The CO₂ desorption performances in rich MEA solutions were quantified in terms of the CO₂ desorption rate (V). An enhancement factor (E_{de}) was defined as the ratio of V with and without nanoparticles to evaluate the enhancement effect of nanoparticles. CO₂ desorption rate and desorption enhancement owing to nanoparticles under different working conditions were thus systematically investigated in the packed tower. The results show that the addition of nanoparticles in the MEA solution improves the CO₂ desorption rate greatly. At the same desorption rate, the presence of nanoparticles can lower the desorption temperature and the height of desorption tower. Therefore, the use of nanoparticles results in a reduction of energy consumption. Possible mechanisms can be due to the fact that nanoparticles affect the bubble shape in the solution and improve the thermal conductivity of rich MEA solution.

11b.2 (11:15-11:35) Effect of Shell Thickness of Core Shell MOF on CO₂ Adsorption and Separation

Xiaoqian Ju, Zhiyuan Yang, Yuhang Zhai, Xinbo Duan, and Changguo Wang
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There are all different proportions of CO₂ in landfill gas, coalbed methane, goaf gas, biogas or low-grade natural gas. The existence of CO₂ is not conducive to the utilization of methane, and will occur certain corrosion to the equipment. So, we prepared a core-shell metal organic framework (MOF) by room temperature crystallization method. The XRD diffraction peaks of core-shell MOF and monomer zeolitic imidazolate framework (ZIF) are consistent. We studied the effect of the different shell thickness on CO₂ adsorption and separation. The core shell MOF also shows the regular dodecahedron structure. The synergistic effect of core and shell increases the adsorption capacity of CO₂. When the ratio of shell to core is 0.5, the CO₂ capacity reached 204.58 cm³-g⁻¹. Furthermore, the shell of core shell MOF did not increase the adsorption capacity of CH₄. This will facilitate the separation of CH₄ and CO₂. More notably, the core shell MOF is a potential CO₂ separation material.

11b.3 (11:35-11:55) Hydrogen for Decarbonized Electricity and Industrial Sectors—An R&D Perspective

David Lyons,
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Hydrogen will play an essential role in the future decarbonization of the electric power and industrial sectors. There are opportunities for large-scale production and deployment of clean hydrogen from carbonaceous fuel (waste coal; plastics; biomass; and natural gas) coupled with carbon capture, utilization, and storage (CCUS). Future plants that produce and utilize or store clean hydrogen will be pivotal for achieving the current administration's goal of a zero-carbon power sector by 2035. In addition, deployment of clean hydrogen technologies in the industrial sector is an important component to meet the administration's economy-wide 50% carbon dioxide (CO₂) reduction target of 2030 and to achieve the goal of a zero-carbon economy by 2050. Clean hydrogen could be widely deployed by 2030 with targeted research and development (R&D). This research is critical to making clean hydrogen production processes cost-effective with net-zero, or even net-negative, carbon emissions.

This presentation will provide a review of U.S. Department of Energy (DOE)/National Energy Technology Laboratory (NETL) R&D efforts to enable deployment of clean hydrogen in the power generation and industrial sectors, along with a discussion of advances in technologies that will serve as the foundation for future low-cost, low-carbon emissions power and industrial systems.

SESSION 12 (9:55-11:35) SUSTAINABILITY AND THE ENVIRONMENT Massood Ramezan and Richard Winschel

12.1 (9:55-10:15) Sustainable Development Model on Coal Supply for Coal-Fired Power Plants by using Multi-Objective Optimization with Economic, Environmental, and Social Aspects Consideration

Firly Rachmaditya Baskoro, Keisuke Nagasawa, Katsumi Morikawa, and
Katsuhiko Takahashi,
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Energy is one of vital part to achieve the Sustainable Development Goals (SDGs). Coal is considered as one of the most abundantly and the cheapest available energy source, particularly in the developing country. Indonesia is one of a country that still heavily rely on coal to fulfill its national primary energy demand, particularly for electricity generation which in majority is generated by coal-fired power plants. Coal holds major role as raw material to generate power, as well as key component in metal production. However, coal utilization is facing greater challenges in terms of economic, environmental, and social concerns. In order to optimize coal utilization in Indonesia, it

is necessary to consider these three factors which in the existing condition only economic aspect that has been considered. Therefore, economic-environment-social model will be constructed to solve the problem by using multi-objective optimization method with epsilon-constraint method. In this study, cost represents the economic aspect, while CO₂ emission represents the environmental impact. Social aspect will be represented by the corporate social responsibility (CSR) programs as well as the human development index (HDI) in several province with high coal dependency. Most research considering social aspect in optimization were conducted by using the number of workers, which often neglects the fact that the same job can have different social benefits in different regions. The utilization of HDI which consider education, healthiness, and economic level of a region may give better understanding on social impact from coal mining industry to the society. Prioritization for underdeveloped and fast-growing region will be considered in the optimization. The optimization will consider several aspects for coal blending, such as coal quality, power plant's specification and demand, and ship type selection. The results of the research perhaps can be utilized by the decision makers to improve the coal utilization towards the sustainable development.

Keywords: social benefits; carbon dioxide emission; sustainable development; multi-objective optimization; coal

12.2 (10:15-10:35) Enhanced CO₂ Physical Solvents for Biogas Upgrading

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Biogas is a renewable energy source which can be used directly as fuel or indirectly as a raw material for synthesis gas or H₂. The main constituents of biogas are CH₄ and CO₂, along with N₂, O₂ and trace amounts of undesirable compounds like H₂S and NH₃. The utilization of biogas presents many environmental advantages, including the fact that it is a renewable energy source. Furthermore it reduces emission of the greenhouse gas CH₄ into the atmosphere, and it can be used as a substitute for fossil fuels. The removal of CO₂ from the CH₄ in biogas can be accomplished in different ways, to include pressure swing absorption, water scrubbing, and chemical scrubbing using either chemical or physical solvents. Because CO₂ is more soluble in organic solvents than water, the use of organic physical solvents can reduce the volume of liquid flow and hence reduce the size and cost of the unit performing the biogas upgrading. The solvent is regenerated via temperature and/or pressure swing processes.

The primary organic physical solvent used for biogas upgrading is Selexol™, which is a mixture of oligomers of polyethylene glycol dimethyl ether. This solvent requires relatively low process temperatures to avoid evaporation and to maintain high concentrations of dissolved CO₂ in solution and tends to absorb water easily, which reduces the ability to take up CO₂. A new family of organic physical solvents has been found which are prepared easily from simple reagents and exhibit greater CO₂ uptake, improved working capacity and CO₂:CH₄ selectivity, and less hydrophilicity. These new solvents were tested over a range of temperatures and CO₂ pressures using a Hidden IGA microbalance and were shown to absorb CO₂ easily and desorb it using a thermal swing process. These solvents have low viscosities, have lower operating costs than Selexol, and are stable towards hydrolysis.

12.3 (10:35-10:55) Reactive Transport Modeling of Coal Fly Ash, A Column Study

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In this study, a reactive transport model was developed using the CrunchFlow code to predict the long-term leaching of coal fly ash deposits in a laboratory-scale column. The fly ash composition was introduced via primary and secondary host phases, determined by characterization techniques. The model considered dissolution/precipitation reactions with thermodynamic and kinetic data (i.e., solubility constants, rate constants, and specific surface area) and transport parameters (i.e., advection and dispersion). The calibrated model predicted the concentration of major and trace elements (As, Mo, Se, B) within 10 years of leaching. Wash-out phase was the result of easily dissolvable minerals dissolution, and was known by release of high contents of Na, K, Mg, Ca, S, B, and Mo. Kinetically controlled reactions occurred in the time scale of 100 days, by depletion of gypsum and calcite, and formation of secondary minerals (such as calcium silicate hydrates, clay minerals, and iron oxyhydroxides). Congruent dissolution of glass phase continuously released its components (i.e., Si, Al, Fe, K, Mg, Se, and As) in long-term leaching. The iron concentration was controlled by formation of ferrihydrite with high specific surface area. The leachate composition at early ages of leaching exceeded the environmental limits for S, B, Mo, and Al. However, in long-term the effluent composition met the leaching limits except for Al content. The porosity of compacted fly ash started to raise from the top layers, and along 30 years of weathering it increased from 28% to 45%, which can significantly affect the stability and transport properties in fly ash deposits.

12.4 (10:55-11:15) Characterization of Fine Coal Processing Waste and Its Technological Applications

Julia Meller Mendes Silva, Elen Machado de Oliveira, Elis Machado de Oliveira, Camila Machado de Oliveira, Thuani Gesser Muller, Gracieli Daniel Zanette José Luiz Westrup, and Michael Peterson,
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Sabrina Tavares, and Rosimeri Venâncio Redivo,
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Brazil's main coal reserves are located in the southern region where, due to the geological characteristics of the region, a large amount of waste is generated in its mining. The fine coal processing waste is an environmental problem and therefore it is necessary to find an alternative use for these tailings. The aim of this work was to characterize the waste from the coal beneficiation stage in terms of moisture, ash, carbon, sulfur, etc., as well as to characterize the waste after thermal activation and its efficiency as a methylene blue dye (MBD) adsorbent. Different temperatures were tested for the activation of the waste, as well as the ideal amount of mass to be used in the adsorption. The study showed that the fine coal waste samples achieved a better performance when activated at a temperature of 500 °C, with a percentage of MBD adsorption of approximately 83%. The amount of mass that had greater efficiency in the adsorption process was 1 g, adsorbing approximately 99.0% of the color. The results show that there is the possibility of using fine coal processing waste in adsorption processes and, consequently, reducing the environmental impacts caused by the beneficiation of coal.

12.5 (11:15-11:35) Life Cycle Water Consumption of Biomass Co-Firing Power Plants with Carbon Capture and Storage

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In the near-to-medium term, co-firing biomass and coal for electricity generation provides the most promising route to bioenergy with carbon capture and sequestration (BECCS), a key mitigation option proposed widely to control global warming below 1.5 –2.0 °C. The objectives of this study are to estimate the consumptive blue water use of coal-biomass co-firing power plants with CCS and then quantify its variability and uncertainty on a life cycle basis. The fuel-based life cycle analysis reveals that for a given location, compared to the case of complete coal combustion with CCS, co-firing biomass at pulverized coal power plants with CCS increases the life cycle blue water consumption by a factor up to about 9, which depends highly on the biomass type and co-firing rate. Biomass-dedicated combustion with CCS further significantly increases the consumptive blue water use by a factor up to 58; the life cycle blue water use also varies with the biomass production location; and among the numerous stages across both coal and biomass fuel cycles, the biomass production is the dominant stage accounting for approximately 70% or more of the life cycle blue water consumption, which indicates the importance of advancing agricultural practices and technologies to reduce the overall water use. Large-scale BECCS deployment would pose a challenge for local and world water sustainability. Thus, this study highlights a strong need for a close coordination of technology, resource, and policy in addressing the complex nexus of climate change, energy, and water resources toward a sustainable net-zero carbon future.

SESSION 13 (12:35 – 14:15) CARBON MANAGEMENT – 2 Nicholas Siefert and Bingyun Li

13.1 (12:35-12:55) Preparation and CO₂ Adsorption Properties of MOF Composites Doped by Ionic Liquid

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Carbon dioxide capture and separation are significant transition technology before the maturity of clean energy, which is of great importance for mitigating greenhouse effect. In this study, 1-butyl-3-vinylimidazolium bis(trifluoromethanesulfonyl)imide ([BVM][TFSI]) is introduced into the pores of ZIF-8, and then the composite structure of imidazolium-based poly ionic liquid (polyILs) shuttling through the ZIF-8 pores, namely polyILs@ZIF-8, was obtained by copolymerization. Stable multiphase composites are formed by in-situ polymerization of ionic liquids in the pores of ZIF-8, and the materials can retain the inherent properties of the two components, which is conducive to the adsorption of CO₂. The composites were characterized by powder X-ray diffraction (PXRD), N₂ adsorption isotherm, CO₂ selective adsorption, FT-IR spectra, energy dispersive X-ray (EDX) and thermogravimetric analysis (TGA). The

adsorption and selection of MOF-based composites for CO₂ were studied systematically by means of experiment and theory.

13.2 (12:55-13:15) Characterization, adsorption isotherms and adsorption rate modelling of activated carbon sorbents for carbon dioxide capture

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Engineering, North-West University, Potchefstroom, South Africa.

An investigation was undertaken involving the determination of accurate adsorption kinetics of selected commercially available activated carbon sorbents for the capture of carbon dioxide, suitable for advanced process CFD modelling and design of circulating fluidized bed absorbers. Four commercially available activated carbon samples (CQ006, CQ30P, CQ650 and PCX1) derived from coal, coconut shells and wood feedstocks respectively were investigated. The samples were characterized using methods such as proximate analysis, ultimate analysis, surface area analysis, pore size distribution and volume analysis, as well as scanning electron microscopy analysis. The activated samples were found to have acceptable surface areas and micropore structures for carbon dioxide capture, with the highest BET surface area and micropore surface area equivalent to 735 m²/g and 517 m²/g, respectively, characteristic of the CQ650 (coconut shells) sorbent. The average pore diameter was determined to be within the range of 3.92–4.13 Å with porosities as high as 27.7 %. Scanning electron microscopy analyses revealed cracks and crevasses, displaying a very uneven surface. The carbon dioxide adsorption isotherms for each activated carbon sample were evaluated at low pressures, ranging from 0 to 114 kPa, at 0 to 55 °C. and it was found that the Dubinin–Radushkevich (D-R) adsorption isotherm model was found to be the most accurate model. Adsorption capacities derived from the D-R equation for CQ650 was found to be 7.6 mmol/gr at 0 °C which compared well to other activated carbons. The adsorption rates of the activated carbon samples were evaluated at 40, 55, 70 and 85 °C with inlet carbon dioxide concentrations of 5, 15 and 25 vol% at a pressure of 1 bar. A differential fixed bed reactor was designed, constructed and operated successfully to determine the adsorption rates under adsorption controlled (intrinsic rates) conditions only. Experimental results were used to determine the most suitable adsorption rate model involving well-known adsorption rate models which included the pseudo first order, pseudo second order, Elovich, Avrami and the fractional order adsorption rate models. It was found that the results from the Avrami and fractional order models compared exceedingly well with all the results obtained at the different temperatures and at 1 bar pressure. The saturated adsorption capacity and activation energy for CQ650 at 40 °C was found to be equal to 0.174 mmol/gr and 7.13 kJ/mole respectively at 1 bar pressure. The quantification of the carbon dioxide adsorption rates (adsorption controlled) for commercial activated carbon sorbents involving the Avrami adsorption rate equation with the relevant parameters has been achieved.

13.3 (13:15-13:35) Viscosity-Reducing Additives for Water-lean Solvents for Carbon Capture

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Shiaoguo (Scott) Chen,
Carbon Capture Scientific, LLC, Bethel Park, PA, USA
and Hyung Kim,
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Commercially aqueous amine scrubbing is the most mature technology available for CO₂ capture. The overall process consists of two columns employing an amine solution. The first column is used to selectively absorb CO₂ (absorber column) in the amine solvent which is then moved into a heated secondary column (stripper column) to release the CO₂ from the solvent. Critical parameters affecting the overall cost and performance are 1) how much CO₂ can be absorbed by the solvent, 2) how much CO₂ can be released, and 3) how much energy is needed for regeneration. The aqueous amine solvents are expensive mainly due to the latent heat of vaporization of water and corrosion to these columns. To decrease the overall cost of capture several new water lean solvents systems have been reported. Overall, the designer water-lean solvents hold great promise. It is important to point out that most water lean solvents have significant increase in viscosity upon the uptake of CO₂. This increase in viscosity results in lower mass transfer and increase in capital cost.

We have taken a different approach which is based on understanding amine reactions with CO₂ at a molecular level and how the long-range interactions exist within these systems upon the adsorption of CO₂, how the unique thermodynamic and physical properties of water-lean solvents are manifested. We used this knowledge to break the long-range interactions within these solvents, via an additive approach with the specific goal to reduce viscosity. In our on-going DOE-funded project (FE0031629), the team developed viscosity-reducing additives for water-lean solvents using the hydrogen bonding (HB) disruptor approach. Figure 1 shows our approach on breaking the large HB network into small clusters using HB disrupting additives.

Our results are extremely encouraging. The amine systems with our additives on average showing a decrease in viscosity of 50% when compared with systems without our additives upon CO₂ uptake. The initial preliminary engineering analysis of the impacts of solvent viscosity on the capital cost and operational cost for CO₂ capture process. Our quantitative correlation between viscosity of the solvent and the equipment cost and operation cost developed has demonstrated that the potential solvent with additive will save capital cost by about 16% or even more just by viscosity reduction assuming a 50% reduction in viscosity. A hypothetical example would be a water-lean solvent with viscosity of 50 cP that drop its viscosity to 5 cP would result in over 120 MM savings. Similar trend is observed in the annual operating cost.

These additives are non-reactive and thus can be used as a viscosity modifier in ionic liquids and polymers with a wide range of applications including pre-combustion separation, battery electrolytes, and as in heat transfer applications.

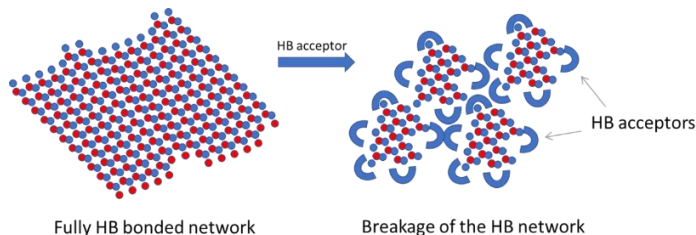


Figure 1. Illustration of fully HB network (left) and the breakage of the HB network by addition of HB acceptors (right).

13.4 (13:35-13:55) Section 45Q Tax Credit Impacts on Carbon Management: Case Study Findings and Modeling Developments

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The Section 45Q carbon oxide sequestration tax credit (45Q) is a federal general business tax credit that provides an incentive for carbon dioxide (CO₂) capture and storage and improves the finances of carbon capture and storage (CCS) networks. The National Energy Technology Laboratory (NETL) has completed initial work to reasonably assess 45Q's impact on carbon management costs, which has led to further analysis and model development to enhance understanding of this area. NETL modeled the impact of 45Q on CCS network scenarios in the central United States (U.S.) from a CO₂ source's perspective utilizing saline aquifers for CO₂ storage, and a combination of self-shelter, transfer to storage company, and tax equity partnerships to optimize 45Q monetization. A variety of CO₂ sources were assessed, including coal-fired power plants and cement manufacturing. In all modeled case study scenarios, 45Q alone was found to not close the financial gap required to make CCS deployment the lowest cost option for the CO₂ sources modeled. NETL assessed additional hypothetical carbon management policies, such as social cost of carbon levies and enhancements to current 45Q, to quantify their impacts on carbon management economics. Currently, NETL is developing a 45Q Tax Credit Monetization Model (45Q Model) that incorporates the finances of both capture and storage companies. This model honors the Internal Revenue Service and U.S. Treasury regulations and guidance on 45Q and tax equity partnerships. The 45Q Model will enable a more robust approach for evaluating the impact of the 45Q tax credit for sources interested in capturing and storing CO₂. When complete, the model will assess the amount of subsidy (equivalent to the financial gap) required to make uneconomic scenarios economical. The 45Q Model also demonstrates how 45Q value is distributed and monetized among capture, storage, and tax equity investor participants in a tax equity partnership.

Disclaimer:

This project was funded by the Department of Energy, National Energy Technology Laboratory, an agency of the United States Government, through a support contract. Neither the United States Government nor any agency thereof, nor any of its employees, nor the support contractor, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

13.5 (13:55-14:15) Dual CO₂ Capture System to Process Flue Gases from Coal or Natural Gas Fired Boilers in One Train Plant

Ahmed Aboudheir, and Walid Elmouadir
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Usually, a post-combustion CO₂ Capture plant would be designed for processing one single source of flue gas stream or a blend of several gaseous streams with slight fluctuation in flue gas composition and conditions. In the frame of reducing greenhouse gas emissions, Capital Power is planning to convert their coal fired boilers to nature gas fired boilers in the coming few years. Further to reduce their emissions to atmosphere, Capital Power is proceeding with plans to build the world's largest commercial scale production facility of carbon nanotubes (CNTs) at their Genesee Generating Station, Alberta, Canada. The design phase of Genesee Carbon Conversion Centre (GC3) is underway with commercial operations expected in the first half of 2022. GC3 will have an initial CO₂ capture plant production capacity of about 30 ton per day (TPD), which will be utilized to produce 2,500 ton of carbon nanotubes (CNTs) per year and once completed will be capable of producing up to 7,500 ton annually.

Delta technology was the selected CO₂ capture technology to capture 30 TPD of CO₂ from the coal fired boiler in the first few years and then continue to produce the same CO₂ production capacity with same CO₂ specification when the power plant is converted from coal fired boiler to nature gas boiler. A comprehensive design exercise is conducted based on both flue gases, coal fired flue gas and natural gas fired flue gas, to meet the cleanup targets and the production capacity in one train and a modular design. A rate-based modelling approach was implemented in the design using commercially available solvents, enhanced process configurations, and optimum operating parameters to achieve the production capacity at minimum emission to atmosphere and minimum capital/operating expenditures.

Also, a modular design and fabrication approach has been adopted for the Genesee CO₂ Capture plant that provides the following main benefits: (1) the process units will be fabricated and tested in a controlled environment (2) it is a cost effective way to transport the skids to the site; (3) it provides a small footprint, flexible equipment arrangement, and accessible layout; and (4) It provides easy site installation and semi-ready for commissioning once all tie-in are completed. In this paper, the innovative design and modular fabrication approach used to meet the production capacity in one train based on coal or natural gas fired boilers' flue gas will be presented.

SESSION 14 (12:35 – 14:15)

COAL ASH MANAGEMENT

Tarunjit Butalia and David Lyons

14.1 (12:35-12:55) Transforming Rare Earth Oxides into Individual REE Metals

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Leveraging the findings of J. Willard Gibbs at Yale (click on link) in the late 1800s, that molecules, when exposed to extreme heat, break apart when their atomic bond energy is exceeded and recombine, when cooled, as simpler and predictable. Similarly, smelting rare earth oxides (REOs) does yield each of the 17 REEs and 16 critical elements; each has a unique temperature at which they boil and subsequently condense, transformed into unique piles of metals.



Clockwise from top center, are praseodymium, cerium, lanthanum, neodymium, samarium, and gadolinium.

14.2 (12:55-13:15) Rapid Spectroscopy Method for Determining Adsorption Properties of Flyash in Concrete Admixtures

Yongjun Chen, E. S. Arun Thamban, and Hisham Menkara,
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Flyash (FA), a coal-combustion residual by-product from power generation facilities, is known to be highly beneficial as a partial replacement of cement in concrete mixtures. However, unburnt carbon residuals in FAs can interfere with the air bubble forming process during concrete mixing by adsorbing commonly used air-entraining agent (AEA) additives. This in-turn affects the long-term stability of concrete used in buildings/bridges/roads during freeze-thaw cycles commonly encountered in extreme weather conditions. Knowing the exact amount of AEA adsorbed by the FA during the mixing process enables better optimization of AEA dosage in concrete mixtures for adequate air-entrainment. Recently, a novel spectroscopy-based process and instrument (IDSpectra™ or IDS) has been developed to determine the amount of AEA adsorbed by FA in concrete admixtures. The process has been shown to be highly effective for quantitatively determining the concentrations of several commercial AEAs solutions and in evaluating the adsorption properties of flyash compositions in several AEA-FA admixtures under concrete mixing concentrations and conditions. The results obtained using this process are found to correlate well with the traditional foam index test (FIT). The instrument also provides the means to measure/monitor several adsorption related parameters such as initial AEA concentration, post-adsorption AEA concentration, and adsorption amount at various concentrations of AEAs in mixtures. Therefore, various AEA-FA systems can be characterized and classified based on their adsorption properties in order to effectively determine their utility as building materials. The IDS device is semi-automated, portable, low power, and has potential to be a versatile analytical tool not just for concrete preparation but also for any application in research or industry that requires rapid quantification and monitoring of small parts-per-million (ppm) changes of analyte concentrations in solutions.

14.3 (13:15-13:35) Nu-Rock Process to Convert All Ash from Coal Fired Power Stations into a Usable Product and Abates Carbon Dioxide Emissions and Uses 2% of the Embodied Energy of a Concrete Product or Clay Fired Product

Maroun George M. Rahme,
Nu-Rock Technology, Piper Power Station - Portland NSW Australia

Nu-Rock has just won the best Green Building product in Australia awarded by the Housing Industry association with more 25,000 builders across Australia. Previously Nu-Rock won the award as the best Site remediation technology in the world from Care CRC which is awarded every 3 years and beat Chevron who were the runners up to the award. Nu-Rock is offering Coal fired power stations, Steel mills, Smelters and Alumina plants a total clean up solution for 25% of any other companies cost of remediation or Liability transfer of the site. In Australia it has been out lawed to transfer an environmental liability from the company that caused the liability to another company, which in turn disappears.

Nu-Rock is offering a solution to ash dams where, Nu-Rock will use the ash dam completely and leave a green field site at the end of life of the power station. Nu-Rock will also create Carbon Abatement credits at the same time which it retains. The way this works is that the Power Station pays a portion of the plant cost so Nu-Rock can build a processing module on their site. The standard module is a 300,000 ton per annum (250,000 ton) a year ash processed per annum and the cost is \$15 million USD. Nu-Rock requires the utility to invest \$8 million USD to receive a shareholding in the Site specific Special unincorporated Joint Venture, that will to the utility will be \$8 million USD per annum when the module is at full capacity selling its entire product made from the ash as a rebate for the ash for their investment. If the power station is producing 300,000 tons of ash a year and 300,000 tons (250,000 ton per annum) of ash being added to the landfill Ash Dam. In this example the power station has an ash dam with 4.5 million tons in the ground, Nu-Rock would set up two modules on the power station so that at the end of life of the power station say for example this was 10 years. All of the fresh ash and portions of the ash dam would be used each year so, by the end of life of the power station the ash dam would have been consumed completely and the site a green field.

14.4 (13:35-13:55) Dewatering & Monitoring CCR - The Current State of Practice

Pierre Gauvin, and Greg Landry
Keller North America, Rockaway, USA

The past several years have seen numerous applications of dewatering techniques in CCR. Those techniques include rim ditching and sumping, wellpoints, and deep wells, and accompanying instrumentation to monitor the direct and indirect effects of dewatering.

Dewatering is an effective geotechnical tool for removing pore water from CCR to increase its shear strength. Temporary dewatering during closure can also be an effective

first step in remediation as it helps to prevent off-site migration of groundwater. The filter pack of a properly constructed dewatering device also acts as an initial treatment step in the removal of constituents of concern by preventing the pumping of excessive solids and the metals sorbed to them.

Access to the surface of any ash pond still remains the initial challenge. Deeper ponds lend themselves to the use of widely spaced wells for dewatering, however, wells are typically installed with sizable drill rigs. Access had been facilitated with floating roads or a shallow crust provided with wellpoint dewatering. Wellpoints are now commonly installed by hand from very wet and unstable pond surfaces.

Based on preliminary CPT data, the target depth of penetration of the dewatering system is anticipated. CPT data will provide some indication of the ponds hydrogeological behavior. Early field testing is typically performed to verify the hydrogeological behavior and depth of penetration of the dewatering devices. Pilot tests have been performed with shallow wellpoints and wells up to 150 ft in depth.

Instrumentation for monitoring CCR includes strategically placed piezometers, inclinometers and shape arrays. Recent advances in transmitting the monitoring data allow practitioners to see real-time results remotely and even to use data to warn workers on the pond of potentially unstable conditions before they happen. This presentation will include many case histories and widely varied applications and techniques.

KEYWORDS: fly ash, dewatering, wellpoints, wells, sumps, rim ditches, instrumentation

14.5 (13:55-14:15) Environmental Justice Initiatives, Risk Assessment, and Coal Ash Management

Ari S Lewis,
Gradient, Boston MA, USA

The Biden administration has made addressing environmental justice (EJ) concerns a top priority. The administration is dedicating significant resources to support EJ goals, which include explicit consideration of EJ issues in federal rulemaking and permitting, increased enforcement activities, and investment in the science that will support scientifically defensible implementation. At the same time, states are developing independent initiatives that attempt to meet similar goals. This presentation provides an introduction to EJ initiatives with a focus on the approaches that are being used to identify and assess risk in communities that have EJ concerns. These include existing and planned geographical information system (GIS) and tracking tools that will be used to support screening efforts, as well as risk assessment approaches that will be used to inform regulations. While the developing EJ activities will affect many industries, this presentation will focus on the intersection between EJ and coal ash and other utility-related environmental issues.

SESSION 15 (14:25-16:25) **CARBON MANAGEMENT - 3** *Nicholas Siefert and Bingyun Li*

15.1 (14:25-14:45) Highly Efficient Photocatalytic Structures and Processes for CO₂ Reforming to Solar Fuels

Yongjun Chen, E. S. Arun Thamban, and Hisham Menkara,
PhosphorTech Corporation, Kennesaw, Georgia, USA

Solar energy driven photocatalysis is a promising artificial photosynthesis approach to generate solar fuels from CO₂ and water. However, such a “green” technology has not yet gained traction in any industrial application on a commercial scale. Recent achievements will be reported in the design and development of semiconductor-metal photocatalytic structures for CO₂ reforming along with demonstration of a pilot scale prototype solar-driven reactor system for CO₂ conversion to solar fuels with improved energy efficiency (e.g., above 0.2%). The latest results demonstrate that semiconductor-metal structures are promising photocatalytic systems, which can have great potential for solar fuel generation from CO₂ in a photocatalytic reactor system as well as a photo-electrochemical system (i.e., photoanode catalytic coatings and cathode metal as electrocatalyst). However, significant scientific challenges still exist and have to be addressed before any commercial use of such technologies for oxygenated hydrocarbon solar fuel generation from CO₂ and H₂O. This presentation will discuss findings associated with the development of such photocatalytic structures, including the importance of a fundamental understanding of the physicochemical properties of such semiconductor-metal photocatalytic structures, and how various operation parameters and preparation conditions can affect performance as well as issues associated with solar light management and their effect on reactor design and scale up.

15.2 (14:45-15:05) Chemical Energy Storage by Means of Carbon Dioxide Capture and Utilization

Mauro Mureddu, Sarah Lai, Francesca Ferrara, and Alberto Pettinau,
Sotacarbo, Carbonia, ITALY

Climate change, global warming, fossil fuel depletion and rising fuel prices have created great incentives to seek alternative fuel production technologies. Carbon dioxide capture and utilization (CCU) technologies are attracting interest of the scientific and industrial community not only as an approach for the production of clean fuels from a waste gas, shifting an environmental problem into a resource, but also as a very promising strategy for chemical energy storage of the overproduction of electricity from renewable sources (with the additional advantages of balancing the electric grid and promoting a further diffusion of non-programmable renewable plants). These renewable electricity-derived fuels (“e-fuels”, i.e. methanol, dimethyl ether, methane, gasoline, diesel, naphtha and many more) are carbon-neutral and very clean, free of the contaminants that can be found in the corresponding fossil-derived fuels and also in biofuels. In fact, they do not come from oil refining, but from synthesis processes from high purity chemical compounds. And they are completely renewable allowing, according to IEA’s estimations, a reduction of greenhouse gas emissions up to 93%. They can represent a key solution for the application in several hard-to-abate sectors – in particular for heavy duty trucks or for aviation and shipping – in place of their fossil-derived counterparts. Finally, CO₂-derived fuels (especially methanol) are characterized by an increasing market, since they can be also used as precursors for the production of countless chemical products.

CO₂ hydrogenation technologies to e-fuels have been developed in several demonstration-scale units in Europe, but the pathway to make e-fuels competitive with their fossil-derived counterparts is still very long, due to the need to cut the conversion costs.

In this context, Sotacarbo is working on the development of processes and catalysts for CO₂ hydrogenation to e fuels, especially methanol and dimethyl ether (DME). This work is focused on an innovative nano-catalysts preparation of both copper/zinc oxide@SBA-15, and copper/zinc oxide/zirconium oxide@SBA-15 systems via a novel combined strategy of impregnation-sol-gel auto-combustion whose behavior in methanol synthesis from carbon dioxide hydrogenation was investigated at 250 °C and 3.0 MPa with the aim of correlating the catalyst's performance with its physico chemical features. The product –international patent application – is characterized, with respect to its competitor, by better performance in terms of production yield and selectivity and it is tolerant to oxygen, which makes it particularly interesting for some specific applications, such as for oxy combustion processes. But, above all and differently from all the other catalysts developed for such a process, it doesn't need any activation pre-treatment (with significant advantages in terms of costs, shut-down duration and safety issues). Characterization of the nano-catalysts clearly shows that the synthesis procedure is efficient in obtaining nanometric particles, even if a difference in terms of active phase crystallinity and dispersion has been observed from the XRD and TEM results. A remarkable space time yield of methanol referring to the active phase is shown; at variance with the case of the unsupported catalyst (10 mg CH₃OH h⁻¹ gcat⁻¹), the methanol yield 37-fold higher is shown for the supported catalyst (376 mg CH₃OH h⁻¹ gcat⁻¹) with a Cu/Zn molar ratio of 1.0 mol mol⁻¹ and a total active phase loading of 20 wt.%.

A remarkable STY of 450 mg CH₃OH h⁻¹ gcat⁻¹ and a methanol selectivity of 36 mol% have been obtained for the catalyst not subject to the activation procedure, being slightly higher than that of the catalyst subject to a reduction treatment (STY of 376 mg CH₃OH h⁻¹ gcat⁻¹ and methanol selectivity of ca. 31 mol%).

In parallel, a new pilot-scale plant is under design (it will be completed in early 2022) to test and develop the integrated power-to-liquids (mainly methanol and DME) and power-to-gas (methane) processes in different operating conditions, with particular reference to process optimization to improve its operation flexibility.

Reference:

(1) Mureddu et al., Applied Catalysis B: Environmental 2019;258:117941.

15.3 (15:05-15:25) Open and Detailed Core Data from Domestic Carbon Storage Field Sites

Dustin Crandall, Thomas Paronish,
NETL, Morgantown West Virginia, USA
Rhiannon Schmitt,
NETL and ORISE, Morgantown West Virginia, USA
Sarah Brown,

West Virginia Geological & Economic Survey, Morgantown West Virginia, USA

At the National Energy Technology Laboratory (NETL) in Morgantown, West Virginia Computed Tomography (CT) and Multi-Sensor Core Logging facilities are being utilized to characterize large volumes of rock core associated with field scale carbon storage in the United States. The data is being disseminated in the public domain via the Energy Data eXchange (EDX) and sample information is made available via the online

System for Earth Sample Registration (SESAR). A primary impetus of this work is to digitally capture pertinent features of cores from potential geologic carbon storage formations and openly provide this data for further characterization and model development. Collaborations between universities, industrial partners, state geologic surveys, and NETL have been forged to collect, describe, and publish this information.

Data generation utilizes medical and industrial grade CT to capture the internal structure and variation in the rock cores at scales ranging from mm down to microns. These measurements are coupled with P-wave velocity, resistivity, magnetic susceptibility, and X-ray fluorescence spectroscopy measurements every several centimeters along the core length with NETL's core logging facility. The resultant large datasets are made available in their raw format and as condensed technical reports on the EDX. All analyses are non-destructive and provide a detailed digital record of the core, while enabling utilization of samples for future studies. The combination of medical CT imagery and high-resolution core logging measurements provide a means to quickly and non-destructively determine areas that are ideal for more rigorous quantitative analysis. This methodology provides a multi-scale description of the core at that is easily accessible. The SESAR system provides a simple, central location for data to be queried; providing the existing suites of geomaterials (subsurface cores, outcrop fragments, and specimens remaining after in-house experiments) and their metadata (including, where available, sampling location, rock type, etc.) located at NETL in Morgantown, WV to the public.

15.4 (15:25-15:45) U.S. Department of Energy National Carbon Capture Center, Supporting Technology Development for Carbon Capture, CO₂ Utilization, and Direct Air Capture

Michele Corser

National Carbon Capture Center, Southern Company, Wilsonville, AL, USA

Sponsored by the U.S. Department of Energy (DOE) and operated and managed by Southern Company, the National Carbon Capture Center (NCCC) is a cornerstone of U.S. innovation in advancing the development of technologies to reduce greenhouse gas emissions. Bridging the gap between laboratory research and large-scale demonstrations, the Center works to accelerate the development of carbon capture technologies from coal- and natural gas-based power plants. The facility evaluates next-generation carbon dioxide (CO₂) reduction processes from third-party developers, focusing on the early-stage development of the most promising, cost-effective technologies for future commercial deployment.

Since its creation in 2009, the NCCC has performed more than 115,000 hours of technology testing. Through pilot testing of more than 60 technologies, the Center has directly participated in the reduction of the projected cost of carbon capture from fossil power generation. As the demand for post-combustion carbon capture options grows, work in this area continues to reduce costs and bring new technologies closer to the marketplace. Evaluation of developing second-generation and transformational carbon capture technologies using actual flue gas under industrial conditions provides critical information on material and process suitability for scale-up to commercial applications. The Center has broadened its research scope to expand testing of carbon capture technologies for natural gas power generation in addition to its existing coal-fueled testing capability. Integration of the new natural gas flue gas equipment with the existing infrastructure will allow each carbon capture project to receive either natural gas or coal flue gas independently of other projects.

In addition, testing at the NCCC now supports research and development (R&D) of CO₂ utilization technologies that will efficiently, economically, and cleanly transform CO₂ into value-added products. As its focus broadens to negative carbon concepts, the Center is also extending its research to help advance direct air capture technologies.

Zero-carbon goals by many organizations worldwide have become a significant driver for the development and deployment of carbon capture technologies. Results from NCCC testing can contribute to the evaluation of alternative zero-carbon pathways. The NCCC seeks input and support from organizations with zero-carbon goals as the NCCC test plan evolves in support of the energy transition.

Because the reduction of CO₂ emissions is an international issue, the NCCC provides global technology development leadership—it co-founded the International Test Center Network (ITCN), a global coalition focused on research, development, and deployment of carbon capture, use, and storage (CCUS). Formed in 2012 in collaboration with DOE's Office of Fossil Energy, the ITCN facilitates knowledge-sharing among carbon capture test facilities around the world to accelerate the commercial deployment of carbon capture technologies. The ITCN now has 14 member test facilities.

The NCCC has also been active in establishing test collaborations with international groups. The Center has successfully tested technologies from seven different countries. In addition to the important work of developing cost-effective technologies, many other aspects of successful commercial deployment must be mastered. Establishing relationships to secure funding, gaining management support, meeting test goals, and satisfying the legal requirements of both international organizations and the NCCC are significant achievements and form a strong basis for future partnerships for larger-scale

development. Oil and gas companies have joined the NCCC and have a strong international presence which will support global collaboration.

Unanticipated benefits to the NCCC's international collaboration have emerged in addition to sharing public information and establishing relationships that could form the basis for partnerships for scale-up of technology. These benefits include (1) adding value to CCUS technologies by meeting requirements of international markets, (2) increasing the value of input into studies, roadmaps, and policy development by including international perspective, and (3) attenuating inconsistent support of CCUS R&D among individual countries. The NCCC hopes to build on the established international relationships to contribute to the important progression of moving from early-stage R&D projects to commercial products.

In conclusion, the NCCC has demonstrated its ability to bring on board and manage a multitude of projects to develop the most promising technologies for clean, efficient fossil-fuel energy production with ultra-low CO₂ emissions. Operations at the Center have resulted in significant scale-ups, process enhancements, and technological breakthroughs. The NCCC is also providing international leadership to promote the level of readiness for CCUS technologies. This paper will detail the Center's capabilities, role in supporting international collaboration, and support of zero-carbon plans.

15.5 (15:45-16:05) TEA of a Unique Process for Producing High-value Nanomaterials or CO₂ Capture and Sequestration

Rui Wang ^a, Husain E. Ashkanani ^a, Bingyun Li ^b, and Badie I. Morsi ^a

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- b. Department of Orthopaedics, School of Medicine, West Virginia University, Morgantown, WV, USA

A uniquely flexible process using aqueous sodium glycinates (SG) solutions for CO₂ capture from a split stream of the flue gas from the 600 MWe clean coal power plant, used in the Wolverine Clean Energy Venture (WCEV) project, was developed in Aspen Plus v.10. This flue gas contained 0.0023 mol% SO₂ and 13.33 mol% CO₂. The process was designed to remove all SO₂ and capture 90 mol% of CO₂ in the flue gas stream. The complete removal of SO₂ from the flue gas using deionized water (DIW) was carried out in a washing unit (WU), which was a countercurrent fixed-bed packed with a structured packing (Mellapak 250 Y). The used DIW was sent to a reverse osmosis unit (ROU) to remove the dissolved sulfuric acid and the cleaned DIW was recycled back to the WU. The CO₂ capture from the desulfurized flue gas stream using the SG solutions took place in an absorber, which was also a countercurrent fixed-bed packed with same structured packing. The clean gas exited from the top of the absorber, whereas the CO₂-rich stream coming from the bottom of the absorber was further processed.

The flexibility of this process resides in the fact that this CO₂-rich stream exhibits a phase-separation into a CO₂-rich phase, consisting mainly of sodium bicarbonate (NaHCO₃) nanomaterials, and a CO₂-lean phase, consisting mainly of glycine and water and hence this process has two Pathways (i) and (ii) on going forward. In Pathway (i), the NaHCO₃ nanomaterials were separated using a ultrafiltration unit (UFU) and sold as a useful product to offset the overall CO₂ capture costs. In Pathway (ii), the CO₂-rich phase was regenerated in a stripper and the recovered CO₂ was compressed to 15.27 MPa using a multi-stage compressor in preparations for sequestration into geological formation of saline aquifers.

In this study, the total flue gas flow rate used in the process was 44.75 ton/h (at 353.15 K and 101.325 kPa). The hydraulics and mass transfer characteristics of the SO₂ WU and CO₂ capture absorber were calculated and discussed. Also, the techno-economic analyses (TEA) of the process two pathways were performed using Aspen Plus v.10. The capital expenditure (CAPEX), operating expenditure (OPEX), and the Levelized cost of CO₂ captured (LCOC) were obtained to draw a direct comparison between the process two pathways. These data were obtained under the following conditions, power plant lifetime of 30 years, discount rate of 10%, capacity factor of 0.8, capital recovery factor of 0.106, and operating and maintenance cost (O&M) of 4% of the total CAPEX.

The calculated hydraulics indicated no flooding in the entire process, and the gas-side mass transfer coefficients were orders of magnitude greater than the liquid-side mass transfer coefficients. The pressure drops in the WU and CO₂ absorber were 0.07 and 0.006 bar, respectively, and the behaviors of the liquid holdup and normalized packing specific wetted surface area were similar in both units. The calculated CAPEX, OPEX, and LCOC for pathway (i) were \$4,456,975, 223 \$/h, and 35.63 \$/ton respectively. Also, 8.144 ton/h of CO₂ were captured to produce 15.545 ton/h NaHCO₃ nanomaterials. On the other hand, the calculated CAPEX, OPEX, and LCOC for pathway (ii) were \$12,113,705, 250 \$/h, and 52.79 \$/ton of CO₂ captured, respectively. The higher CAPEX values of the pathway (ii) than pathway (i) were due to the required larger absorber and stripper in addition to the need for a reboiler and condenser for pathway (ii). The higher OPEX values of pathway (ii) than pathway (i) were attributed to the reboiler duty for solvent regeneration. Also, the LCOC values of pathway (i) were 32.5% lower than pathway (ii), which led to conclude that pathway (i) was more cost-effective than pathway (ii).

15.6 (16:05-16:25) Pre-combustion CO₂ Capture using Ionic Liquids

Husain E. Ashkanani ^{a,b}, Rui Wang ^{a,b}, Wei Shi ^{a,c}, Nicholas S. Siefert ^a, Robert L. Thompson ^{a,c}, Kathryn H. Smith ^{a,b}, Janice A. Steckel ^a, Isaac K. Gamwo ^a, David Hopkinson ^a, Kevin Resnik ^{a,c}, and Badie I. Morsi ^{a,b}

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- Leidos Research Support Team, NETL, Pittsburgh, PA, USA

Aspen Plus v.8.8 was used to perform techno-economic analysis (TEA) of the CO₂ capture process in a pre-combustion 543 MWe power plant using 11 ionic liquids (ILs) at different temperatures from 0 to 50 oC. The process capital expenditure (CAPEX), operating expenditure (OPEX), and levelized cost of CO₂ captured (LCOC) were calculated using literature data [1-4] to evaluate its feasibility. The process hydraulics (pressure drop, liquid holdup, specific packing wetted area), and mass transfer (gas-side and liquid-side mass transfer coefficients) were also calculated. The flow rate of the sulfur-free shifted fuel gas used in the process was 521.367 ton/h at 51.4 bar and 35 oC, and it contained 40.78 mol% of CO₂ and 56.82 mol% of H₂. At 0 oC, the solvent flow rates varied from about 6,480 to 15,840 ton/h based on the IL.

The CO₂ capture process included a countercurrent packed-bed absorber with a structured packing (Mellapak 250Y), followed by three flash drums for the CO₂-rich ILs regeneration, and a multi-stage compressor to boost the CO₂ pressure to 152.7 bar in preparation for subsequent sequestration. In addition to no flooding in the CO₂ absorber, the key process constraints were (1) 90% CO₂ capture from the sulfur-free shifted fuel gas, (2) less than 0.5 mol% fuel gas and a maximum of 600 ppm water in the CO₂ stream ready for sequestration, and (3) the height to diameter ratio of the absorber should be greater than or equal 6 to avoid gas-liquid segregation and channeling.

The PC-SAFT Equation-of-State was used to model the solvent density and vapor-liquid equilibria of the gas-liquid systems, while other physico-chemical properties of the ILs and flue gas species were acquired from experimental data and literature. Also, under all operating conditions used, flooding in the absorber was checked using the generalized pressure drop correlation (GPDC) by Leva [5].

Aspen Plus calculations indicated that due to the extremely low vapor pressure of the ILs used (less than 10⁻⁵ Pa), the solvent loss in the process was negligible lowering the OPEX. However, due to the high viscosity of the ILs (up to 1.4 Pa.s), high pumping costs were required increasing the OPEX. Since CO₂ solubility decreased while H₂ solubility increased with temperature in the ILs, operating the process at low temperatures reduced the required solvent flow rates, equipment size and the operating and maintenance (O&M) cost lowering both CAPEX and OPEX. Also, among the 11 ILs used in the process, [emim][Tf₂N] exhibited the lowest LCOC, using our baseline assumptions for the costs of the solvents. Depending on the actual cost, the process modeling conducted here revealed how operating conditions should change to lower the cost of CO₂ capture as function of the solvent cost.

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SESSION 16 (14:25-16:25)

VALUE-ADDED PRODUCTS FROM COAL - 2

Tarunjit Butalia and Joseph Stoffa

16.1 (14:25-14:45) Preparation and HRTEM Characterization of Symbiosis of Coal-based Graphene and Coal-based Graphene Quantum Dots

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Yangquan Xinyu
Geotechnical Engineering Co., Ltd., Yangquan, China

In this study, Baozi anthracite (BZ-2#-M4, BZ-2#-KC) and Xinjing anthracite (XJ-8#-M6) from Qinshui coalfield of Shanxi Province were selected as carbon sources. Based on the modified Hummers redox method, the amount of acid and reducing agent and the time of ultrasound were properly adjusted in the experimental process, and a symbiosis of coal-based graphene and coal-based graphene quantum dots was prepared simultaneously, and the final products was characterized by high resolution transmission electron microscopy (HRTEM). The results show that coal-based graphene and coal-based graphene quantum dots can be prepared simultaneously and coexist stably. In the symbiosis of coal-based graphene and coal-based graphene quantum dots, graphene quantum dots were not embedded in the graphene sheet layer, but they were distributed in different layers. Graphene quantum dots were densely distributed in the edge and fold of graphene sheet layer, and less distributed in the flat lamellae in the middle of graphene sheet layer. Among the three products, the number of layers of graphene was 3-7, most of which were 5. The average layer spacing was 0.37 nm, and the number of layers had a negative correlation with the reflectance of coal samples. The particle size of graphene quantum dots was uniform, ranging from 3.14 nm to 5.02 nm, with an average size of 3.87 nm and an average lattice stripe spacing of 2.72 nm. The size of graphene quantum dots had a positive correlation with the number of graphene layers and a negative correlation with the reflectance of coal samples.

Keywords: coal; graphene; graphene quantum dots; symbiosis; HRTEM

16.2 (14:45-15:05) Application and Development of X-MAT® Coal Core Composites for Building Components

William Easter
Semplastics, Oviedo, FL, USA

Using coal for value added products is an important goal for the continued economic health of coal producing communities. To that end, recent X-MAT® Research and Development activities have resulted in an alternative use for raw coal particles as a key component for building components used in the housing industry. X-MAT® technology combines proprietary chemical formulations with raw coal powders (approximately 70% by mass of the composite) and transforms these materials into an inert coal core composite. Even though a key component is flammable coal particles, the coal core composite does not burn in an open flame due to the transformation process.

The Department of Energy National Energy Technology Laboratory (NETL) awarded Semplastics a Phase 2 Small Business Innovative Research (SBIR) grant in 2019 to continue X-MAT® R&D activities with coal. The specific purpose of this DoE-funded research is to produce coal-core composite roof tiles, which have key advantages in weight, fire resistance, and durability over the conventional alternatives.

In addition, several additional Research Contracts have been awarded by the NETL to Semplastics to produce additional coal core composite building materials. These coal-derived building components include bricks, blocks, facades and panels.

This talk will highlight the current status of the coal-based roof tile project as well as initial experimental results regarding coal-derived bricks, blocks, facades, and panels.

16.3 (15:05-15:25) Taking Advantage of Oxygen Rich Subbituminous PRB Coal to Produce Hybrid Asphalt Additives using Renewable Carbon Sources

Jeramie J. Adams, Western Research Institute, Laramie, WY, USA
Devang Khambhati, Jianqiang Huo, William Schaffers, David Bell, Richard Horner,
University of Wyoming School of Energy Resources, Laramie, WY, USA
Jean-Pascal Planche, Western Research Institute, Laramie, USA

Currently, about 25 million tons of asphalt binder are used each year in North America for paving and roofing applications, and more than 100 million tons are used each year globally. Asphalt binder is currently produced from crude oil residue bottoms left after making fuels during petroleum refining. Changes in feedstocks and refining practices in the quest to improve profitability and yields of higher value products - have severely impacted asphalt quality in recent decades. There has also been a significant increase in thermal and catalytic process to upgrade residue bottoms to higher value fuels affecting availability of some residue bottoms. This, coupled with an increasing shift by refiners to make less fuels and more petrochemical products, further detracts from the availability of high volumes of high quality petroleum asphalts. The increasing electrification of vehicles may also further detract from availability of a robust asphalt pool and potentially strain future supplies.

Coal derived asphalt products could potentially provide a new, vast, controlled and highly engineered feedstock to produce consistent and reliable alternatives to petroleum derived asphalt, and asphalt additives, for the future.

Solvent extraction of PRB subbituminous coal provides phenolic rich compounds that can be further reacted with various forms of renewable carbon triglyceride oils to produce viscous liquids and viscoelastic materials with the appropriate solubility and mechanical properties suited for asphalt paving applications. The understanding gained by developing asphalt additives are helping to develop strategies to produce a complete

petroleum asphalt replacement product. A significant concern with using coal is the health and safety of the coal based asphalt products. Careful work has shown that the uniqueness of PRB coal, along with careful processing, can produce a low PAH containing fractions amenable for asphalt work with a very low carbon footprint.

Coal derived asphalt additives that support recycling of aged oxidized petroleum asphalt - the most recycled material in the world—have been developed from coal. Also, some SuperPave performance graded (PG) asphalt materials have also been developed. Some of these chemistries can be applied to coal extracts while other can be applied directly to coal and solvent extraction residues. This presentation, will highlight select developments and approaches to make coal derived asphalt products that conform to industry standards, along with describing the characterization of the coal materials by unique methods.

16.4 (15:25-15:45) Conversion of Coal Liquids to Isotropic Pitch for the Production of Mesophase Pitch

Cierra Crowe, E. Ashley Morris, Rachel Kaplan, and Matthew C. Weisenberger
University of Kentucky Center for Applied Energy Research,
Lexington, KY 40511, USA

Carbon fiber produced from coal tar pitch has recently gained renewed interest for low cost and high-performance carbon fiber. As steam coal production in the U.S. declines, uses for coal in value-added materials including carbon fiber are being investigated. Low severity solvent extraction of coal slurries is one method that allows for the production of a variety of heavy coal liquids, with coal conversion upwards of 80 wt.%. This paper reviews our current work converting such coal liquids to isotropic pitch by vacuum distillation. Recovery of the distillates is also included. A nominal softening point temperature of 100 C was targeted for the isotropic pitch and monitored as a function of the distillation vapor temperature and pressure. All else equal, the pitch yield was found to dramatically increase for coal liquids containing approximately 20% coal by weight, compared to the 0% coal-in-solvent baseline. Hot-stage microscopy of the resultant isotropic pitch was used to probe mesophase formation at 410 C over up to 8 hours in real-time. Mesophase was observed to readily form from the baseline pitch, but not from the coal liquid derived pitch. Organic sulfur composition may play a role in this. Realizing a simple path to economically and environmentally sustainable coal to mesophase pitch, is important for the concept of coal to carbon fibers.

16.5 (15:45-16:05) The Use of Softening Point and QI Content to Tune the Conversion of Isotropic Coal Tar Pitch to Mesophase Pitch Toward the Development of Multifilament Spinning for Carbon Fibers

Kirk Norasak, George Frank, Justin Lacy, John J. McHugh, and Matthew C. Weisenberger
University of Kentucky Center for Applied Energy Research,
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PAN based carbon fiber has long dominated the commercial carbon fiber industry. However, mesophase coal tar pitch derived carbon fiber is building interest due, in part, to lower base material costs and higher yield% by weight after thermal processing. Therefore, understanding control of a stable multifilament spinning process of coal tar mesophase pitch could reduce the production costs of carbon fiber while also paving new opportunities for U.S coal markets and industries. In this investigation an isotropic coal tar pitch was converted into mesophase pitch through thermal processing under flowing nitrogen. Dynamic mechanical analysis (DMA), and the ASTM "Standard Test Method for Quinoline-Insoluble (QI) Content of Tar and Pitch" process was used to characterize the softening point (Tsp) and quinoline-insoluble fraction (QI%) respectively for the converted mesophase pitch. After analyzing the processing conditions, correlations were observed between Tsp, QI%, and average soak temperature. These relationships allowed for a predictive process tuning of the isotropic coal tar pitch to mesophase pitch. Moreover, it was determined that the Tsp and QI% correlated linearly with the average soak temperature with a R² value of 0.92 and 0.88 respectively. Thus, an empirical formula was established from these linear relationships that allowed for Tsp and QI% to be predicted based off average soak temperature and therefore tuned to targeted values that produce stable multifilament mesophase pitch melt spinning. Tsp control is key since it sets the processing conditions for melt spinning. QI% impacts mesophase melt spinning stability so this variable must be controlled tightly as well. Hence, predictive process control of Tsp and QI% is paramount for the success of producing stable multifilament spinning of coal tar mesophase.

16.6 (16:05-16:25) Formation of Coal Liquids from Various Seams of Coal with Direct Solvents

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Carbon fiber has been produced from various precursors for several decades. Pitch-based carbon fiber has long drawn interest as a potentially ideal combination of low cost

and high performance. Commercially, isotropic and mesophase pitch fiber has been produced from petroleum and coal tar derived precursors. The current work involves combining various coals with different solvents to yield liquids that can form pitch and eventually mesophase, carbon fiber, and composite materials. These studies are currently being conducted on two scales: a microreactor scale using small stainless steel tubes for analytical purposes (to study coal conversion percentages with the various combinations), as well as a 2 L Parr reactor scale to produce sufficient quantities for downstream processing. This presentation will cover the analyses of coals from the Springfield, Herrin, and Blue Gem seams combined with several solvents that will form homogeneous liquids with the coals over a heat treatment of 30 minutes at over 400°C at autogenous pressure, and the resulting coal liquids. Stark differences have been observed with the various coal / solvent combinations. Current studies are focused on the effects of coal and solvent on the coal conversion, yield, % sulfur, % ash, and molecular weight distribution of the combinations and their resulting ability to form mesophase.

SESSION 17 (8:00 – 9:45)

POWER PLANTS - 1

Ting Wang and Francis Lau

17.1 (8:05-8:25) Removal of SO₂ and NO_x from Flue Gas by Adsorption over Activated Carbon at Cold Temperatures

Shiqing Wang, Lianbo Liu, Jinyi Wang,
Huaneng Clean Energy Research Institute, Beijing, CHINA
Shiwang Gao, Hongwei Niu,
Beijing Key Laboratory of CO₂ Capture and Process, Beijing, CHINA

SO₂ is an acidic gas and can be removed by reacting with alkalic agents (CaCO₃, CaO, NH₃, Na₂CO₃, MgO, seawater, etc.) and forming stable sulfates. NO_x is mainly composed of nitrogen monoxide (NO) which can be either reduced to non-toxic gas N₂ or oxidized to nitrogen dioxide NO₂ which can be scrubbed by alkalic solutions. These mature technologies have been widely deployed in power plants but face a common problem: the massive consumption of chemicals such as limestone and ammonia, which can also cause the emission of secondary pollutants. In addition, adsorption technology has also been successfully demonstrated for flue gas desulfurization, in which activated carbon or coke is used as the adsorbent. However, NO_x which is mainly composed of nitrogen monoxide is unable to be removed through adsorption due to its poor adsorbability. Instead, NH₃ is used to remove NO_x through catalytic reduction over activated carbon or coke, which has a deNO_x rate of about 70%.

In a recent study, the research team has discovered that NO can be effectively adsorbed by activated carbon with an astonishing adsorbing capacity when the flue gas is cooled to below room temperatures. With an initial concentration of NO=200 ppmv, the specific adsorption capacity increases from 3.8 to 169.1 mg/g when the temperature decreases from 80 to -20 °C. Meanwhile, the SO₂ adsorption capacity is also significantly enhanced. With an initial concentration of SO₂=1000 ppmv, the specific capacity increases from 12.9 to 123.1 mg/g when the temperature decreases from 80 to -20°C. The impact of oxygen and water content over the adsorption of SO₂ and NO at various temperatures are studied. It is found that NO can be oxidized to NO₂ efficiently at low temperatures over activated carbon with the presence of oxygen, which causes the substantial increase of adsorption capacity. A novel cold oxidation adsorption process (COAP) is developed to simultaneously remove SO₂ and NO_x from flue gas. A pilot-scale system with a flue gas flow rate of 3600Nm³/h is built to test the performance of COAP technology. The SO₂ and NO_x emission is lower than 1 mg/Nm³ and the removal efficiency of SO₃, Hg, HCl and VOCs are over 95%. The energy penalty of COAP process is analyzed based on the pilot test results as well as Aspen Plus modeling. The ambient temperature has a significant impact on the electricity consumption for flue gas cooling and the overall consumption is around 2-3% of the installed capacity. A pre-feasibility study of COAP flue gas treatment facility based on a 300MW unit is also conducted. The CAPEX is about 92 USD/kW and the OPEX is around 2.77 USD/MWh.

17.2 (8:25-8:45) High-Temperature Multi-Process Sensor Development for a PC-fired Unit

Hong-Shig Shim, Zhonghua Zhan, Kevin Davis, Andrew Chiodo, Marc Cremer,
Reaction Engineering International, Boulevard, Midvale, UT, USA

Condition-Based Monitoring (CBM) is a maintenance philosophy that actively monitors the health of assets to predict and prevent failures and maximize power plant's availability and generating capacity at a reduced cost. The electric power industry is experiencing a push toward using big data to develop advanced automated control and smart maintenance management. CBM systems can provide boiler condition data that the advanced control system can utilize for plant performance optimization, which is

increasingly relevant as coal power plants shift from predominantly base-load operation to predominantly transient operation involving large load swings. A transient operation can create fluctuating local stoichiometries at tube surfaces in high temperature regions, as well as reduced back-end temperatures creating acid dew-point corrosion concerns.

Reaction Engineering International is developing a multi-process sensor that is capable of monitoring real time boiler conditions including electrochemical noise-based metal attack/wastage as well as metal surface temperature, heat flux and deposition under the US Department of Energy's Crosscutting Technology Research program (DE-FE0031680 and DE-FE0031682). This electrochemical noise-based technology has been put through various tests to ensure accuracy and repeatability for metal wastage measurements and has shown a possibility to be used in combustion tuning/optimization by simultaneous monitoring of other aspects of boiler performance. Through these projects, REI re-designed and assembled new monitoring equipment, enhanced software by converting legacy code and implementing new process correlations, performed pilot-scale testing, and demonstrated the multi-process monitoring system in two full-scale PC-fired units with a range of fuels from lignite to bituminous coals. In this paper, REI will discuss the progress of the projects including new sensor design efforts for self-regulating control, electronics development, and the CFD modeling of the demonstration units as well as the findings from the full-scale demonstration.

17.3 (8:45-9:05) SO₃/H₂SO₄ Continuous Real-Time Sensor Demonstration at a Power Plant

Jason Kriesel, Ilya Dunayevskiy,
OptoKnowledge Systems, Inc., Torrance CA, USA
Brent Spang, Gary Shiimoto, Lawrence Muzio,
Fossil Energy Research Corporation (FERCo), Laguna Hills, CA, USA
Andrea Biasioli, Yu-Chien Chien, Derek Dunn-Rankin,
University of California, Irvine (UCI), Irvine CA, USA
Richard Himes,
Electric Power Research Institute (EPRI), Palo Alto, CA, USA

We will present results from field testing of a new, innovative sensor developed to measure SO₃/H₂SO₄ continuously and in real time at a coal-fired power plant. The system utilizes the sensitivity, specificity, and real-time capabilities of mid-infrared (Mid-IR) laser absorption spectroscopy, along with a close-coupled cell mounted directly to a power plant duct.

Measurements were made by the laser sensor over a 3-day period and compared to results from the accepted method, EPA 8A, also referred to as "controlled condensation". The condensation method requires a 30-minute collection, labor intensive processing, and off-site analysis at a lab. In contrast, the laser sensor continuously samples flue gas and reports measurements of the concentration of SO₃/H₂SO₄, SO₂, and H₂O in real-time ever second with unattended operation.

This initial demonstration proved the sensor concept and identified specific aspects requiring further optimization, paving the way for sensor use for controlling sorbent injection used to neutralize SO₃/H₂SO₄. Optimized sorbent injection will enable significant cost savings associated with efforts to mitigate the presence and effects of SO₃/H₂SO₄ such as "Blue Plume", air heater fouling, and duct corrosion. In particular, the real-time, actionable information will enable better control of additive injection in flue conditions and with variable fuels.

17.4 (9:05-9:25) Rapidly ramp cryogenic air separation unit without loss of O₂ product purity—application for low-carbon fossil-fuel plants

Mao Cheng, Piyush Verma, Zhiwei Yang, and Richard L. Axelbaum,
Washington University in St. Louis, MO, USA

The rapid integration of intermittent renewable sources into the electricity grid is driving the need for low-carbon, fossil-fuel power plant capable of rapid ramping. Therefore, a cryogenic air separation unit (ASU) as part of low-carbon, fossil-fuel power plant should be capable of rapid ramping. However, highly integrated and nonlinear processes of the ASU would significantly restrict this rapid ramping. To overcome this fundamental issue, we study the basic dynamic process of a state-of-the-art double-column ASU. A flow-driven dynamic model was established in Aspen Plus Dynamics, assuming perfect flow controls, to capture the basic dynamics of ramping ASU. We find the vapor-liquid counter-current flow structure in the low-pressure column is critical to the air separation when rapidly ramping the ASU. This flow structure is established based on a complicated heat integration process. It is simplified as an apparent counter-current heat transfer process in this work, which greatly reduces the complexity for studying the dynamics of ASU. For keeping this basic flow structure, the heat integration is maintained as its heat duty follows the ASU load, through several basic feed-forward and feed-back controllers on the critical stream flowrates. Moreover, we find a fundamental issue of mismatched dynamics in the low-pressure column, resulting in a significant loss of O₂ product purity when rapidly ramping down the ASU and an obvious fluctuation of O₂ product purity. Based on these explorations, we propose a basic control method for rapidly ramping the ASU without loss of O₂ product purity.

Results show the ASU basic dynamic process successfully ramps at a rate up to 10%/min (40-100% load) while maintaining the O₂ product purity within 95.2-95.6 mol%.

17.5 (9:25-9:45) Simulation Study of the Start-up Period of Once-Through Boilers

Xuandai Ngo, Byungho Song*
Department of Chemical Engineering, Kunsan National University, Gunsan, Korea
Jaehyeon Park, Dowon Shun and Jaegoo Lee
Korea Institute of Energy Research, Daejeon, Korea

A mathematical model of once-through boiler at circulating fluidized bed combustor is developed to analyze the boiler's transient behavior. The start-up scenario of the once-through boiler at subcritical and/or supercritical 2 MW CFB combustor has been simulated and analyzed by the present model. The model is established by applied mass, energy, and momentum balance equations for the general block units which could be any compartments in the once-through boiler system. Therefore, the behavior of whole once-through boiler can be simulated by connecting each block models all together. The above model approach might be applied to supercritical once-through boilers with the other configurators. The model can be used to check the safety of newly proposed operational scenarios of boilers before implementing the actual power plant. The models also can be further enhanced to simulate special conditions such as the shut-down process.

Keywords: mathematical model; once-through boilers; circulating fluidized bed; start-up period.

SESSION 18 (9:55-11:55)

POWER PLANTS - 2

Ting Wang and Francis Lau

18.1 (9:55-10:15) Waste Heat Recovery in a Simulated Liquefied Natural Gas (LNG) Plant

Shisir Acharya, and Ting Wang,
Energy Conversion and Conservation Center, University of New Orleans, New Orleans, LA, USA

Natural gas (NG) has a lower level of and cleaner emissions as compared to other fossil fuels such as coal and petroleum. Thus NG gas has been widely used in recent years to replace coal, diesel, or other petroleum derived fuels to generate power. However, many nations in the world have limited or minimal NG resources. Importing liquefied Natural Gas (LNG) has become the only method for countries where transporting natural gas through land-based piping is not sufficient or not available, for example, Japan, South Korea, Taiwan and Pakistan, to name a few.

LNG can be obtained when natural gas is refrigerated to a temperature around -260°F (-162°C). At this temperature, the original volume of the natural gas is reduced by 600 times. To reach this temperature, a multi-stage refrigeration system with intercooling and regeneration is required. The process of producing LNG is an energy intensive process, which demands a large amount of compression from multiple compressors. Each of these compressors is directly driven by a gas turbine. The gas turbine exhaust contains a large amount useful energy, but often much of the energy is released into the atmosphere and ultimately wasted. The objective of this study is to identify methods to utilize this hot wasted exhaust and recover energy from it. Firstly, this paper provides a generic review of various existing commercial LNG production processes. Then a cascade LNG process is simulated to utilize up to four succeeding (cascading) vapor compression refrigeration loops to achieve a cryogenic temperature around -260°F (-162°C). This gas turbine is then combined, and the energy is recovered through a Heat Recovery Steam Generator (HRSG) to power a Rankine cycle power plant to produce electricity. The result shows that the HRSG combined with a Rankine cycle can recuperate up to 47% of the waste energy.

18.2 (10:15-10:35) Optimization by Automatic Control with Acoustic Gas Temperature Measurement – Improvement of Efficiency, Emissions, and Plant Availability

Matthias Ritter, Manfred Deuster, Atul Sharma,
Bonnenberg & Drescher GmbH, Aldenhoven Germany

The solid fuels are heterogeneous due to varying composition and different heating values which makes the combustion and operations in power plants complex. Additionally, high efficiency (low excess air) and low emission values require careful fuel/air control. This applies especially to old plants with low design reserves.

The temperatures in the combustion chamber, their temporal fluctuations and local imbalances are available for routine boiler operation with the introduction of the acoustic gas temperature measurement. The outstanding characteristics of the acoustic

measurement, i.e., no ageing, no drift, no influence by the heat radiation and the high local resolution due to the use of combined operating sensors, allow a highly accurate and reliable diagnosis of the furnace temperatures (balancing).

Local temperature imbalances and strands correlate very sensitively with the stoichiometric conditions in the combustion chamber. They are caused or reduced by small changes in the fuel/air system. Thus, their exact diagnosis and adjustment is the key for a furnace operation with the lowest possible air ratio and low CO values. The relationships are described by examples.

There are economically significant examples in which the corrosion was substantially reduced by active control of the combustion air (incinerators) or by targeted trimming of the fuel/air distribution in power plants up to 900 MW in Europe.

The automated active balancing control through the acoustic measurement has been implemented for a hard coal furnace for the first time in a steam generator of a power plant in Poland. In combination with a combustion optimizer, the active balancing control achieves an operational optimum concerning gas-burnout, NO_x, steam parameters and denitrification. This combination of the acoustic temperature measurement and a combustion optimizer has now also been implemented in more than 15 power plants with lignite coal furnaces. The results are presented.

The control of SNCR plants by acoustic measurement has become routine for incinerators and power plants. Balancing is mandatory for high NO_x reduction and low specific consumption of the reacting agents.

Today, acoustic measurement technology allows the fast and simultaneous measurement of an unlimited number of paths. In the past systems were limited to 24 paths measured in 1–2 minutes. Modern systems measure > 200 temperatures in <15 seconds. Such applications are standard in blast furnaces in combination with new local high-resolution tomography methods. In hard coal-fired power plants with SNCR systems, high-resolution measurement systems provide temperatures from several levels for the control of more than 50 injection positions in the boiler.

18.3 (10:35-10:55) Development of Adsorbents for the Removal of Elemental Mercury from Coal Gasification Gas

Md. Azhar Uddin, Kento Fujiyama, and Yoshiie Kato
Graduate School of Environmental and Life Science, Okayama University Japan

Integrated gasification combined cycle (IGCC) power generation from coal is receiving increased attention for its high efficiency. Fuel gas generated from coal gasification also contains elemental mercury. To date, most of the research activities, both practical and fundamental, have focused on the removal and conversion of elemental mercury from real or simulated coal combustion flue gas. Very little attention has been paid to the capture of elemental mercury from coal-derived fuel gas.

The purpose was to develop metal oxide adsorbents suitable for removing mercury from coal gasification gas atmosphere. Particularly, Iron oxide-cerium oxide adsorbents was developed with varying composition and they were tested for elemental mercury removal from simulated coal gasification gas. The durability and regenerability of the adsorbents were also investigated.

18.4 (10:55-11:35) Unit Flexibility: Keep Your Coal Unit Viable and Marketable

Bruce J. Ogden,
EAPC Industrial Services

Extended and frequent unit low load operation and increased ramp rates can make you coal fired unit marketable and valuable in a renewable energy driven market. Understanding most coal-fired units were originally designed to be base loaded, extreme low load operation and high ramp rates presents numerous challenges. This paper will provide a high-level approach to meeting those challenges, including a methodology for exploring and evaluating the various obstacles. Some of the obstacles to be discussed will be boiler typical low load failure modes, boiler operating modes, turbine low load failure modes, and numerous auxiliary equipment considerations. In addition to the technical challenges the biggest challenge can be retraining the operations department to operate the plant at very low loads and avoiding unit cycling. The focus of this presentation will be on-site Unit Flexibility Testing results.

18.5 (11:35-11:55) Filling the Gaps: What Impacts Hydrated Lime Dry Scrubbing Performance?

Ian Saratovsky,
Lhoist North America, Fort Worth, TX, USA

Which hydrated lime properties matter most for acid gas (i.e. SO₂, SO₃, HCl, HF, etc.) capture in dry scrubbing applications? During the early days of dry sorbent injection (DSI) hydrated lime with high purity was considered important. It turned out that at > 90 %, purity is not critical since only the outer 20-50% of the sorbent is utilized in most

applications. After years of operating experience, importance was placed on particle sizes and surface area. While intuition indicates that smaller particles and more surface area would improve performance, this isn't the case. Two decades of R&D work in the laboratory, pilot and full-scale studies, have demonstrated that pore characteristics (e.g. pore volume and pore diameter) are the most critical hydrated lime property. While surface area is important, not all surface area is the same/has the same reactivity with acid gases. Increasing surface area can be accomplished through particle size reduction or introducing many, small pores into the sorbent. Shrinking particle size results in an insignificant increase in reactive surface area of typical 20 m²/g sorbents: for example -shrinking particles from 10 μm to 2 μm marginally increased surface area from 0.3 m²/g to 1.4 m²/g. Introducing many, small pores also increases surface area; however, small pores tend to rapidly plug, restricting additional flue gas penetration into the internal pores. For optimized acid gas reactivity in dry scrubbing applications, hydrated lime sorbents with engineered pore characteristics (i.e. optimized pore volumes and pore diameters) minimize pore pluggage, maximize sorbent utilization, and exhibit the greatest adsorption capacities to continue reacting with acid gases while residing on particle control devices (e.g. fabric filter or ESP). In this presentation, results from full-scale, laboratory, and pilot-scale tests illustrate that hydrated lime pore characteristics are the most important parameter impacting acid gas removal performance in dry scrubbing applications.

SESSION 19 (12:35 – 14:15)

POWER PLANTS – 3

Eric Grol and Ting Wang

19.1 (12:35-12:55) Accelerating Large-Scale Decarbonization of Coal Power Plants Through Improving Condenser Efficiency

Vinod Veedu, Matthew Nakatsuka, Sumil Thapa, and Alexander Ventura,
Oceanit, Houston, TX, USA

Decarbonization of the power sector is often framed in terms of the inevitable substitution of renewable energy sources for fossil fuels, as well as developing carbon capture, utilization, and storage technologies to cover the rapidly growing demand for power. While these may be possible paths for addressing climate issues in nations that have viable and cost competitive fuel alternatives, in much of the world a lack of available financial resources has stymied efforts at rapid transition. To encourage development, new technologies must not only have a public benefit in reducing emissions, but an immediate economic value to the operator that can reduce existing operating expenses or increase production.

The idea of doing “more with less” through improving plant operations is one potential way to better enable decarbonization globally. This work will outline efforts in developing a way to improve heat transfer efficiency in coal-fired power plants through a pilot deployment of an ultra-thin, low-surface energy treatment on the tube side of heat exchanger and condenser units. The tube side is typically exposed to untreated cold water from neighboring bodies of water, meaning that this area is at risk of developing thick layers of insulating biofilm and scale, tube blockage through marine growth, and pit formation due to silt and mineral erosion. Reduction in heat transfer and flow disruption within the tubes can lead to significant losses in plant capacity and increased fuel usage.

By deploying this long-lasting surface treatment on heavily worn units in lieu of full tube replacement, significant performance gains were noted, while maintenance costs and total downtime were greatly reduced for the operator. Additionally, this deployment was capable of being directly integrated into a regularly scheduled maintenance stop, with full application completed within 14 days despite heavily fouling of the equipment prior to the introduction of the surface protection treatment. Analysis of the post-treatment performance showed that efficiency gains up to 7% were viable, meaning that the calculated effect of biofouling could be almost eliminated and mitigated. Direct calculation of the effect on power plant emissions was also calculated, with an estimated 150,000 Ton reduction at a 500 MW plant over the course of 12 months.

19.2 (12:55-13:15) FGD Effluent Treatment Modeling and Speciation Analysis Before & After Phys/Chem/Biological Treatment using Aqueous Chemistry Software

Nicholas Siefert, NETL, Pittsburgh, PA, USA
Britley Jones
Chemical and Biological Engineering Department, Princeton University,
Princeton, NJ, USA

As part of the U.S. Environmental Protection Agency (EPA) Effluent Limitation Guidelines (ELGs), the EPA measured the concentrations of nearly all elements in flue gas desulfurization (FGD) wastewater and in the streams after different steps in the

treatment process. In this project, we focused on three of the power plants the EPA studied and three separate locations in the treatment process. For example, we analyzed the EPA data for (a) the FGD influent, (b) the intermediate stream leaving the Physical/Chemical treatment system, and (c) the effluent stream after the Bioreactor. For each of these three stream locations, we averaged the measured elemental concentration over multiple days, e.g. Se. An aqueous chemistry software (OLI Studio) was used to check for charge balance, to estimate missing species, to reconcile pH, and to estimate speciation of these averaged streams, e.g. SeO_4^{2-} . In addition, we used OLI Flowsheet to model a theoretical reactor (to mimic a biological reactor without kinetic limitations) to compare the experimental results after the biological reactor with a theoretical Gibbs minimizing reactor. This presentation will review the results of this analysis, as well as highlight trends and patterns in the data collected. Analyzing this data is an important step towards understanding how to lower the cost of treating FGD effluent using Physical/Chemical precipitation and Biological reactors.

19.3 (13:15-13:35) Effective Removal of Trace Levels of Toxic Heavy Metals from Flue Gas Desulfurization Wastewater Using SiO₂ Supported Hydrogel Sorbent

Qiuming Wang, Walter C. Wilfong, Brian Kail, Tuo Ji, Fan Shi, Support Contractor NETL, Pittsburgh, PA, USA
McMahan Cray, NETL, Pittsburgh, PA, USA

Flue Gas Desulfurization (FGD) wastewater generated from fossil fuel thermoelectric power plants contains potentially harmful heavy metal pollutants, such as Copper (Cu), Zinc (Zn), Cadmium (Cd), Mercury (Hg), Lead (Pb), Chromium (Cr), Iron (Fe), Nickel (Ni), Arsenic (As), Selenium (Se), Cobalt (Co), Manganese (Mn), and Aluminium (Al). Among these heavy metals, the U.S. Resource Conservation and Recovery Act (RCRA) classified a group of eight heavy metals, including As, Cd, Cr, Pb, Hg, Se, Ba, and Ag, as extremely toxic at even small concentrations (RCRA metals) because they can accumulate in the human body and cause serious health disorders. In November 2015, the US EPA promulgated the Effluent Limitations Guidelines (ELG) for the steam electric power generating sector to eliminate or lower permissible discharge limits for six wastewater streams produced at coal fired power plants, including FGD wastewater. In this work, we present a stable PEI-MBAA 3D crosslinking network functionalized SiO₂ solid sorbent material (PMS-1.2/1/4) and investigated its adsorption behaviors toward heavy metals in different solution environments. Particularly, the adsorption kinetics and capacity of six of the toxic heavy metals (As, Cd, Cr, Pb, Se, and Hg) were evaluated using an ideal solution prepared with single elements in MilliQ water. The kinetic experimental data were used to analyze the effect of the external film boundary layer and intraparticle mass transfer resistance on the sorption process and its significance. The adsorption selectivity of metals was investigated using authentic industrial FGD wastewater and Se/Hg spiked industrial FGD wastewater. Initial results showed PMS-1.2/1/4 achieved superior removal of Se, Cd, U, and Al down to below their reporting limits, while simultaneously capturing ~90% Ni and Zn, ~80% Cu and Hg, and ~60% Cr and Co. The reusability of the sorbent was studied through five adsorption-desorption cycles using industrial FGD water.

19.4 (13:35-13:55) Development of a Novel Thermal Battery for the Flexibilization of Fossil-Fired Power Plants

Julio Bravo, Justin Caspar, Sudhakar Neti, Zheng Yao, Alparslan Oztekin, Carlos Romero, Shuoyu Wang, Ahmed Abdulridha, Clay Naito, Muhannad Suleiman, Spencer Quiel, Lehigh University ATLSS Engineering Research Center, Bethlehem, PA, USA
Yue Xiao, Devon Jensen, Chien-Hua Chen, Advanced Cooling Technologies, Lancaster, PA, USA

As the need for more flexible power generation systems grows, energy storage is now more important than ever to compensate the phase shift between renewable energy availability and grid demand. Among the different options for energy storage, thermal energy storage is a natural option for integration with Rankine and Brayton power cycle systems. Sensible heat, solid state energy storage offers the potential for competitive cost advantages (\$/kWh), material stability as well as flexibility of integration with the power plant thermal cycle. However, issues related to thermal and mechanical performance need to be addressed to offer a solution that provides large enough energy storage capacity (MWh) and fast energy charge and discharge rates (kW/min) for the dynamic operation of plants. This paper introduces research carried out at Lehigh University on the development of a thermal battery for applications in coal-fired power plants. The battery consists of an advanced cementitious formulation and configuration for optimal heat storage capacity and mechanical performance, and a heat transfer design that includes efficient transient heat transfer to/from the storage media. Design study information and experimental results from a 10 kWh prototype are reported in this paper. Repeated charging and discharging cycles (6 and 4 hours, respectively) proved the feasibility of the concept in terms of energy storage in the solid media, design operating temperatures of 400 °C, storage capacity, and rapid charge and discharge of the battery. Future work will move the prototype to a 100 kWh scale for demonstration at a Dominion Energy's coal-fired station.

19.5 (13:55-14:15) Hydrogen Blending with Natural Gas for Transportation Via Pipeline: Current Issues and Potential Solutions

David Lyons
U.S. DOE, National Energy Technology, Morgantown, WV, USA
Alfred Chang, Henry A. Long, III, Christopher Munson, Massood Ramezan
KeyLogic Systems, Inc.

As the need for more flexible power generation systems grows, energy storage is now more important than ever to compensate the phase shift between renewable energy availability and grid demand. Among the different options for energy storage, thermal energy storage is a natural option for integration with Rankine and Brayton power cycle systems. Sensible heat, solid state energy storage offers the potential for competitive cost advantages (\$/kWh), material stability as well as flexibility of integration with the power plant thermal cycle. However, issues related to thermal and mechanical performance need to be addressed to offer a solution that provides large enough energy storage capacity (MWh) and fast energy charge and discharge rates (kW/min) for the dynamic operation of plants. This paper introduces research carried out at Lehigh University on the development of a thermal battery for applications in coal-fired power plants. The battery consists of an advanced cementitious formulation and configuration for optimal heat storage capacity and mechanical performance, and a heat transfer design that includes efficient transient heat transfer to/from the storage media. Design study information and experimental results from a 10 kWh prototype are reported in this paper. Repeated charging and discharging cycles (6 and 4 hours, respectively) proved the feasibility of the concept in terms of energy storage in the solid media, design operating temperatures of 400 °C, storage capacity, and rapid charge and discharge of the battery. Future work will move the prototype to a 100 kWh scale for demonstration at a Dominion Energy's coal-fired station.

SESSION 20 (14:25-16:25)

CLEAN COAL DEMONSTRATION AND COMMERCIAL PROJECTS

Thomas Sarkus and Eric Grol

20.1 (14:25-14:45) An Integrated Energy System for Thar Coal in Pakistan

Dr. Farid A. Malik,
FC College, A Chartered University, Ferozpur Road, Lahore Pakistan

An integrated coal based energy system has been developed for the 175 billion ton deposit at Thar. Initially a five phase program was developed that consisted of; Concept Report and Scoping Study, Mining Study together with a Test Pit Design, Test Pit Construction, Project Management and Mine Development, Co-production Plants Set Up. An IGCC (Integrated Gas Combined Cycle) approach was proposed with power generation, CTL/FTD (Coal to Liquids, Fischer Tropsch Diesel), Urea and SNG (Substitute Natural Gas) production.

In 2018 the first open pit mine with an output of 3.8 million tons per year (mtpa) came on line which has now been up-graded to 7.6 mtpa. Power generation units have also been synchronized to the national grid for 660 MW. One 7.8 mtpa project has also been approved under CPEC for CTL/FTD, SNG production.

Out of the 12 demarcated blocks, 4 have been allocated, rest are available for prospective investors. A simple one window approach mechanism has been developed through TCEB (Thar Coal Energy Broad). Thar has the potential of emerging as an energy power hub of the Middle East and Asia.

This presentation will discuss the integrated approach adopted for development of Thar Coal all the way from mine development to downstream utilization with emphasis on gasification of coal for multiple applications.

20.2 (14:45-15:05) Slipstream Testing of Amine-Based Solvents at a Low-Rank Coal-Fired Power Plant

Joshua Strege, Jason Laumb, John Kay, and John Oleksik
University of North Dakota Energy & Environmental Research Center
Grand Forks, ND, USA

Although amine-based postcombustion carbon capture (PCCC) technology has the potential to reduce CO₂ emissions from large stationary power sources, the fine aerosols present in flue gas from low-rank coals such as North Dakota lignite may present a challenge for amine-based capture. Aerosols provide nucleation sites where volatile amine vapors can condense as flue gas rapidly cools at the absorber column outlet. These amine-laden aerosols can then escape the column and lead to accelerated solvent losses. Moreover, several of the components present in the fine particulate from low-rank coal combustion can react with amines or catalyze amine degradation to deactivate solvent

and cause fouling. Past testing conducted by the Energy & Environmental Research Center (EERC) has shown that while a wet electrostatic precipitator (WESP) can be an effective means of reducing aerosol-based solvent losses, WESP performance is highly dependent on many variables, and the optimum flue gas pretreatment configuration for minimizing solvent losses is likely to be site-specific. To better assess mitigation strategies for aerosol reduction to extend solvent life, the EERC installed a pilot-scale CO₂ absorption system at a lignite-fired plant in central North Dakota. The pilot-scale system was operated using both commercial KS-1™ solvent and advanced KS-21™ solvent provided by Mitsubishi Heavy Industries (MHI). MHI's proprietary amine emission reduction unit (AERU™) technology was installed downstream of the absorber columns to reduce solvent losses by recovering amines at the system outlet. Fine particulate loading was measured throughout the capture system with and without a WESP operating and using both solvents. Captured particulate was brought back to the EERC to be analyzed for chemical composition and to be examined by scanning electron microscopy for particulate structure. These variables were then correlated to performance of particulate control devices in reducing aerosol formation and solvent losses.

20.3 (15:05-15:25) ODYSSEUS - Coal-to-Liquids Supply Chain Integration in View of Operational, Economic and Environmental Risk Assessments Under Unfavorable Geological Settings

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Sam Parsons, Vasilis Sarhosis,
University of Leeds, Leeds, UNITED KINGDOM

ODYSSEUS is an R&D project initiated in 2019 and funded by the European Research Fund for Coal and Steel. The project partners from the European coal industry, research organizations and universities focus on the Coal-to-Liquids Supply Chain (CLSC) integration and enhanced assessment of operational, economic and environmental risks during or after mine operation in unfavorable geological settings for potential high coal production areas in European medium- to low-grade coal deposits. For that purpose, technological CLSC integration and optimization are the main objectives, supported by laboratory- to demonstration-scale experimental activities on upgrading coal-derived liquids and by-product beneficiation, integration of conventional and innovative mine development as well as enhanced techno-economic and environmental risk management. The present contribution will provide insights into the CLSC integration strategy developed for a European hard coal deposit and an operating lignite mine based on the combination of in-situ coal conversion with conventional extraction, findings from laboratory- and demonstration-scale coal-liquefaction experiments at surface and in-situ conditions, techno-economic assessments and numerical modelling of coupled processes for the elaboration of a robust environmental risk assessment framework.

20.4 (15:25-15:45) Design and Performance Considerations for the FEED Study of an Advanced Pressurized Fluidized Bed Combustion Power Plant with Carbon Dioxide Capture and Storage

Stephen E. Winter, Daniel P. Connell, Jacqueline M. Fidler,
CONSOL Energy Inc., Canonsburg, PA, USA

At the 2020 International Pittsburgh Coal Conference, CONSOL Energy presented conceptual and pre-FEED (front end engineering and design) study results from its transformative power plant project as part of the U.S. Department of Energy, National Energy Technology Laboratory's (DOE NETL) 21st Century Power Plant Program (formerly Coal FIRST). This presentation will provide an update on the project and will outline the design and performance considerations for the recently commenced FEED study phase of the project.

The project is based on using an advanced pressurized fluidized bed combustor (PFBC) to fire fine wet waste coal and seeks to capture and permanently sequester 97% of the generated CO₂ emissions. To ultimately achieve a net zero or net negative CO₂ emissions performance, the plant also is being designed to include a BECCS (bioenergy with carbon capture and storage) strategy to co-fire up to 10% wet biomass produced through a regional farming network. Air pollution control and wastewater treatment

technology will be integrated to deliver near-zero air emissions and zero liquid discharge operation, which further enhances the plant's positive environmental profile. The location of the plant is expected to be at or near CONSOL Energy's Pennsylvania Mining Complex (PAMC), where the potential for integration into existing mine site infrastructure promotes the sustainability of the coal supply chain. The scope of work for the FEED study includes two phases: the first exploring value engineering tasks focused on optimizing plant configuration and technology, and the second involving the detailed FEED study, lifecycle analyses to assess emissions performance, and development of the final investment case. Both phases also include parallel task streams to define and understand CO₂ geologic storage and disposition opportunities in Northern Appalachia in the vicinity of the PAMC.

While preliminary results have indicated that the overall plant concept is expected to achieve favorable fuel and variable O&M costs in the range of ~\$18-21/MWh with an effective dispatch cost of less than zero (when applying a CO₂ capture tax credit), the capital costs for the plant remain a primary focus for the FEED study. The presentation will discuss several equipment design and performance areas and considerations where potential improvements may be realized. These include boiler design and fabrication, waste fuel processing, and strategies to right-size environmental controls and CO₂ capture and storage systems. Other aspects of the project related to minimization of water consumption, characterization of CO₂ storage reservoirs, and the development of nearby biomass and carbon pipeline networks will also be presented.

The project endeavors to complement developing renewable power systems and changing market dynamics while providing a CO₂-neutral, cost competitive power supply to meet the needs of an evolving electric grid and social landscape. Importantly, aspects of the project that support environmental justice, workforce development, and community growth initiatives will also be discussed.

Given favorable economics and an efficient design, construction of the plant could commence in ~2024, with commissioning targeted in ~2028.

20.5 (15:45-16:05) Flameless Pressurized Oxy-Fuel (FPO) Technology Update & Commercialization Objectives

Massimo Malavasi, Richard A. Homer,
School of Energy Resources, University of Wyoming, USA

Flameless Pressurized Oxy-fuel Combustion (FPO) technology has many attractive benefits that can support the continued responsible use of fossil fuels in stationary electrical and power generation, notably as the urgency of the energy transition unfolds. Not only is FPO capable on operating on multi-fuels, including coal, natural gas, biomass and waste, it can be configured in any practical scheme to operate in differing fuel types together. The integrated combustion and carbon capture capability means that the system power recovery efficiency is around 42% and 53% operating on coal and natural gas respectively, meaning that economic returns on deploying FPO technology are favorable when compared to post carbon capture technology additions on existing air fed combustion systems.

The engineering modularity of FPO, means that a facility can largely be constructed and commissioned offsite, with minimum site activity required. Integration into an existing fossil fuel facility can be carried out quickly, with the minimum of disruption, downtime and inconvenience. Retrofit options to existing facilities operating on coal when compared to adding post carbon capture solutions are attractive.

Operationally, FPO offers load following performance that supports ability of the combustor and energy recuperation scheme to rapidly respond to frequent unscheduled changes in the market and customer demand for energy. Even when the combustor is operating at low capacity, it can still generate energy at close to the optimum efficiencies. The response time to changing demand for energy -until steady state operation is achieved, in less than 15 minutes operating on solid fuel and even faster on natural gas.

Any incombustible material left in the combustion chamber when operating on coal, is vitrified and therefore benign, so it can be collected and sold for use in road and building construction materials.

FPO technology has been proven and demonstrated on various fuel types including coal, natural gas and waste refuse and plastic. While a first of a kind commercial scheme - including carbon dioxide utilization in below ground reservoirs is still to be built, a number of privately funded projects are currently being investigated, notably in Wyoming. The focus and intent of these projects will generally be described.

20.6 (16:05-16:25) Combustion Related Considerations in the Retrofit of a Pulverized Coal Fired Boiler Utilizing Oxy-Coal Technology

Andrew P. Chiodo, Kevin A. Davis, Brydger Van Otten,
Reaction Engineering International, Midvale, UT, USA
and Steve Krinsky,
Jupiter Oxygen Corporation, Des Plaines, IL, USA

A feasibility study was performed to evaluate Jupiter Oxygen Corporation's (JOC) patented high temperature oxy-combustion technology for retrofit in an existing coal-fired boiler. This technology utilizes an oxygen stream rather than air with minimal flue gas recycle (FGR) to produce a high temperature flame (~4500°F). This high flame temperature increases radiant efficiency in the boiler. Additional FGR outside of the burner zone is used to balance convective heat transfer downstream of the boiler in order to maintain the final system steam requirements. Detailed Computational Fluid Dynamics (CFD) modeling as well as process modeling has been performed to aide in a conceptual design of the high temperature retrofit. An air-fired baseline model (based on current plant operation) was first developed to demonstrate a thorough understanding of the unit. Over 50 oxy-fired CFD simulations were carried-out to investigate heat transfer, burner geometry optimization, operational tuning, load variations, and flue gas recycle rate. Metrics for evaluations focus on performance characteristics such as flame location/stability, local peak tube/burner temperatures and heat fluxes, carbon conversion (CO and carbon-in-ash), NO_x emissions, particulate carry-over, tube corrosion, and ash deposition/sintering. Once the CFD modeling has been performed, the predicted radiant heat transfer is input into a detailed process model of the entire power plant system. Here the fire-side and steam-side circuits are integrated to develop a complete representation of the retrofit system and how final steam production will be impacted. At the conclusion of the feasibility study, a conceptual design was produced which showed:

- Increased radiant heat transfer in the boiler
- Balanced convective heat transfer achieved with an optimized FGR rate
- Final superheat and reheat steam production in agreement with current air-fired production
- Acceptable furnace exit gas temperature
- Maximum heat flux and tube temperatures within acceptable limits
- Improvements in carbon-in-ash
- Higher concentrations of trace pollutants (CO, NO_x), but lower emissions on a mass basis
- Acceptable performance at turndown conditions with optimized FGR rate
- Lower deposition rates when compared to air-firing

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