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COAL CONFERENCE

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ABSTRACTS BOOKLET

Clean Coal-based Energy/Fuels and the Environment

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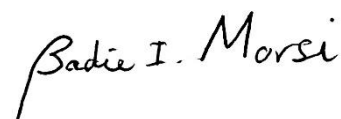
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On behalf of the Thirty-Seventh Annual International Pittsburgh Coal Conference, we wish to express our sincere appreciation and gratitude to Ms. Kristen Harper for her meticulous leadership and control of the entire operation of the conference and to Mr. Husain Ashkanani, Mr. Rui Wang and Mr. Sai Kundan Vena for their invaluable assistance in preparing this Abstracts Booklet.

Thank you,

Badie I. Morsi

Badie I. Morsi, Editor
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SESSION 1
GASIFICATION TECHNOLOGIES – 1
Diane Revay Madden and Alberto Petttinau

1.1 Size Distributions and Chemistry of Inorganic Particles in Residues Produced from Two Commercial Entrained-Flow Coal Gasification Plants in China

Yafeng Wang, Yuegang Tang, China University of Mining and Technology (Beijing), CHINA; John P. Hurley, University of North Dakota, USA; Xin Guo, China University of Mining and Technology (Beijing), CHINA; Robert B. Finkelman, University of Texas at Dallas; Shane K. Butler, Alexander Azenkeng, University of North Dakota; USA.

Computer-controlled scanning electron microscopy (CCSEM) with Bruker's ESPRIT Feature module is an advanced technology that can be used to measure the sizes and chemistry of inorganic particles in geologic materials on an individual particle basis. In the present study, the feed coals used in the two gasification plants are high volatile C bituminous coals prepared into a coal–water slurry and pulverized coal for General Electric (GE) and Gaskombinat Schwarze Pumpe (GSP) coal gasification, respectively. The coarse residues derived from the crushed bottom slags and the fine residues separated from the syngas were collected from the bottom of the gasifiers and the filters in the syngas purification system, respectively. The sizes and chemistry of inorganic particles in the fine fractions (<75 μm) of four residues were measured using CCSEM-Feature. More than 30,000 inorganic particles were detected in the fine fractions of GE Coarse Residue (GE-CR), GE Fine Residue (GE-FR), GSP Coarse Residue (GSP-CR), and GSP Fine Residue (GSP-FR). The size ranges of the particles determined based on the equivalent diameter (minimum diameter of 0.5 μm) were 0.5–67.8 μm, 0.5–46.9 μm, 0.5–74.7 μm, and 0.5–56.7 μm, respectively. About 90% of the particle counts in each sample were in the range of 0.5–2.5 μm. The fine residues generally contained more spherical particles as indicated by the circularity that can be observed in the SEM images. The inorganic particles in the coal gasification residues were predominantly silicates. Na-Fe silicate and Mg-Fe silicate were the main silicate phases in the GE gasification residues; however, Mg-Fe silicate and Fe aluminosilicate in the GSP gasification residues had the dominant calculated weight percent (wt%) of the total particles based on particle area. Quartz particles (with Si>80%) in the GE-CR, GE-FR, GSP-CR, and GSP-FR were 7.0 wt%, 11.6 wt%, 6.9 wt%, and 9.9 wt%, respectively. The inhalable quartz particles ($PM_{2.5}$ and $PM_{10-2.5}$) in the GE-CR, GE-FR, GSP-CR, and GSP-FR were 6.3 wt%, 28.1 wt%, 9.6 wt%, and 19.5 wt%, respectively. Generally, the mineral transformations in the coal gasification processes resulted in the increase of the fractions of the aluminosilicate and silicate in the residues. The equivalent diameters of most quartz particles were larger than 10 μm. Iron-containing phases such as Fe silicates, aluminosilicates, and iron oxides were generally the main carriers of potentially hazardous trace elements including V, Cr, Mn, Co, Ni, Cu, Zn, As, Sr, Mo, Cd, Sb, Tl, and Pb. The size distributions and chemistry of inorganic particles in the coal gasification residues will provide an understanding of the mineral behavior during the coal gasification processes and the associations of potentially hazardous trace elements to the particles are probably useful for the control of the hazards.

1.2 CFD Simulation of the Two-Stage Dry Feed Entrained Flow Gasifier

Bo Zhang, Shaoping Shi, Yanfei Mu, Yan Shu, PhD State Key Laboratory of Coal-Based Clean Energy (Huaneng Clean Energy Research Institute), CHINA

A computational fluid dynamics (CFD) model was constructed for a two-stage dry feed entrained flow gasifier developed by China Huaneng Group. The CFD model employs the discrete phase model to describe the two-phase flow of gases and solids, the detailed chemical kinetics to model the reactions during the gasification process and the discrete ordinates radiation model for radiation simulation. The errors of the calculated mole fraction of CO, H_2, CO_2 in the product syngas and the temperature at the outlet compared with industrial operational data are all within 5%. This demonstrates the effectiveness using the developed CFD model to study the gasifier and the gasification process. With the CFD model, the effect of flow rates of steam and coal injected into the second stage on the performance of the gasification process are further analyzed.

1.3 Performance Evaluation of Coal Pyrolysis-Based Staged Conversion Polygeneration System Coupling with a 2×300wme CFB Power Plant

Kaikun Li, Qinhui Wang, Mengxiang Fang, Zhongyang Luo, Zhejiang University, CHINA

For a long time, most of China's electricity supply comes from coal-fired power plants. The total installed capacity of China was 1899.67GW in the end of 2018, in which approximately 60% was contributed by thermal power. However, directly combusted of coal not only causing environmental problems, but also wasting its high-value added inherent components. Therefore, many efforts have been made to develop a clean coal utilization technology. In this paper, a transformation scheme of a 2 ×300MWe circulating fluidized bed (CFB) coal power plant was presented, and its performance evaluation was conducted based on simulation results. In aforementioned modified system, coal was first pyrolyzed to produce char, tar and hot coal gas. Then the hot char generated in the fluidized pyrolyzer was combusted in the CFB boiler with air for subcritical steam. The high-temperature ash was used as solid heat carriers for coal pyrolysis process. Based on the coal pyrolysis coupled with char combustion process, two kinds of technical routes were proposed, (a) tar was reacted with H_2 which was separated from the clean syngas to synthesize crude light oil, coal gas after cooled and cleaned was sent to format synthetic natural gas (SNG). Char was fired in the CFB power plant for electricity; (b) Coal gas for methanol production, char for power generation, and tar to produce crude light oil. Simulation of the two polygeneration transformation plants was conducted using Aspen Plus. Two RYield modules were used to simulate the coal pyrolysis and char decomposition process, respectively. Combustion of char was modeled by the RGibbs module, based on the Gibbs free energy minimization method. Moreover, MHeatX module for heat recovery, Sep module for acid gas removal process, REquil modules for SNG formation reactors, and RPlug module for methanol synthesis. Several turbine blocks were used to simulate different pressure cylinders for power generation. According to the results obtained from the simulation, thermodynamic analysis was calculated and discussed. For both cases, the coal consumption was set at 680.60t/h, which was calculated to match the amount of char combusted in the CFB boiler. Simulation results showed that in case (a), the production of SNG, crude light oil and net electricity power can reach 65833.49Nm³/h, 19.85t/h and 605.86MW respectively. For case (b), it obtained 56.34t/h of methanol output, 19.85t/h of crude light oil production and 825.13MW of net electricity power. It should be noted that the higher generating capacity of case (b) was due to the gas turbine installation. The total energy efficiency of plant (a) and (b) can reach 53.59%, and 50.74% respectively, which was much higher than that of original CFB coal-fired power plant. In conclusion, there are practical advantages to conduct transformation of traditional CFB coal-fired power plant on the strength of coal pyrolysis-based staged conversion polygeneration technology co-producing electricity and high value-added chemicals.

1.4 Research and Development of New Biomass-Coal Co-Conversion Technology

Fan Lulu, Co-Authors Chen Hui, Meng Xianliang, Zhou Min, Yan Xinlong, Wan Yongzhou, Xiao Lei, China University of Mining and Technology, CHINA

Biomass energy is a kind of renewable energy, but its low energy density and immobility restrict its large-scale application. To make it truly an alternative energy source for fossil fuels, the key is to convert low-grade biomass energy into efficient, clean, high-grade energy. Therefore, based on the solidification and molding of coal and biomass, this paper develops a new high-temperature plasma biomass/coal co-conversion unit to study the characteristics of biomass-based coal gasification. The results show that the addition of mineral compounds can promote the pyrolysis of biomass briquette. The addition of mineral compounds reduces the pyrolysis activation energy of biomass briquette in the main reaction zone, making the pyrolysis reaction of biomass briquette easier to proceed. The material compounds can also promote the production of H2, CO, CO2 and CH4 during the pyrolysis of biomass briquettes. Based on this discovery, a new type of high-temperature plasma torch biomass/coal co-conversion device was designed and processed in this paper to realize efficient methanation of biomass / coal. With calcined dolomite or Ni/Al2O3 as the catalyst, the addition of steam in the tar catalytic cracking can not only increase the gas production rate, but also increase the hydrogen content and improve the gas production quality. In addition, a three-dimensional simulation model of plasma ultra-high temperature gasification melting furnace was constructed in Fluent simulation software. Based on the principle of fusion pyrolysis and diffusion mechanism, the co-gasification matching law of plasma torch and coal/biomass, the temperature field, fluid field and concentration field distribution of the gasifier are

simulated and studied. The temperature in the gasifier meets the test conditions for biomass/coal co-conversion, laying a foundation for the smooth progress of the pilot test research.

1.5 Coal Hydrogasification for Aromatics and Methane Process Innovation and Industrialization

San Zhou, Guoqing Wang, Zhichao Ma, Haoqiang Wang, Lirong Ma, ENN Science & Technology Development Co., Ltd., CHINA

(1) Background

With the rapid growth of global energy consumption, the intertwined energy and environmental problems have attracted increasing concerns. The extensive use of coal is in urgent need of transformation, and it is of great significance to achieve the clean and efficient conversion of coal resources. ENN has developed its own proprietary coal hydrogasification technology for producing aromatics and methane from low-rank coal. The novel process integrates the advantages of coal-to-gas and coal-to-oil technologies, achieves the clean utilization of coal and improves the energy conversion efficiency, which is significant for deploying clean coal technologies and diversifying the raw materials for energy and chemical industries.

(2) Technology introduction

Coal hydrogasification process involves fast pyrolysis of pulverized coal under hydrogen atmosphere, secondary cracking reaction of the volatile and hydrogasification of the active char at moderate temperature (800-1000℃) and high pressure (5-10MPa), producing methane, aromatics and char. It is a highly-efficient, environmentally-friendly and economic novel gasification process, which is one of the most advanced clean coal conversion technologies to realize the comprehensive, efficient and clean conversion of coal through the cascade, grading and staged utilization strategy.

(3) Demonstration Progress

ENN's coal hydrogasification technology development, which was initiated in 2012, has been through lab-scale study, 10 tons/day PDU test, 50 tons/day pilot test and 400 tons/day industrial demonstration plant test. The industrial demonstration plant is currently at the stage of system operation and optimization.

The 400 tons/day coal hydrogasification process is composed of sections such as pulverized coal preparation, dense-phase conveying, hydrogasification, cooling and dust removal. The core technologies and equipment include dense-phase conveying system of pulverized coal, gasifier, high-temperature and high-pressure hydrogen combustion nozzle and char-cooling fluidized bed. The key equipment includes waste heat boiler, crude gas filter, hydrogen heating furnace, etc. The process flow diagram is shown in Figure 1.

The raw coal is first dried and prepared to pulverized coal with particle size <75 μm, and then pneumatically transported to the dense-phase conveying system. The pulverized coal flows through the variable pressure and the high pressure coal lock hoppers, and then is transported to the nozzle and injected into the entrained bed gasifier via the dense phase conveying with high pressure hydrogen. The hydrogasification reaction generates the char, gaseous aromatics and crude gas. The char is discharged from the bottom of the gasifier into a fluidized bed for char cooling and heat recovery after de-dusting by baffles. The crude gas and gaseous aromatics together with a small amount of char is cooled to 300℃ by the waste heat boiler and then enters the crude gas high-temperature metal filter for fine dust removal. Subsequently, the crude gas and gaseous aromatics is cooled to 40℃ by multistage intercoolers, and the products methane and aromatics are obtained after separation and purification.

A 72-hour continuous operation of the 400 tons/day coal hydrogasification demonstration plant was conducted in September 2019, verifying the reliability of the core technologies and key equipment such as dense phase conveying technique, nozzle, gasifier and char-cooling equipment.

The demonstration test shows excellent performance of the coal hydrogasification technology, including ≥50% total carbon conversion rate, 11-15% yield of aromatics, 0.5-0.8Nm³/kg-C direct yield of methane and above 90% conversion efficiency of hydrogasification island. The hydrogasification technology is clean and environmentally friendly, achieving the direct conversion from coal to target products. Moreover, the aromatics produced are simple in composition and easy for separation, which greatly improves the technical and economic advantages of this technology.

(4) Outlook

At present, the demonstration plant is under long-term system optimization and modification, and stable production is planned in December 2020. With the stable operation of the 400 tons/day demonstration plant, coal hydrogasification technology will complete the process development phase and be ready for commercial deployment. Meanwhile, ENN will devote itself to the development of kiloton process package and process optimization, and actively seek partners for industrial promotion, realizing the ultimate goal of the comprehensive, efficient and clean coal transformation.
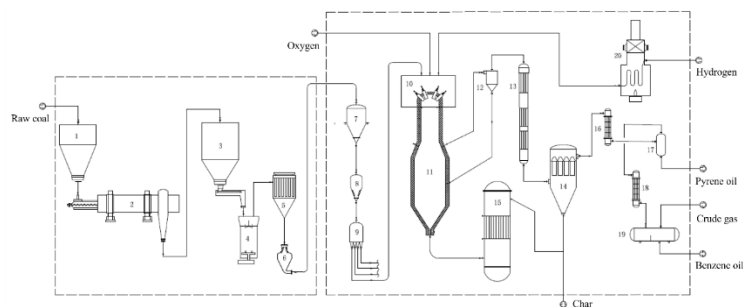

Figure1. Process flow chart of coal hydrogasification for aromatics and methane
1-raw coal bunker; 2-drying machine; 3-crushed coal bunker; 4-coal mill; 5-bag-type dust remover; 6-eductor; 7-pulverized coal bunker; 8-variable pressure coal lock hopper; 9-high pressure coal lock hopper; 10-high-temperature and high-pressure hydrogen combustion nozzle; 11-gasifier; 12-cyclone separator; 13-waste heat boiler; 14-crude gas filter; 15-char-cooling fluidized bed; 16- secondary heat exchanger; 17-primary separation tank; 18-primary heat exchanger; 19-secondary separation tank; 20-hydrogen heating furnace

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SESSION 2
COMBUSTION TECHNOLOGIES – 1
Evan Granite and Johan Van Dyk

2.1 The Effect of Alkaline Earth Metals on Soot Formation and Devolatilization Kinetics During Coal Pyrolysis

Yifan Wu, Yu Zhang, Jiankun Zhuo, Tsinghua University, Qiang Yao, Tsinghua University & Xinjiang University, CHINA

Mineral components in coal have significant influence on pyrolysis kinetics and product distribution. Many studies have shown positive effect of alkali metals on soot elimination, while the effect of alkaline earth metals is still unclear. In this work, the effect of calcium on soot formation were investigated with experimental methods. Coal samples, treated by acid wash and calcium ion exchange, were pyrolyzed using a Hencken flat flame burner. A two-stage quenching system was installed to collect the entire particulate matters. The devolatilization kinetics under high heating rate were estimated by sampling char at different residence time. The results indicated that calcium could notably hinder the formation of soot, and change the size distribution of fine particulate matters. The soot elimination effect depends on coal rank and calcium existing form. Loading of calcium could also shift the pyrolysis kinetics and the ultimate char yield.

KEYWORDS: Alkaline earth metals, Soot formation, Resident time, Coal Pyrolysis

2.2 Fireside Corrosion of Ni-Fe Based Alloy GH984G for Ultra-supercritical Coal-fired Power Plants

Jiali Wang, Jiankun Zhuo, Tsinghua University, CHINA

The advanced ultra-supercritical technology (operating at 760ºC and 35Mpa) is promising for the future development of world electric power generation due to its high thermal efficiency, low pollution and sustainability compared to traditional fossil-fired power plants. Considering the more severe working circumstances of heat transfer components, a critical limiting factor to enhancing steam parameters in future ultra-supercritical power plants are the materials of construction, that were required to have the appropriate combination of high creep rupture strength(100Mpa/10^5h) and corrosion resistance (<=2mm cross-section loss in $2*10^5$h). Currently used advanced ferritic and austenitic stainless steels would no longer be able to meet the new stringent material targets. Therefore, many projects have established to evaluate and develop advanced materials applied to the advanced steam cycles in coal-fired electricity generation plants. Ni-based superalloys are the promising materials for A-USC application with outstanding high-temperature mechanical properties and oxidation resistance. However, the high cost of the solid solution strengthening element Co, Ni and Mo with high costs of manufacture and fabrication in comparison with steels affected the promotion of Nickel base alloys in large components. Recently, some novel Ni-Fe based alloys (excluding precious element Co) with superior high temperature creep strength, high thermal conductivity and cost-effective/ have attracted much attentions as interesting alternatives. More recently, a new Ni-Cr-Fe-based high-temperature wrought superalloy GH984G possessing excellent stability of microstructure and mechanical properties has

been specially developed for highly efficient power plants by metal research institute, Chinese academy of sciences. Research showed that GH984G possessed superior processing properties and thermal conductivity, furthermore exhibited prominent microstructure stability, mechanical properties, and steam-side oxidation comparable to the advanced Ni-based candidate alloys such as Inconel 740 and Inconel 617 in highly efficient power plants conditions. However, the fireside corrosion resistance of GH984G wrought alloy has rarely been reported in A-USC conditions. For this purpose, fireside corrosion performance of GH984G under different temperatures and deposit environments to represent the metal temperature of superheater/reheater components designed in A-USC PP was investigated; meanwhile the other three protential candidates were detected for comparison. The process of the corrosion was determined using traditional weight change method and dimensional metrology of sample cross-sections. The Morphological characteristics of corrosion products were researched utilizing SEM, EDS and XRD. Results were focused on oxidation process, and sulphur induced corrosion. Results showed that relationship of corrosion rates to temperature followed a linear kinetics in the range of 600ºC-780ºC in the absence of ash conditions for all selected Ni-Fe based alloys, and GH984G showed comparable to the advanced Ni-based candidate alloys in the coal-ash environment. The results are being used for providing recommendations for the suitable alloys which have the strength for superheaters and reheater tubes of A-USC.

2.3 Ignition Characteristics of Single Coal Particle under Pressurized Oxy-fuel Conditions

Qianyun Chen, Yusheng Wang, Jing Li, Zhaohui Liu, Chuguang Zheng, Huazhong University of Science and Technology, CHINA

Pulverized coal combustion in pressurized oxy-fuel condition is accepted as one of the most promising technology for carbon capture and storage. In this study, the ignition characteristics of single coal particles were investigated in an optically accessible pressurized flat-flame reactor (OPFR). Three different rank coals were investigated, namely Powder River Basin (PRB) subbituminous coal, Shenhua bituminous coal (SH) and Shanxi anthracite coal (SX). Experiments were conducted under 20%O2/CO2 atmosphere with the gas temperature of 1400K, and the pressure at the range of 0.1-1 MPa. A Particle Tracking Image Pyrometer (PTIP) method was developed to get the particle velocities, diameters, temperatures simultaneously by means of non-intrusive optical measurements. Ignition characteristics such as ignition delay time, ignition mode and volatile combustion duration time etc. are deduced then. The results demonstrate that the elevated pressure retards the onset of ignition and increases the duration of volatile combustion for all three coals. For PRB coal and SX coal, the ignition times vary monotonously as pressure increase, while a single-peak tendency of increasing under lower pressures (0.1-0.7 MPa) and decreasing under higher pressures for SH coal. The effect of elevated pressure on coal ignition and volatile combustion can be explained by its higher heat capacity and higher O2 pressure. At lower pressure, the heating process of coal particles was slowed by the higher heat capacity of the surroundings, which led to longer ignition delay. While at higher pressure, the increase of O2 pressure accelerates the homogeneous or heterogeneous ignition of coal particles.

2.4 Elemental Mercury Removal by I- doped Bi$_2$WO$_6$ with Remarkable Visible-Light-Driven Photocatalytic Oxidation

Yili Zhang, ZhuoXiong, Yongchun Zhao, Junying Zhang, Huazhong University of Science & Technology, CHINA

Gaseous elemental mercury removal from coal-fired power plants has been a great challenge in the field of environmental protection. Among several methods for removing elemental mercury, photocatalytic oxidation is a clean and effective one. Bismuth tungstate (Bi$_2$WO$_6$) is a widely used visible light catalyst. And the band gap of BiOX depends on element X (X = I, Br, and Cl); among these, BiOI exhibits the smallest band gap, which may indicate that iodine reduces the band gap of the semiconductor. In this work, I⁻doped Bi$_2$WO$_6$ nanocomposites with different iodine contents were synthesized by a one-step hydrothermal method. Detailed experimental and density functional theory (DFT) studies were conducted to analyze the performance of I⁻-doped Bi$_2$WO$_6$ in Hg^0 removal when irradiated by visible light.

The results showed that at an iodine concentration of 1.0 wt.%, the doped Bi$_2$WO$_6$ exhibited the optimal Hg^0-removal efficiency of 87.6% and 97.5% under N$_2$+O$_2$+CO$_2$ and N$_2$+O$_2$+CO$_2$+SO$_2$+NO conditions, respectively. The Hg^{0}photooxidation efficiency of the synthesized I⁻ doped Bi$_2$WO$_6$ was much higher than that of pure Bi$_2$WO$_6$(9.1%). There were three main reasons on the improved photocatalytic activity of modified Bi$_2$WO$_6$. Firstly, I–doping reduced the band gap of the semiconductors by decreasing the potential energy of the conduction band, thus preserving the oxidation capability of the material. Secondary, I⁻ doping decreased recombination rate of electron-hole pairs. Lastly, I⁻ doping reduced the impedance of the material; further, the separated electrons and holes could be quickly transferred to the interface surface to participate in the photocatalytic reaction. Through density functional theory calculations, we showed that

iodine was doped in the (WO$_4$)$^{2-}$ layer and oxidized HgO can be adsorbed on the surface of I⁻-doped Bi$_2$WO$_6$. The O$_W$ site was found to exhibit weak adsorption with respect to HgO, implying that it is most conducive to the desorption of HgO, which can provide guidelines for the selection of sites to be exposed in the preparation of catalysts. Finally, the photocatalysis mechanisms elaborated and that h$^+$ and •O2$^-$ were the predominant active sites.

2.5 Experimental and Modeling Investigation of Coal/Biomass Particle -wall Collision Behaviors

Jingyu Wang, Tsinghua University; Lele Feng, China University of Mining and Technology; Yuxin Wu, Guangxi Yue, Tsinghua University; CHINA

The particle-wall collision behaviors are important to the performance of gas-solid flows in pulverizers, which affects the combustion efficiency in coal-fired boilers. Typical fuel particles have irregular shapes and exhibit complex behaviors after colliding with rough walls. In this paper, particles-wall collisions with coal and biomass particles on steel walls were studied experimentally using high-speed photography. The effects of key parameters including particle non-sphericity, wall roughness and impact angle were analyzed.

The rebound velocities of the non-spherical particles were highly scattered, and different approaches were compared to model the distributions. By regrouping the results by the measured impact velocity and angle, the collision coefficients could be analyzed statistically. These coefficients for fuel particles were found to be similar to the values for non-spherical glass particles. With an existing 4-parameter semi-empirical model, the cases with fuel particles and rough steel walls could be predicted with relatively low errors.

For more accurate descriptions of the rebound behaviors, the neural network methods were applied to the data. The network consisted of fully connected hidden layers and a probability distribution output layer, with the mean and the standard deviation as output parameters. It was trained on each experimental condition with the log-likelihood as the loss function. Compared with the traditional statistical method, the predicted functions of the impact angle showed smoother trends. The predicted log-likelihood increased by up to 0.2 for fuel particles, especially when the data were not heavily filtered during pre-processing.
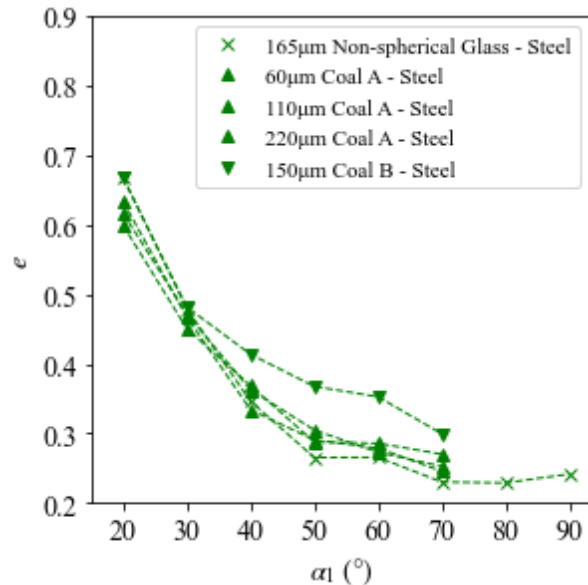
SESSION 3
CARBON MANAGEMENT – 1
Nicholas Siefert and Omar Basha

3.1 120,000t/A Post-Combustion CO2 Capture Unit Upgrading and New Solvent Performance Verification

Jinyi Wang, Hongwei Niu, Dongfang Guo, China Huaneng Clean Energy Research Institute; Lianbo Liu, Beijing Key Laboratory of CO2 Capture and Process; Shiwang Gao, State Key Laboratory of Coal-Based Clean Energy, CHINA

CO2 capture is an important carbon management route to mitigate the greenhouse gas emission in power sector. Chemical absorption based post-combustion CO2 capture (PCC) technology is the leading one in large scale demonstration for PC power plant. Lowing the capture cost and energy penalty is the key to promote the application of CO2 capture, enhancing the equipment performance and the innovation in the chemical solvent used for capture is the main solution to improve the PCC system.

Huaneng Shanghai 120,000 t/a PCC located in Shidongkou No.2 Power Plant, Shanghai, China, is the first one of this scale in the world. As part of the US-China Clean Energy Research Center - Advanced Coal Technology Consortium (CERC-ACTC) cooperation, the system was retrofitted and upgraded in 2017, including replacement of column parts of different geometry features, and applying surface treatment to the column. New type of column packings and internal parts such as distributors are designed and selected through computational fluid dynamics simulation and bench testing in the lab. After equipment upgrading, the mass transfer in the columns is greatly enhanced, the height of the new packing is reduced by 20%. Surface coating was applied to the carbon steel inner wall of CO2 absorber, the corrosion rate of the column slowed down, as the iron ion concentration in the process solution was decreased by some 60%. The overall system operation performance and efficiency were improved by 15% due to upgrading, which provides options to reduce the CAPEX investment of PCC system in the future.

New solvents were developed through screening on blended amines, the screening combines true heat flow (THF) calorimetric test on reaction heat and Vapor-Liquid Equilibrium (VLE) studies. A new solvent, HNC-5, was put into long term operation for more than 2000h after equipment retrofit. The reboiler heat duty for CO2 regeneration in stripper is <3.0GJ/tCO2, the solvent loss rate is <0.5kg/tCO2, and the unit operation cost after applying HNC-5 is reduced by about 15%, regardless of the equipment upgrading.

3.2 Simultaneous Removal of Carbon Dioxide and Multi-pollutants from Flue Gas by Cryogenic Pentane Scrubbing

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

The combustion of coal has powered the world for centuries, but has also brought the earth enormous environmental problems due to the emission of greenhouse gas carbon dioxide as well as noxious pollutants such as SOx, NOx, HCl, HF and Hg. Nowadays, various mature technologies are available for pollutants removal and carbon capture, such as selective catalytic reduction (SCR) for NOx removal, wet-limestone scrubbing for SOx removal and amine scrubbing for carbon capture. However, these classical technologies can only treat CO2 and pollutants individually. In recent years, cryogenic CO2 capture technology, in which carbon dioxide is separated from flue gas by desublimation at cryogenic temperatures, was developed and demonstrated by pilot-scale field test. By cooling the flue gas to around -120°C, 90% of the CO2 is captured in the form of dry ice. The field test results indicated that pollutants such as SO2, NO2 and Hg can also be removed effectively removed in cryogenic temperatures. One major challenge of cryogenic CO2 capture process is that flue gas has to be dehydrated by molecular sieve before cooling to frosting temperatures to prevent ice formation in the heat recovery exchanger where flue as is pre-cooled by cold clean flue gas. The deploy of molecular sieve dehydration system for large scale flue gas is practically impossible.

In this study, a novel cryogenic Pentane scrubbing process is developed to achieve carbon dioxide capture and multi-pollutants removal simultaneously. Flue gas with water moisture can be directly cooled to cryogenic temperatures by pentane scrubbing without dehydration pretreatment. H_2O, CO2 and pollutants in their solid or liquid phase can be separated from liquid pentane due to their insolubility with each other. Process modeling study is conducted by Aspen Plus^{TM} based on a 600MW$_e$ coal-fired unit to evaluate the capture rate of CO2, removal efficiency of pollutants, and overall energy penalty. At a scrubbing temperature of -117°C, a capture rate of 90% is achieved for CO2, and a removal rate close to 100% is reached for pollutant component SO2, SO3, NO2, HCl, HF and Hg. A three-stage cooling process is adopted, in which H_2O, SO2 and CO2 are removed and recovered successively. The overall energy penalty is around 0.97 MJe/kgCO2 if the captured CO2 is recovered as liquid and is reduced to 0.68 MJ$_e$/kgCO2 if the captured CO2 is recovered as gas, which is about 30% lower than that of amine-based CO2 capture technology.

3.3 CO2 Capture by Supported Phosphonium Dual Functionalized Ionic Liquids @ MCM-41

Rui-nan Wang, Taiyuan University of Technology; Cui-ping Ye, Taiyuan University of Technology, Training Base of State Key Laboratory of Coal Science and Technology Jointly Constructed by Shanxi Province and Ministry of Science and Technology; Xia Gao, Taiyuan University of Technology; Wen-ying Li, Training Base

of State Key Laboratory of Coal Science and Technology Jointly Constructed by Shanxi Province and Ministry of Science and Technology; CHINA

The CO2 discharge from the combustion of the fossil fuels leads to the explosive growth of the amount of CO2 in the atmosphere, causing serious climate change and environmental damage. The flue gas from power plant is one of the main sources of CO2, and it is generally difficult to capture since the low CO2 concentration, normally between 10% -15%. Among the capture media, ionic liquids (ILs) have the advantages of good thermal stability, tunable and environmentally benign, which have been as a kind of efficient and reversible solvent used for CO2 capture. The incorporation of functional groups greatly improves the CO2 trapping capacity of ILs. For example, the CO2 capacity reaches to 1.58 mol CO2/mol ILs using anion-functionalized ILs, [P_{66614}][2-Op]. The ILs fixed to mesoporous materials not only has high adsorption properties, but also is easy to be recovered and separated. A strategy for improving CO2 capture capacity by dual functionalized ILs with multiple active sites has been proposed. Three ILs containing different anions ([aP_{4443}] [2-Np], [aP_{4443}] [2-Op] and [aP_{4443}] [Triz]) were synthesized, and [aP_{4443}] [2-Np] had a higher CO2 capacity of 1.88 mol CO2 /mol ILs. The infrared spectra analysis confirmed that the feasibility of introducing functional group to improve the capacity of CO2, and the amino and hydroxyl react with CO2 to form $NHCOO^-$ or CO_3^-. [aP_{4443}] [2-Np] supported on MCM-41 through a wet impregnation-vaporization method was studied under different loading ratio, temperature and different CO2 partial pressure. It was found that 30% [aP_{4443}] [2-Np]-MCM-41 had the best CO2 adsorption performance up to 3.19 mmol/g (theoretical data was 3.35 mmol/g) under the atmosphere of CO2:N_2 (15%:85%) at 30 ℃, 0.1 MPa. The cyclic experiments showed that the thermal stability of 30% [aP_{4443}] [2-Np]-MCM-41 was good, and after 6 cycles, the adsorption property reduced indistinctively. The pseudo-second-order model and internal diffusion model were used to analyze the adsorption kinetics for a better understand of the CO2 adsorption behavior and mechanism of supported ILs. Combined with the activation energy calculation results, we could get that the adsorption process of CO2 by [aP_{4443}] [2-Np]-MCM-41 was a physical adsorption process, and the internal diffusion was a speed control step.

3.4 Oxidation States of Pt Nanoparticles Induced Selectivity Change of Photocatalytic CO2 Reduction Over Pt/TiO2 Catalysts

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As a CO_2 emission reduction technology with mild reaction conditions, low cost and environmental friendliness, photocatalytic CO_2 reduction technology deserves wide attention. In this paper, PtO and Pt cocatalysts were deposited on the surface of TiO_2 and both of them improved the photocatalytic CO_2 reduction activity, while Pt/TiO_2 showed a good product selectivity for CH_4. It is found that the chemical states and distribution of Pt species were the main reasons for the change of photocatalytic activity and product selectivity. Both PtO and Pt inhibited the recombination of photogenerated electron-hole pairs, whereas Pt^0 had a stronger ability to capture photogenerated electrons. Denser distribution of PtO would occupy the active sites on the catalyst surface, leading to the decrease of CO adsorption capability. Meanwhile, coordination oxygen bound to Pt^{2+} can over-stabilize, inhibiting subsequent reduction of CO into CH_4. The Pt nanoparticles would migrate and grow during the photochemical reduction of PtO into Pt, retarding excessive CO adsorption. In addition, Pt^0 was easier to form linear adsorption with CO, which was conducive to further activation and reduction of CO, thus increasing the yields of CO_2 reduction and promoting selective generation of CH_4. Models of CO adsorbed on Pt/TiO_2 and PtO/TiO_2 surfaces were built on the basis of the density functional theory (DFT) calculations, the results showed that CO adsorption on Pt/TiO_2 surface was stronger than that of PtO/TiO_2.

SESSION 4
GASIFICATION TECHNOLOGIES – 2
Andreas Richter and Rolf Maurer

4.1 Underground Coal Gasification as a Transitional Fuel in South Africa

David Love, Golder; Johan Brand, Africary; Robert Gumbi, Oxeye Energy; Shehzaad Kauchali, University of the Witwatersrand; Shaun Pershad, Eskom Holdings SOE; Christien Strydom, North West University and South African Underground Coal Gasification Association; SOUTH AFRICA

South Africa's National Climate Change Response Strategy, notes that it is a significant contributor to climate change, with greenhouse gas emissions from its energy intensive, fossil-fuel powered economy, almost 4 times the world average. By later this century, South Africa should have achieved an environmentally sustainable society, expanded low-carbon economy and reduced emissions, through a Just Transition, which encompasses a range of social interventions needed to secure workers' jobs and livelihoods, and wider society, when economies are shifting to sustainable production,

including avoiding climate change. South Africa's thermal power stations, which currently provide by far the bulk of the country's electricity generation, with all but two power stations scheduled for decommissioning by 2050, over half within the next decade. Ramping up of electricity production from renewable sources will be gradual during this period.

Underground coal gasification provides an opportunity for closing the loop in solid waste, emissions and dirty water, through co-firing or sole-firing of thermal coal power stations during the three decade transitional period when the thermal coal fleet will still be operating. This can include:

1) Closing the loop in solid waste through the UCG process: coal is gasified in in the coal seam, only syngas comes to the surface. There is no surface exposure of coal, no spoils or discard dumps on the surface and so no acid rock drainage affecting surface water or usable shallow groundwater. A residue of slag, ash and salts remains in the gasified zone.

2) Closing the loop in emissions is a progressive target: UCG with closed-circuit gas turbines produces very little NOx and SOx and produces 28% less CO2 emissions than coal combustion thermal power. The CO2 emissions can be progressively reduced by using renewables for operations electricity demand and then by using solar ignition. Carbon capture (from the power station) and storage (in the spent gasifier zone of the coal seam) is the next stage, followed by carbon reuse and reinjection as an input to the UCG process, reusing the carbon dioxide rather than emitting it.

3) Closing the loop in dirty water needs to be understood in the context that UCG makes use of saline water from the coal seam aquifer, water that is very high in salts an unusable for agriculture of domestic purposes. Water reuse is possible, through recovery of the water content of syngas from gas turbines (rather than release as flue gas) and reuse and reinjection of condensate. It is also planned to use of external dirty water: mine water decant from one of the coal mines that currently supplies the power station could be injected into the gasifier.

UCG can be implemented in the same coalfields and at the same power stations that large parts of South Africa's Highveld depend upon for their livelihoods. This creates opportunities to deliver sustainable development projects for the coalfields, as part of the Just Transition to low-carbon economy. The presentation will unpack three projects in different locations in South Africa and how each can contribute.

4.2 Geochemical Assessment of the Underground Coal Gasification Geo-reactor

Lehlohonolo Mokhahlane, University of the Witwatersrand, SOUTH AFRICA

The Eskom UCG pilot site is located near Majuba Power Station in the Mpumalanga province of South Africa. During high temperature coal conversion (1200 – 1400 °C), minerals contained in coal will undergo transformation into various phases and forms. The gasification process also leads to the formation of ash, tars and void spaces in the coal seam. These void spaces are due to the mass transfer of solid coal into gaseous phase that ultimately creates a cavity in the coal seam which gets partially filled with residue products. The mineral content of the coal is responsible for the composition of the ash generated by the gasification process. At the completion of the UCG process, the geo-reactor shuts down when the injection of oxidants is discontinued and ultimately cools down by natural influx of groundwater into the gasification zone. The shutdown process can be expedited by injecting surface water into the gasification chamber. Ultimately the geo-reactor will be flooded with water which interacts with the residue products leading to possible leaching of environmentally toxic material.

Leaching of coal ash generated from surface gasifiers have has been explored quite extensively in a number of studies which show heavy metals and trace elements being leached at rates that pose an environment risk. Post gasification, there is a need to establish if the UCG cavity is environmentally neutral or a potential source of pollution to the surrounding groundwater. The geochemical environment in the post-reaction area of UCG is different from the atmospheric conditions that most surface waste is exposed to and hence there is a need to determine the leaching dynamics of post-process chamber under field representative conditions. There is also a need to cater for possible development of acidic conditions due to geochemical transformations of residue with time especially given the inherent sulphide mineralization in coal that can cause acid rock drainage (ARD).

This study offers a modified elution method that uses deionized water, hydrogen peroxide, and sulphuric acid as leaching agents. Hydrogen peroxide provides for elution under complete oxidation as it is a strong oxidizing agent that provides for efficient dissolution of even inert sulphides such as pyrite. The elution tests will further incorporate leaching by groundwater taken from the UCG carven from the study area. The groundwater elution tests will be carried out in temperatures recorded from the study site in an attempt to simulate field conditions. The results show that the geo-reactor is not a neutral carven and leaching of metals and trace elements can be expected. Acid base accounting also indicates that the UCG chamber is likely to be a source of acidic

conditions going forward. All of this shows that there is a need to have a rehabilitation plan for the UCG chamber post gasification in order to avoid potential environmental risks especially to groundwater.

4.3 Particle Morphology Evolution During Char Conversion Process Applied for CFD Modeling an Entrained-Flow Gasifier

Cong Bang Nguyen, Johannes Scherer, Mathias Harwich, Andreas Richter, TU Bergakademie Freiberg, GERMANY

The change in a particle's morphology affects both its trajectory and its carbon consumption rate, hence the performance and efficiency of an entrained-flow gasifier. Among key processes taking place inside the gasifier, the char conversion process is a limiting step for the overall carbon conversion. For that reason, the presentation presents the evolution of morphology of char particles during conversion process. To monitor the morphology evolution, particle-resolved transient CFD calculations were performed to estimate changes in shape, density and volume of a char particle under different condition processes. The complex physical and chemical processes taking place in the vicinity and the interior of the char particle were observed in detail. Analyses of the numerical data obtained from the transient CFD calculations were carried out. As a result, new expressions related to drag coefficient, parameters of particle conversion model were emerged. The new expressions were applied for modeling a pressured entrained-flow gasifier at laboratory scale. The numerical results of the gasifier show good agreement with the experimental data and the improvement of the applied sub-model particle.

4.4 Numerical Study on the Effect of Particle Residence Time on Kinetics Evaluation of Gasification Reaction in a Drop-Tube Furnace

Fengbo An, Andreas Richter, TU Bergakademie Freiberg, GERMANY

Kinetics of heterogeneous reaction measured in a drop-tube furnace can better reflect environmental conditions of the particles in the entrained-flow gasifier. However, the hydrodynamics and thermo-chemical processes can be complicated in drop-tube furnace. A special attention should be paid to particle residence time, since it directly affects the conversion rate. Due to the non-equal distributions of gas temperature and concentrations, and due to a distinct particle size distribution, the particle trajectories vary significantly and cannot be estimated by use of different drag force models. The present work studies the particle trajectories in a high-pressure drop-tube furnace by use of CFD and experiments. It can be shown that using of different drag force models can evoke large errors and cannot be used to obtain correct kinetic parameters. To overcome this limitation, drag force terms for different particle sizes are analyzed and modified, which shows a very agreement with experimentally obtained particle residence times. Furthermore, the effect of particle residence time on the kinetic evaluation will be discussed in detail.

4.5 New Approach for Flame Image Segmentation Based on Machine Learning Algorithms

Mohsen Gharib, Andreas Richter, TU Bergakademie Freiberg, GERMANY

The characteristics of the flame have a significant effect in the global reforming process of syngas from any feedstock. Some of these characteristics are the flame shape and size. Hence, the determination of the flame borders is an essential task to differentiate between combustion regions with high reaction rates and reforming regions with low reaction rates. Nowadays, digital image processing methods play a big role in flame monitoring systems. In this study, flame images were acquired using a high-speed camera, which is attached to an optical system. Afterward, the output videos/images are imported to an in-house optical data analysis software for preparation and analysis steps. This software was developed to combine flame image processing methods with model-based flame and process analysis tools and to provide a user-friendly GUI that can be used by everyone. The scope of this study is on developing a machine learning algorithm based on random forest model to provide auto adaptive segmentation of flame images. This algorithm is used to extract the most important features from the flame image and then predict the flame edges in unseen images based on what it was trained on. Furthermore, a comprehensive comparison was done to compare this approach with the traditional images processing methods like manual thresholding, edge detection algorithms and histogram-based image segmentation. The present study shows that using machine learning tools for flame image segmentation provides a flexible and reliable method, even in comparison with traditional methods. Finally, the results were compared with numerical results from CFD calculations in order to complete the analysis.

SESSION 5
COMBUSTION TECHNOLOGIES – 2
Evan Granite and Thomas Sarkus

5.1 Dynamic Simulation of the Flue Gas Behavior in a Conceptual 10 Mw$_{th}$ Oxy-Circulating Fluidized Bed Combustor

Hoangkhoi Nguyen, Byungho Song, Kunsan National University; Dowon Shun, Jaehyeon Park, Jaegoo Lee, Korea Institute of Energy Research; SOUTH KOREA

Oxy-fuel circulating fluidized bed (oxy-CFBC) has been considered as a promising technology to facilitate high separation of CO_2, and low pollutant emission of SO_x, NO_x, CO in the flue gas. In this study, an oxy-combustion process model was established using a 10 MW$_{th}$ oxy-CFBC test facility. The dynamic model was based on the mass, energy balance and the reaction kinetics of coal combustion in oxy–fired condition. At the steady-state, the predicted flue gas concentrations are 88.2 % of CO_2 and 3.4 % of O_2. A smooth switching from the air-fired to oxy-fired was explored within 12 min, and of 10 min for vice versa process. The sensitivity of dynamic analysis revealed that the high CO_2 purity was strongly affected by the air-leakage amount. The CO_2 was reduced by 25 % (from 88.2 to 66 %) with 5% of air ingress. In addition, the relationships of load change inputs and the response of the flue gas and temperature have been evaluated. The comparison of the simulation results with the experimental results showed a good agreement. The presented results could be a good reference for the real operation of oxy-CFBC plants.

5.2 The Pressurized Oxycombustion Behavior of Turkish Lignites in the Bubbling Fluidized Bed Combustor

Ufuk Kayahan, TUBITAK Marmara Research Center Energy Institute; Nevzat Ula, Marmara University; Berrin Engin, Aslı Sayar, Namık Ünlü, TUBITAK Marmara Research Center Energy Institute, TURKEY

In this study, the combustion of two different Turkish lignites in a 30 kW thermal capacity of bubbling fluidized bed combustion system was carried out in order to compare their combustion characteristics in the air, atmospheric oxyfuel and pressurized oxyfuel environments. The combustor has 120 mm inner diameter, 2250 mm height (from distributor plate), and double layer refractory. The moisture, ash and volatile matter contents of the lignites were in the range of 16-36%, 30-31% and 6-27%, respectively.

Combustor was operated in the temperature range of 745-855 °C, 760-835 °C and 750-860 °C air, atmospheric oxycombustion, pressurized oxycombustion (4 barg) respectively. CO_2, CO, O_2, NO, N O_2 and S O_2 emissions in the flue gas were continuously measured and recorded by an online Gasmet FTIR DX 4000 type gas analyzer.

The oxy-fuel combustion experiments were done with %21 O2/ %79 C O_2 and %40 O_2 / %60 CO_2 mixture. Emissions of both NOx and SO2 appeared to be considerably affected by combustion atmospheres. In the oxyfuel combustion both the NOx and S O_2 emissions were higher than that in the air combustion and increased with increase in the O_2 concentration in the feed gas. In the oxyfuel combustion processes, CO_2 concentrations of up to 96% in the flue gases were reached on dry basis.

5.3 Characterization of Oxy-Coal Swirl Injector

MD. Mohieminul I. Khan, Ana Rios, Mehrin Chowdhury, Ahsan Choudhuri, The University of Texas at El Paso, USA

The article presents the design and testing of a coal-slurry swirl-pintle injector for high-pressure oxy-coal combustion systems. Pressurized oxy-coal combustion-based systems have the potential to improve efficiency by recovering latent heat of the steam in flue gas and achieve 90% CO_2 capture. In oxy-coal combustion, coal is burned in the presence of pure oxygen, which results in higher efficiency and less greenhouse gas in the exhaust. With the advancement of pressurized oxy-coal combustor research, there is a need to investigate injector technology suitable for this unique combustion approach. Effective atomization and mixing of coal-slurry and oxidizer pose a challenge for the efficient burning of coal particles. A swirl-pintle type injector was designed and tested to enhance the atomization of the coal-water slurry spray by adding a swirl to the oxygen flow path. Although pintle type injectors are traditionally used in rocket engines, they present a promising approach in clean coal combustion technology due to higher mixing effectiveness and enhanced performance. The mixing behavior of three pintle injectors with different swirl numbers (S = 0, 0.9, and 1.2) was tested using a high-speed shadow sizing technique. Mixture ratios of 30%, 40%, and 50% (by mass) coal-water slurry were studied. The droplet diameter and dispersion characteristics were determined from shadow images of coal-water spray. The jet breakup length, droplet number, total moment ratio (TMR), and Ohnesorge number were then calculated to compare the performance of different injectors. The paper presents an empirical correlation of the TMR with droplet size and spray regimes. For a pintle injector with S = 1.2 swirler, the average droplet diameter was found to be in the range of 1.3 mm to 1.6 mm for different mixture ratios. The jet breakup length was also shorter in comparison to S= 0 and 0.9 injectors. A second atomization zone was also observed at 2 and 5 diameters downstream of injector exist at spray edge and jet core respectively.

5.4 Effects of Supercritical, CO_2-dilution on the Flame Dynamics and Morphology in a Coal-Fired Allam Cycle Combustor

Samuel Ogunfuye, Abdulafeez Adebiyi, V'yacheslav Akkerman, West Virginia University, USA

The current global demand for energy has prompted developing next generation energy systems. Advanced combustors to be used in these next generation energy systems have been a research focus, as these energy systems looks promising in achieving high efficiency and lower emission. Coal-fired Allam cycle, which is a direct-fired supercritical carbon dioxide (sCO$_2$) power cycle developed for gasified-coal combustion, is one of such promising technologies. The focus of this work is to investigate the combustion physics occurring in an advanced combustor used in this power plant technology. In the present work, the syngas fuel, which is a product of coal gasification, is modelled as methane to ensure adaptability for both coal and natural gas fired Allam cycle. In this respect, the present work extents our earlier works on sCO$_2$ combustion by considering the effects of CO_2 dilution on oxy-methane flame morphology and propagation at supercritical conditions, $CH_4 + 2O_2 + nCO_2 \rightarrow CO_2 + 2H_2O$. The computational simulation of the fully compressible supercritical reacting flow equations was carried out with various dilution ratios, $\beta \equiv n/(n+2)$ in the range $0 \leq \beta \leq 80$ % at constant pressure and temperature of the fuel mixture. It is shown that a flame slows down with dilution resulting in the thickening of the flame front at supercritical condition similar to atmospheric conditions, since flame temperature reduces with the dilution ratio. At supercritical condition, flame propagation demonstrates an initial exponential trend, which became quasilinear with time, though similar to atmospheric condition has a relatively higher magnitude. The laminar flame speed and heat release values have also been observed to decrease with the increase in the dilution ratio β, in agreement with earlier works performed at atmospheric conditions. Also, the effect of β on the flame structure is also evident as the scaled acceleration rates increased with dilution rate for smaller channel width when $\beta < 80$ %. As channel width increases, the scaled corrugated flame velocity grows mostly exponentially with time, and an increase in β results in a decrease in the exponential acceleration rates as long as $\beta < 80$ %.

5.5 Developing an Intensified and Cost-Effective Coal-Fueled Chemical Looping Combustion Process

Ayo Omosebi, Kunlei Liu, University of Kentucky, USA

Each year, electricity demand continues to grow from increases in population and economic development, and while coal is a low-cost energy source for power generation, increasing legislative controls on CO_2 emissions is putting coal at a disadvantage in a carbon-constrained world because coal is the most carbon-intensive fuel for power generation (1-2). Coal-fueled chemical looping combustion offers the simultaneous benefit of power generation and carbon capture without the need for add-on solvent-based capture systems that are required by conventional coal-fired power generation plants. While similar to oxy-combustion, it avoids the use of an air separation unit by using the redox states of oxygen carriers to facilitate coal conversion (3). While there is already significant body of knowledge on key component technologies that support coal-fired CLC like coal feeder, gas-solid fluidized bed, cyclone, loopseal, steam turbine, and heat recovery steam generator, however, oxygen carrier development, cost, reactivity, and attrition remain key issues CLC, coupled with long-term operation and performance stability under tar and slag forming conditions (4).

University of Kentucky's Center for Applied Energy Research (UK CAER) is currently exploring coal-fueled pressurized CLC using red mud derived from abundant bauxite waste for coal conversion in a 50 kWth unit. Cost-effective OC material development and methods to improve the overall reaction rate are extensively studied at bench scale, followed by pilot plant testing with direct coal feed, without the need for external coal pyrolysis and tar cracking to eliminate the solid agglomeration that occurs for many CLC technologies. UKy-CAER's approach reduces the technical gaps that impede the application of CLC to solid fuel through demonstration of the 50 kWth pressurized facilities. Current results show little to minor char/ash slip from fuel to air reactor and >50% coal conversion using red mud as (OC). Progress on OC attrition will be discussed.

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SESSION 6
CARBON MANAGEMENT – 2
Nicholas Siefert and Bingyun Li

6.2 Evaluation of CO2 Leakage Potential through Injection and Monitoring Wells at The Shenhua CCS Demonstration Project: Impact of Well Permeability Variation

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This study applies the publicly available US DOE's National Risk Assessment Partnership (NRAP) toolset to investigate CO_2 leakage potential through an injection well and two monitoring wells at the Shenhua CCS Demonstration Project in the Ordos Basin, China. The advantage of NRAP lies in its use of Reduced Order Models (ROMs) to estimate potential CO_2 leakage without implementing full-physics numerical simulations. This toolset has been implemented in several CCS and CO_2–EOR projects worldwide. Since the permeabilities of the injection well and the two monitoring wells at the Shenhua site are unknown, this study tests four scenarios with different well permeabilities. In Scenarios 1, 2 and 3, the permeabilities of the three wells are assumed to be 10^{-11} m^2, 10^{-12} m^2 and 10^{-13} m^2, respectively. In Scenario 4, the permeabilities of the three wells are assumed to follow a well permeability distribution based on permeability data collected from oilwells in Alberta, Canada. Simulation results show that only for Scenario 1, there is a low chance to have CO_2 leakage more than 1% of the total injected CO_2 during a 1000-year simulation period. Since the injection well and the monitoring wells at the Shenhua site are new wells, the chance to have those wells with a permeability of 10^{-11} m^2 or higher is extremely low. In summary, the CO_2 injected at the Shenhua site can be safely stored in the subsurface for a period of 1000 years, given a very low potential for CO_2 leakage through the injection well and the monitoring wells.

6.3 Effects of MDEA Concentration and Nanofluid-Types on the CO_2 Absorption and Desorption Performance of MDEA-based Nanofluids

Liu Yang, Chengdong Kong, Zhongxiao Zhang, Jian Liu, Shanghai Jiao Tong University, CHINA

The chemical absorption method is the most promising technique for large-scale CO_2 capture in the short term but still faces significant challenges of high energy penalty during absorbent regeneration. To improve the performance of CO_2 capture by traditional chemical absorbers, novel amine-based nanofluids absorbents were prepared mixing with the traditional chemical absorber (i.e., MDEA). Their absorption and desorption performances of CO_2 under different MDEA concentration (20wt% - 50wt%) and nanofluid types (i.e., TiO_2-MDEA, Al_2O_3- MDEA, SiO_2- MDEA) were studied by using a bubble absorption-desorption experimental system. The experimental results show that with the increase of the MDEA concentration, the absorption enhancement of nanofluids firstly increases and then decreases, and has the maximum absorption enhancement at an MDEA concentration of 30wt%; while the enhancement of desorption rate by nanofluids decreases firstly and then increases with the increase of MDEA concentration, and has the minimum desorption enhancement at an MDEA concentration of 40wt%. Furthermore, in the absorption process, when the mass fraction of nanoparticles is less than 0.08wt%, the TiO_2-MDEA nanofluids has the best absorption performance with an absorption rate enhancement of 82% at a mass fraction of 0.06wt%; in the desorption process, the desorption performance of Al_2O_3- MDEA nanofluid is worse than that of TiO_2-MDEA and SiO_2- MDEA, and the SiO_2- MDEA nanofluid has the best performance. In order to evaluate the overall performance including absorption and desorption processes, the enhancement mechanisms were

further discussed, and an overall enhancement factor was proposed based upon the separate absorption and desorption enhancement factors.

6.4 Renewable Fuels Production from Fossil-Derived CO2: The Sotacarbo Experimental Results

Alberto Pettinau, Mauro Mureddu, Sarah Lai, Francesca Ferrara, Sotacarbo S.p.A., ITALY

Carbon dioxide capture and utilization (CCU) technologies for the production of clean fuels are attracting interest of the scientific and industrial community for a series of possible applications in both power generation and industrial sectors. Firstly, CO_2 can be considered as a feedstock to chemically store 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 characterized by very low pollutant emissions: they can be directly used in transport sector – in particular for heavy duty trucks or for aviation and shipping – in place of their fossil-derived counterparts. Finally, CO_2-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.

Several studies are currently in progress worldwide, the results are very promising, and the first demonstration-scale applications are already available. But the pathway to make e-fuels competitive with their fossil-derived counterparts is still very long.

In this context, Sotacarbo is actively engaged in the development of processes and catalysts for CO_2 hydrogenation to e-fuels, especially methanol and dimethyl ether (DME). In particular, the research is focused on the development of catalysts that – using innovative preparation methods and advanced materials – can allow very high performance.

This work summarizes the most relevant results on the experimental development of advanced processes and catalysts for CO_2 hydrogenation to renewable methanol and DME. In particular, a specific methanol catalyst has been obtained combining the sol-gel method with self-combustion technique to deposit the active phase (based on copper and zinc oxide) on a support composed by a mesoporous silica, with a pore size in the order of few nanometers. The product – international patent application PCT/EP2019/053068 – is characterized, with respect to its competitor, by higher performance[1] in terms of production yield and selectivity[1] 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).

And a new pilot-scale plant is under design (it will be completed within late 2021) to test and develop the integrated power-to-liquids (i.e. methanol and DME) and power-to-gas (i.e. 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.

6.5 Assessment of Microwave CO$_2$ Gasification for Different Rank Coals

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Microwave-assisted CO_2 gasification of coal is studied to assess the feasibility of this technology for different rank coals. A lignite (Mississippi coal), a sub-bituminous (Wyodak) and a low-volatile bituminous (Pocahontas) coal were gasified with CO_2 in both a microwave and conventional reactor for comparison. During a typical experiment, a fixed bed of coal (3 g) was placed in the center of the microwave or conventional reactor and heated under a mixed gas flow of 150 sccm CO_2 and 50 sccm Ar. Gas phase products were analyzed by online MS and micro-GC. For microwave gasification carried out at 700 C, carbon conversion efficiency reached approximately 56% for both low rank coals (lignite and sub-bituminous), whereas conventional gasification resulted in very low conversions (10-12%) at this temperature for the low rank coals. For the low volatile bituminous coal, conversion was much lower, as expected, reaching a carbon conversion efficiency of only 22% under microwave and 4% under conventional heating. Conventionally heated gasification typically requires very high temperatures (900-1200°C) depending on the feed material with greater temperatures needed to convert high rank coals. Microwave gasification was able to reach a high conversion rate under CO_2 at mild temperatures (700°C). As seen by the enhanced conversion rates at mild temperatures, the ability of microwaves to rapidly and

selectively heat materials leads to greater heat transfer efficiencies compared to conventional heat transfer mechanisms. These performance characteristics of microwave-assisted gasification are ideal for a modular gasification system in which rapid start up/shut down times and intermittent operation are required. The conversion efficiencies obtained with CO_2 in this study can be improved with addition of other oxidants such as steam or air, which will be the topic of future work.

SESSION 7
GASIFICATION TECHNOLOGIES – 3
Gary Stiegel and Alberto Pettinau

7.1 Neutron-Scattering Diagnostics for Improved Gasifier Modeling

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Coal gasification is a complex process that generates fuel gas mixtures (syngas) from pyrolyzing coal particles in inert or partially oxidizing atmospheres. Gasification reactions are complex processes, and theoretical simulations are critical to 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 the methodology and results of these experiments to produce nonintrusive visualization data and validation information that enables accurate simulations of coal gasification beds. Cold neutrons interact strongly with hydrogen in coal and weakly with the gasifier vessel (metal or quartz), which provides the unique ability to observe in situ coal pyrolysis and gasification. Our strategy involves using neutron radiography and tomography to map reaction levels in the reactor bed with spatial and temporal variations supplemented by additional measurements of outlet gas compositions and characterization of the solid fuel particles. We will present results from measurements at the Center for Neutron Research at NIST and the High Flux Isotope Reactor at Oak Ridge National Laboratory, along with complementary laboratory measurements. With this study, we seek to produce a map of coal pyrolysis within the vessel to improve the bed-scale modeling component of the overall system CFD model.

7.2 Modeling Updraft Moving-bed Gasifier Performance for Industrial Scale CHP Applications

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Ultra-high efficiency (85 to 90+%) coal and biomass gasification systems for industrial scale (2 to 50 MW$_e$) 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 Sotocarbo 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 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 a commercial-scale gasifier for use at Alaska

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 subbituminous coal in a 1-ft ID refractory lined lab scale gasifier at the Sotocarbo Sustainable Energy Research Center plus similar subbituminous 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 are 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 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 design and operation of downstream components. For example, removal of particulates in the raw gas stream exiting the gasifier is necessary prior to cooling the syngas to condense and recover the pyrolysis tar fog using wet electrostatics to obtain the 99.9+% removal efficiency.

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 at the University of Alaska Fairbanks. Both coal and biomass feedstocks possess volatiles which are released within the devolatilization zone of the reactor. The 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 prior to condensing the pyrolysis vapors. Removal of particulate in the raw gas stream exiting the gasifier prior to cooling the syngas is achieved using hot cyclonic separation prior to condensing the pyrolysis vapor and removing/recovering the pyrolysis tar fog using wet electrostatics with a 99.9+% 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.

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 to predict the devolatilization process and pyrolysis liquid yield with high accuracy for all coals.

7.3 Technoeconomic Analysis of Oxygen-Nitrogen Separation from Air for Oxygen Enrichment Using Membranes

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Enriched oxygen is a valuable commodity and has a range of applications in industries such as agriculture, chemical processing, petrochemicals, oil/gas production, petroleum refining and glass industry. Enriched oxygen is essential for the efficient gasification of coal-derived hydrocarbons. Enriched oxygen can be obtained from air using different processes, such as cryogenic distillation, pressure swing adsorption, membrane-based air separation, etc. Historically, oxygen/nitrogen separation from air is done using cryogenic distillation where the air is cooled down to a low temperature so that component gases are recovered at different temperature ranges. However, this process is known to be complex, expensive, and energy intensive and is most economically viable for very large-scale operations. Pressure swing adsorption has also been used for past several decades to produce high purity oxygen by adsorbing nitrogen from air. For this technology, a packed column is used with adsorbents such as zeolite to adsorb nitrogen at one pressure and release the same component at another pressure. The advantage of this process over the cryogenic distillation is this can be modular and can be used in small to medium scale production of oxygen with relatively low hold time. However, pressure swing adsorption incurs very high capital cost as well as high operating cost. The modules are packed with expensive adsorbents with high regeneration energy and they rapidly degrade in terms of their performance over time.

Membrane-based processes for oxygen enrichment are receiving renewed commercial interest. Using membranes, air can be separated into component gases or as an enrichment of one component gas using less energy and less capital cost than the other technologies. Additionally, membrane processes do not require any regenerative steps and the products can be directly used or discharged. In the literature, there are numerous polymeric membranes reported with a range of separation performances. Polymeric membrane materials are desirable for their availability, easy synthesis, cost, and eco-friendliness. Also, polymeric materials are processible and robust and this allows them to be easily manufactured into high surface area membrane modules. However, the principal disadvantage of polymeric membrane approaches is relatively low permeability and selectivity.

Idaho National Laboratory (INL) is developing novel mixed matrix membranes of both thin-dense and phase inverted films of polysulfone loaded with functionalized nanodiamonds. These membranes are being designed to improve selectivity and permeability over the state of art commercial polymeric membranes plus these new mixed matrix membrane formulations can easily be developed into commercial modules for small scale applications. As a part of the commercial viability study of these membranes, a comprehensive technoeconomic analysis was performed to understand the economics of the oxygen enrichment using these membranes. For this analysis, INL developed a spreadsheet based technoeconomic analysis model that considered numerous parameters including selectivity and permeability of the membranes, performance conditions such as number of stages, permeability factor, module material, electricity cost, membrane cost, driving force, etc. INL calculated the cost of production of product oxygen in $/tonne gas product at different oxygen purities and compared that with cryogenic distillation and pressure swing adsorption processes. This analysis also helped to determine the membrane module scale performance targets in terms of permeability and selectivity of the mixed matrix membrane modules to be economical for a small modular coal-fired power plant.

7.4 Hydrogen Enrichment for a Solid Oxide Fuel Cell/Gas Turbine (SOFC/GT) Hybrid Power Generation System Using Mechanical Gas Separation

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A typical high-pressure coal fired gasifier will produce a syngas stream that is comprised mainly of CO, CO_2, H_2O and H_2. These syngas streams can be effectively used to power a Solid Oxide Fuel Cell/Gas Turbine (SOFC/GT) hybrid power generation system. There are two distinct advantages offered by an SOFC/GT hybrid system over a conventional coal fired power generation system that uses a boiler coupled to a steam turbine. The primary advantage is that the hybrid system has a significantly higher efficiency. Studies have clearly shown that the efficiency of a hybrid system can be twice that of a conventional system. Another advantage of a hybrid system is that it's power output can be variable. This would significantly help in addressing the needs which are brought about by a shifting load demand. This advantage is becoming more significant because with increasing penetration of intermittent renewable power sources such as wind turbines and photovoltaic cells, there is a corresponding increase in the variability of power demand. This presents the greatest challenge to conventional coal fired systems and exposes their most severe limitation. Conventional coal fired systems were designed to run optimally for a constant load. When a conventional system deviates from this base load, the already low efficiency is even further reduced. It is therefore desirable that advanced coal fired power generation systems be designed not only to be highly efficient and clean, but also to meet significant variations in power load demands. The SOFC/GT system is expected to be able to achieve both advantages.

The SOFC/GT system efficiency increases with the hydrogen content of the fuel stream. In a pressurized syngas fuel stream, the hydrogen content of the SYNGAS stream can be maximized using a relatively new gas separation technology which removes both H_2O and CO_2 out of the syngas stream thus leaving a fuel stream with a significantly enriched content of H_2. A fuel stream with an enriched H_2 content significantly boosts the SOFC/GT system efficiency by increasing the Nernst potential and the operating voltage. This in turn can prolong fuel cell life by reducing the localized temperature gradients which are associated with reforming and shift reactions inside the fuel cell. This gas separation technology provides a unique opportunity not only to significantly boost the efficiency of an SOFC/GT system, but also to offset the efficiency penalty which is associated with carbon capture. In this work we present calculations of hydrogen enrichment using this novel separation technology. We show how the SOFC/GT system can be used to provide a significantly higher efficiency coal fired system and at the same time reducing the cost of carbon capture.

7.5 Overview of U.S. Department of Energy Office of Fossil Energy's Solid Oxide Fuel Cell Program

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The U.S. Department of Energy (DOE) Office of Fossil Energy (FE), through the National Energy Technology Laboratory (NETL), is leading the R&D of solid oxide fuel cells (SOFC) technology. The mission of the SOFC program is to enable the generation of efficient, low-cost electricity through natural gas-fueled distributed generation (DG) systems in the near-term and coal or natural gas-fueled utility-scale systems with carbon capture and sequestration (CCS) in the long-term. The program supports R&D that addresses the technical and economic barriers to commercial viability, and the development of prototype SOFC power systems that validate those solutions. The program is a unique balance of strategically oriented research and development activities spanning fundamental research to prototype testing. The accomplishments of these activities will be presented.

SESSION 8
COMBUSTION TECHNOLOGIES – 3
Nicholas Siefert and Ting Wang

8.1 CFD Investigation of the Impact of a Pulverized Coal Particles Size on Staged, Pressurized Oxy-Combustion (SPOC)

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Staged, pressurized oxy-combustion (SPOC) constitutes an advanced low-cost, low-emission, and highly-efficient power generation technology, which has demonstrated a promising enhancement to *carbon capture, utilization, and storage* (CCUS). In the SPOC process, pulverized coal is burned under elevated pressures and low flue gas recycle (FGR). This technology is being experimentally developed at Washington University in St. Louis (WUSTL) using a 100 kW lab-scale combustor, in which an oxy-coal flame is stabilized by having a threshold oxygen concentration in the oxidizer streams. In the present computational fluid dynamics (CFD) investigation, the three-dimensional (3D) unsteady *large-eddy simulations* (LES) of a SPOC combustor, with 90 kW of power generated by pulverized coal and 10 kW by methane, are performed by employing the *Dynamic Smagorinsky-Lilly* sub-grid-scale (SGS) turbulence model. A scrutiny of the Lagrangian physical dynamics of the coal particles is presented to better understand particle dispersion in the combustor. The analysis is devoted to the particle residence time and relaxation time as well as of the characteristic fluid time scale, considering their ratio (the Stokes number, St) as a quantitative measure. Investigation of the Stokes number transition, from St < 1 to St > 1, shows that particles smaller than a critical size disperse well due to the eddy motion in the turbulent flow field. Similarly, the study of the oxidation/gasification reactions, with diffusion and surface mechanisms on char combustion, indicates that particles smaller than such a threshold size can completely burnout in the combustor. For larger particles, the initial momentum from the burner influences the particle trajectories by ballistically ejecting the particles with incomplete burnout, which has the potential to cause slagging if not properly addressed

8.2 Commissioning of a Pilot-Scale, Dry-Feed, Pressurized Oxy-Combustion System

Zhiwei Yang, Dishant Khatri, Piyush Verma, Tianxiang Li, Adewale Adeosun, Benjamin M. Kumfer, Richard L. Axelbaum, Washington University in Saint Louis, USA

Concerns over greenhouse gas emissions from coal-based power plants have prompted the development of next-generation coal combustion technologies for CO2 mitigation. First-generation oxy-combustion, which operates under atmospheric pressure, has shown promise for capturing CO2, yet suffers from significant penalties in plant efficiency and cost. By pressurizing the process, i.e., pressurized oxy-combustion (POC), plant efficiency can improve because the latent heat of flue gas moisture can be recovered and integrated into the power cycle. POC also allows for co-capture of SOx and NOx in a simple water wash column, reducing the cost for emission control compared with traditional power plants. Washington University in St. Louis (WUSTL) has proposed an advanced POC technology, namely Staged Pressurized Oxy-Combustion (SPOC), which can further improve the efficiency and operational flexibility of POC, and reduce costs. In this process, pulverized coal is combusted in a pressurized, oxy-combustion environment, which has not been demonstrated in pilot-scale. To address this technology gap, WUSTL designed and constructed a 100 kWth POC facility, which has a unique burner and furnace design. This paper presents the first results of pilot-scale, dry-feed, POC experiments. The commissioning tests focused on exploring flame stability and shape, char burnout and fine particulate matter formation. Testing results suggest that the furnace has exceptionally good flame stability. The flame shape is consistent with the design philosophy and agrees with large eddy simulations. Importantly, complete char combustion can be achieved with an oxygen mole fraction in the flue gas of only 0.8%, as opposed to a required value of 2.5% for conventional atmospheric pressure furnaces/boilers and first-generation oxy-combustion.

8.3 Oxygen Uncoupling and Reduction Reactivity of Mixed Metal Oxides Cu-Fe and Mn-Fe for High Temperature Coal Chemical Looping Combustion

Ping Wang, Department of Energy (DOE)/National Energy Technology Laboratory (NETL); Co-Authors: Nicholas Means, Chemical Engineer, Leidos Research Support Team; Bret Howard, Department of Energy (DOE)/National Energy Technology Laboratory (NETL); USA

Development low cost oxygen carriers (OCs) is important for scaling up and commercializing coal chemical-looping combustion (CLC), which is a promising technology for CO_2 capture during power generation. Mixed Cu-Fe and Mn-Fe oxides have the potential to be produced at low cost from common minerals (ores). This study investigated the oxygen uncoupling and reduction reactivity of synthesized mixed Cu-Fe and Mn-Fe OCs with an inert support (SiO_2 or ZrO_2) at high temperatures. The OCs were prepared using high pressure pelletization followed by calcination at 950 or 1100ºC. Oxygen uncoupling and reduction reactivity of the prepared OCs were evaluated by two cycle tests using a fixed bed reactor - quadrupole mass spectrometer (QMS) system at 950 and 1050ºC. Fresh OCs and the residues remaining after each test were analyzed for their crystalline phase composition by using powder X-ray diffraction (XRD). The Cu-Fe and Mn-Fe OCs underwent oxygen uncoupling and released gaseous O_2, detected by QMS. Cu-Fe OCs had good recyclability of the oxygen uncoupling as compared to the Mn-Fe OCs due to the phase changes of Mn-Fe OCs after re-oxidation. During the reduction of OCs with coal char, the OCs with a ZrO_2 support had a higher CO_2 conversion efficiency than the same mixed metal OCs with an SiO_2 support. The OCs that calcined at 1100ºC and tested at 1050ºC had lower oxygen uncoupling and CO_2 conversion efficiency than the OCs that were calcined and tested at 950ºC.

8.4 Recycle of Oxygen Carriers in Chemical Looping Combustion: Impact of Coal Ash-derived Chemical Impurities

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Oxygen carriers (OCs) for chemical looping combustion (CLC) have long been thought of as a non-renewable material. As a result, much focus has been allotted for the development of attrition resistant carriers that maintain high oxygen transport capacity (OTC) and high reaction rates. Two problems with this approach are that (1) attrition resistance generally requires a highly engineered support material which drives up the cost of manufacture and (2) even with highly engineered materials, attrition is unavoidable and non-negligible. For this reason, a new approach focused on the low-cost recycle of oxygen carriers is introduced here. Of particular interest is the CLC of coal, since the post combustion waste material contains a mixture of coal fly ash and attrited oxygen carriers. A selective recycle process using chemical leaching – similar to coal demineralization – can be utilized to target the active metal oxide of an oxygen carrier. First, highly soluble compounds such as alkalis can be removed using water and low concentration acids. Then the active metal oxide of interest can be targeted with an acid (or another solvent) that features favorable leaching kinetics with the given metal oxide. Ideally, compounds of low leachability (i.e. Al and Si based compounds) are left in the solid phase. The goal of this work is to investigate the limits of OC recycle with an understanding that simple, low-cost recycling processes generally do not yield high-grade purity. The limits of oxygen carrier recycle are evaluated by assessing oxygen carrier performance after "poisoning" carriers with metal oxides (MeO) that are present in coal ash and that are difficult to separate from the metal oxide system that is responsible for oxygen transport. In the study reported here, cupric oxide (CuO) is the active metal oxide system of interest.

Cupric oxide oxygen carriers were synthesized to give a loading of 30wt% CuO (supported on porous silica) under ideal circumstances. The copper nitrate solutions used during synthesis by dry impregnation were "poisoned" with metal nitrates of the major components in fly ash (Al, Ca, Fe, K, and Na oxides). These compounds represent the impurities that might be removed during nitric acid leaching – a favorable technique for Cu recovery. The loading of each metal nitrate was chosen based on the composition of Powder River Basin coal ashes in combination with literature on the leachability of each major component from fly ashes. Upon calcination, the metal nitrates decompose into metal oxides. The binary pairings of CuO with each ash-derived metal oxide were evaluated based on oxygen transport capacity (OTC) – the weight percentage of an OC available as transportable oxygen, and the oxygen coupling-uncoupling rates. The non-CuO metal oxides were in low concentration with the highest MeO to CuO ratio being 1:20 and the lowest being 1:400. The pure CuO oxygen carrier suffered a near 50% loss in OTC – relative to the ideal case – likely due to sintering effects – a common issue encountered with cupric oxide oxygen carriers. The binary addition of each non-CuO metal oxide caused changes in OTC ranging from a 30% decrease to a 60% increase compared to the pure CuO carrier. The addition of calcium and iron improved the OTC in all cases whereas aluminum had no effect. The alkali compounds (Na and K) had a negative impact on particle performance except at very low concentration (1:400). The results presented in this study help to understand how the ash-derived metal oxides impact oxygen carrier performance and they indicate the allowable level of each

compound that can be present during oxygen carrier synthesis. Though this study is specific to silica-supported CuO oxygen carriers, the framework can be applied to any oxygen carrier synthesis technique that involves solution-based precursors. The implementation of oxygen carrier recycle has the potential to decrease the overall cost of oxygen carrier manufacture and improve the economic outlook of the chemical looping combustion of coal.

8.5 Process Design and Analysis of a Novel Carbon-Capture-Ready Process for Flexible-Load Power Generation: Modular Pressurized Air Combustion

Piyush Verma, Zhiwei Yang, Washington University in Saint Louis, Saint Louis; Scott Hume, Andrew Maxson, Electric Power Research Institute, Inc.; Richard L. Axelbaum, Washington University in Saint Louis; USA

The rapid retirement of dispatchable, fossil-based electricity sources and the influx of intermittent energy sources, both driven by the impetus towards a low-carbon future, have led to concerns about the reliability of the grid. The future need for on-demand, rotating, inertial-based assets that can be low carbon and flexibly meet changing demand to balance against intermittency will be essential. Hence, future fossil-based power generation will need to be highly efficient and flexible, and have the ability to add carbon capture when required. In this study, the process design of a modular pressurized air combustion power plant, which involves burning coal in air under pressure in parallel, modular boilers is described. After treatment, the high-pressure flue gas is passed through a series of turbines and inter-heaters to recover most of the compression work. The high-pressure operation allows for thermal recovery of the latent heat of moisture of the flue gas by integration into the steam cycle, which results in a plant efficiency that is 1.7% higher than that of the conventional atmospheric air-fired power plant. Moreover, the modularity enhances the flexibility of the power plant, with an improved ability for load following. This work also discusses the path to convert the modular, pressurized-air combustion process to a staged, pressurized oxy-combustion process, which is one of the most promising carbon capture processes. This can be accomplished by adding a frontend air separation unit and a backend CO_2 compression and purification unit.

SESSION 9
CARBON MANAGEMENT – 3
Omar Basha and Ahmed Aboudheir

9.1 Synthesis of Tri- and Tetra-esters for Use as Physical Carbon Capture Solvents

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The specific interaction of CO_2 molecules with Lewis base groups, especially carbonyl groups, has also been utilized in the design of CO_2-philic materials. This CO_2/Lewis base interaction with various functional groups containing carbonyl moieties particularly acetate groups has suggested that maximizing the number of acetyl groups in a particular molecule, while maintaining favorable properties such as viscosity and hydrophobicity, could result in useful physical solvent for CO_2. Computational experiments at NETL have identified a family of di-esters which show promise as physical solvents for CO_2, but more recently some common precursor molecules were identified which could provide easy access to small tri- and even tetra-ester products. In this work, the synthesis of 6 tri-esters and 3 tetra-esters are reported. The relevant physical properties, such as viscosity and density, of these solvents were obtained and the CO_2 and H_2O absorption of these solvents were measured by gravimetric absorption on a Hiden IGA system. The results show that these solvents absorb comparable amounts of CO_2 from 25 – 70°C, while absorbing far less H_2O, even at 80% relative humidity in N_2 compared to known physical solvents such as propylene carbonate. Computational values for the prepared solvent molecules, including partial atomic charges and CO_2-carbonyl interaction energies, support the acetate carbonyl groups as the likely sites of CO_2 interaction.

9.2 Joint Study to Develop an Integrated Commercial Scale CCUS Project in the Ordos Basin Presenting

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This research is supported by the Advanced Coal Technology Consortium of US-China Clean Energy Research Center. The goal of the project is working closely with Chinese partners to build a scientific, technological, and engineering framework necessary for a commercial-scale integrated carbon capture, utilization, and storage (CCUS)

demonstration project including CO_2 utilization (enhanced oil recovery- EOR and enhanced water recovery - EWR), and geological storage. The two major objectives of the project are: (1) utilize CO_2 from the coal-to-chemical industries to support CO_2-EOR/EWR projects, and (2) integrate CO_2-EOR/EWR with commercial-scale CO_2 storage. The ultimate goal of the proposed joint research is to develop commercial-scale integrated CCUS demonstration projects in the Ordos Basin and Wyoming Laramide basins.

One of the biggest challenges for developing a sustainable low carbon economy is a dual one: the need to meet rising energy demand while at the same time reducing carbon emissions. To maintain a health and environmentally friendly energy industry future, fossil energy rich regions, such as Wyoming in the United States and the Ordos Basin in China whose economies highly depend on fossil energy industry developments, must attract innovative techniques.

The CCUS has been suggested as one of viable components in a multi-level approach to reduce greenhouse gas in the atmosphere. Even though CCUS has been explored for a long time and is regard as mature technologies in various levels, research gaps and opportunities remain to improve performances, reduce costs, discover new utilizations, and implement regulatory frameworks and international standards to reduce uncertainty in permitting and operation of CCUS projects.

The overlapping development of relatively new coal conversion industries with existing oil and gas industries in the Ordos Basin, China has created a unique opportunity to apply the systematic approach developed in Wyoming: the integration of geological CO_2 storage, enhanced oil recovery (CO_2-EOR) and enhanced water recovery (CO_2_EWR) using anthropogenic CO_2. The results of static and dynamic modeling from this project show that concurrent with the enhanced oil recovery, about half of the injected CO_2 remains in the subsurface during the CO_2-EOR process, while produced CO_2 recycled and recompressed for reinjecting back into the reservoirs. At the completion of production, the EOR project has significant potential to permanently store CO_2 in the depleted oil fields.

One of the greatest strengths of this integrated systematic approach is the cost advantage and sustainability. The integrated approach is considered as the most effective pathway with very high Technology Readiness Levels for large-scale mitigation of CO_2, especially for high-purity CO_2 stream available from the coal conversion plants. In the Ordos Basin, the well-developed coal chemical industry could provide a large volume (over 50 Mt annually) of high-concentration CO_2 (>95%) as a result of the industrial separation during coal gasification/ liquefaction processes. High-concentration CO_2 stream from the coal conversional process requires much less capture effort and reduce costs of CCUS projects dramatically. Compared with other CCS projects, the ability to use CO_2 from the coal conversion industry for CO_2-EOR/EWR and geological CO_2 storage makes these projects in the Ordos Basin more economically feasible and technologically efficient.

In this presentation, we will present a case study to develop a commercial-scale integrated CCUS project in the Ordos Basin with a description of opportunity and challenge for developing a commercial-scale integrated CCUS project based on the results of laboratory experiments and numerical CO_2 injection simulations.

9.3 CO_2-Fracturing Fluid Driven Geochemical Alterations at the Shale Matrix-Fracture Interface

Angela Goodman, Sean Sanguinito, Patricia Cvetic, Barbara Kutchko, United States Department of Energy, National Energy Technology Laboratory; Sittichai Natesakhawat, University of Pittsburgh; USA

With a high demand for an economic energy source but also a concern for increasing greenhouse gas emissions, there is growing consideration in shale production for processes including 1) enhancing hydrocarbon recovery via CO_2 flooding, 2) using CO_2 as a fracturing agent to reduce water usage, and 3) storing CO_2 in shale formations to manage the environmental impact of emissions. To increase fundamental understanding of the reactions that will occur between CO_2, shale, and water/fracturing fluid, we use in situ Fourier Transform infrared spectroscopy, (FTIR), feature relocation scanning electron microscopy (SEM), and surface area and pore size analysis using volumetric gas sorption. Samples from the Eagle Ford and Barnett Shales are analyzed with these techniques with exposure to dry CO_2, CO_2 and water, and CO_2 and a synthetic fracturing fluid. These analyses indicate geochemical reactions are directly related to the mineralogical composition of the shale formation, especially carbonate rich shales. Shales targeted for CO_2-EOR or CO_2 storage will experience two waves of chemical reactivity from fracturing fluid (pH of ~2) as well as carbonic acid (pH of ~5.6). This dual reactivity mechanism drives dissolution and precipitation processes, altering petrophysical properties of the shale, and leading to a significant impact on flow pathways. Barite formation occurs on nucleation sites such as dissolved calcite but is absent on more resistant minerals such as apatite. Sulfur, most likely sourced from kerogen, is readily available for reaction and forms gypsum when shale samples are exposed to carbonated water and forms barite when shale samples are exposed to

fracturing fluid. The abundance reactivity observed in these samples impacts the fracture and matrix interface and altering potential flow pathways in the shale.

9.4 Observed Variation of CO_2-Brine Contact Angles on Sandstone

Foad Haeri, Deepak Tapriyal, Sean Sanguinito, Fan Shi, National Energy Technology Laboratory; Samantha J. Fuchs, The University of Texas at Austin; Laura Dalton, John Baltrus, Bret Howard, Dustin Crandall, Christopher Matranga, Angela Goodman, National Energy Technology Laboratory; USA

In this study, contact angles were measured for CO_2 bubbles on six different sandstones (Navajo, Nugget, Bentheimer, Bandera Brown, Berea, and Mt. Simon) that could potentially represent properties of CO_2 storage depositional environments. The impacts of pressure and temperature were studied by focusing on the CO_2 phase behavior in three different scenarios: gaseous, liquid, and supercritical conditions. Despite controlling the sample preparation and cleanliness, CO_2-brine equilibration conditions, and pressure and temperature, there were inconsistencies in contact angle trends that could largely be attributed to natural sample heterogeneity resulting from localized variations in topography, surface roughness, and mineral composition across the surface. By analyzing more than 1100 measurements, there seemed to be a distribution of angles for all CO_2 droplets with a mean of $22°$. The majority of angles were between $10°$ and $40°$, representing strongly to moderately water-wet behavior. Additionally, super-critical CO_2 showed to be more wetting than liquid or gaseous CO_2. Other factors to consider for a better understanding would be CO_2 adhesion to the rock, chemical reactions at the three-phase contact line, rock surface charge density and ionic strength of the aqueous phase (brine), exposure time of rocks to CO_2, and a closer examination of roughness.

9.5 Valorization of CO_2 Emissions of Steam Methane-Reforming with Co-Production of High-Value Carbon Materials Via MW Plasma

Aayush Mantri, Vignesh Viswanathan, George Skoptsov, President & CEO, H Quest Vanguard, Inc., USA

In 2019, the global fossil-fuel carbon emission estimate stood at 36.8 billion metric tons of CO_2, with over 2% of this amount (0.83 billion metric tons CO_2/year) directly attributable to industrial H_2 production from fossil fuels for petroleum refining, petrochemistry, and fertilizer production. In the US, natural gas is used almost exclusively as feedstock for on-purpose hydrogen production with the steam methane reforming (SMR) process, emitting as much as 25 tons of CO_2 per MMscf of H_2 produced. Given the high yield of H_2, its comparatively low energy requirements, and the already existing vast capacity, fossil-fuel sourced hydrogen production is unlikely to be replaced in the next two decades. Substantial reduction of these associated emissions is impossible without retrofitting the existing processes in a way that is technologically viable and economically attractive.

H Quest Vanguard, Inc. has developed a plasma-catalyzed chemical conversion platform that can enable utilization and conversion of the CO_2-rich exhaust streams from SMR plant hydrogen separation units directly into premium carbons and value-added hydrocarbons (acetylene, ethylene, aromatics). H Quest's electrically-driven process relies on microwave plasma to operate at mild bulk temperatures (~500 C) and near ambient pressure (1~2 atm), lending itself to small-scale, low-cost, and modular deployment without the need for extensive balance of plant installations. Microwave plasma provides a non-uniform, non-equilibrium distribution of energies, with reactions driven by electron kinetics rather than thermodynamics, and allowing rapid quenching of desired products almost immediately after formation. Thus, this process enables reaction pathways that are not easily accessible to conventional chemical processes. More generally, microwave plasmas offer reaction intensification, opening opportunities for reducing system costs and producing portable, modular reactor systems.

The ruggedized microwave reactor system developed at H Quest sidesteps limitations that typically constrain the scale-up and long-term operation of microwave plasma conversion processes. Proof-of-concept, unoptimized CO_2 conversion trials have shown energy requirements <3 kWh/kg-feed conv., with conversion rates >50%, along with a decreasing trend in specific energy requirements, as the process and reactor have matured. These studies have also demonstrated feasibility of utilizing the CO_2 as replacement for the expensive inert plasma support gases (eg: Ar), typically used in the process. Furthermore, the process has proven to be agnostic to the composition of the hydrocarbon feed stream, demonstrating direct, single-step conversion of varying streams of pure methane, ethane, propane, carbon dioxide, and mixtures thereof to higher hydrocarbons (acetylene, ethylene, and aromatics), hydrogen, and high-structure high-purity carbon. This versatility enables any upstream processes to which it may be paired.

This novel approach allows utilization of an otherwise harmfully wasted (or at best sequestered) chemical feedstock (carbon dioxide) in production of value-added products - platform chemicals and high value carbons used in fuels, energy storage and advanced

manufacturing applications. The deployment of these modular systems within industrial SMR plants may substantially reduce (up to 25%) the CO_2 footprint of hydrogen production, while production of premium carbon black, graphene nanoplatelets, and synthetic graphite precursors would further contribute to indirect reduction of emissions by displacing legacy carbon black and graphite burdened with a high CO_2 footprint. The by-product credit from these products will provide a further economic incentive to refiners, and industrial hydrogen producers to meet their zero emission goals.

SESSION 10
SUSTAINABILITY & THE ENVIRONMENT – 1
Leslie Ruppert and Evan Granite

10.1 Net Zero Operation of Coal-Fired Power Plant Using Surplus Renewable Energy

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In order to introduce a large amount of renewable energies, such as wind and solar power, the thermal power plants are requested to operate as a backup of intermittency of the renewable energies to maintain the frequency and demand-supply balance of the power grid. Since coal-fired power plants contribute to the frequency stability at the minimum load condition during the power output from the renewable energy exceeds power demand, lower minimum load is responsible for more introduction of renewable energies to the power grid. Net zero power output condition of the coal-fired power plant is considered in this paper; the power output of synchronized generator (gross power output) is 5% of the rated power output. At net zero power output condition, active power(kWh) is no longer delivered from the power plant, however the other values of the plant, such as an inertia, a reactive power, a speed governing operation, etc. that can contribute to stabilize the frequency is conserved in the power grid. Coal no longer cannot use because the power output is too low to maintain the stable burning of coal, thus the oil is supplied as a fuel at net zero power output condition. A 700MW- class super-critical coal-fired power plant is described. Temperatures/pressures of the high-pressure steam turbine (HP-ST) and the intermediate-pressure steam turbine (IP-ST) at rated power output (100% load) are 538°C/24.2MPa and 566°C/4.1MPa, respectively. At net zero power output condition, the power output of synchronized generator is 35MW (5% load), and the temperatures/pressures of the HP-ST and IP-ST are 465°C/7.85MPa and 455°C/0.49MPa, respectively. HP has a bypass to the re-heater, whereas the IP has one to the condenser. Material and heat balance at net zero power output (gross output is 35MW) of the coal-fired power plant is estimated. Calculated gross efficiency (fuel to synchronized generator efficiency) at 35MW output power is 29.6%. Energy input by oil at 35MW power output is replaced by surplus electricity from renewable energies. In the case that the surplus electricity of 100MW is supplied to the coal-fired power plant, the oil flow rate decreased to almost zero; the coal-fired power plant is operated by the surplus electricity only at this condition. The efficiency at 35MW power output condition gains with the increase of the surplus electricity because the energy loss of the exhausted gas is minimized. The coal-fired power plant could effectively contribute to stabilize the frequency of power grid by its inertia, non-reactive power, etc., without coal or oil (without emitting CO_2) during the period that the power output of renewable energy exceeds the power demand.

10.2 Country-specific Role and Value of Carbon Capture and Sequestration in the Power Systems

Yoga Wienda Pratama, Niall Mac Dowell, Centre for Environmental Policy – Imperial College London, UK

Delivering the Paris Agreement will require a rapid transformation of global energy systems, with the power sector become a key for this transition. Since 2015, there has been significant ambitious net zero targets around the globe. Although the share of fossil fuel in the world's energy consumption has been slightly reduced from 86% 5 decades ago to approximately 81% recently, the evident inertia of the global energy system due to the increasing demand requires us to find a pragmatic solution which must be socially equitable, technically feasible, and financially viable. Among many options, carbon capture and sequestration (CCS) is a key.

CCS is a mature technology which allows sustainable use of fossil and biomass energy resources. The technology can deliver near zero emissions electricity from fossil fuels and is also key to the carbon dioxide removal (CDR) services required to meet the Paris

agreement. However, deployment of CCS has been frequently hindered by perceptions of cost. Moreover, given the rapid cost reduction of intermittent renewable energy sources (iRES), such as wind and solar power, their combination with energy storage technologies is frequently cited as a cost-effective strategy to completely displace fossil energy.

The purpose of this study is to quantify and qualify the role and value of CCS technologies in the electricity system in several key regions around the world, which includes the United Kingdom, Poland, New South Wales in Australia, and the Java-Madura-Bali (JAMALI) system in Indonesia, also the Electric Reliability Council of Texas (ERCOT) and the PacifiCorp East (PACE) grids in the United States of America. To deliver this study, the Electricity Systems Optimisation (ESO) framework was used. ESO is a hybrid capacity expansion and unit commitment model which allows electricity system transitions analysis. ESO is an optimization framework to minimise the cost of system transition while satisfying the grid technical requirements and emission targets. In each case study, a reference scenario, with no emissions target, was developed – Business As Usual (BAU). Then, three scenarios with net zero emissions target by 2050 being imposed were developed, which includes: 1) All Technologies which allows the deployment of all technologies including CCS-equipped power plants, nuclear, iRES, and storage, 2) No CCS – similar to All Technologies but without CCS, and 3) Renewables and Storage scenario which only permits the new deployment of iRES and energy storage technologies.

The core overarching conclusion of this work is that CCS is consistently critical to delivering a resilient and cost-effective zero emissions electricity system. All case studies consistently show that the absent of CCS increases the cost of delivering a net zero system by between two and seven times more expensive compared to the solution with CCS. This study also finds that the highly seasonal power demand may improve the value of CCS due to a stronger requirement of flexibility capability in load following manner. Accordingly, electrification of other sectors in the future, such as heating or transport, can potentially advance this value proposition.

The results also reveal that the No CCS and Renewables and Storage scenarios require an exceptional rate of deployment of iRES and storage technologies. In the BAU and All Technologies scenarios, technology deployment rates were considered to be in line with the historical rates for each region. This is important as the deployment of power generation assets may be unlikely to be able to significantly increase in the short term due to the requirement of integrated value chain. Despite the significant build-rate constraint relaxation, scenarios without CCS cannot match the level of system's reliability can be achieved by system with CCS.

A final important conclusion from this study was that CCS appears to not in competition with iRES deployment as the two technology clearly plays distinct and not competing roles in the system. Thanks to their near-zero marginal cost, iRES will be dispatched ahead of CCS power in all case studies even if the 45Q and 48A tax credits for CCS in the US were included. Those tax credits mechanisms can privilege CCS-equipped coal, gas and biomass over their unabated counterparts, but not over the renewable alternatives. Hence, it is not a case of "CCS or renewables", but rather one of "CCS and renewables".

10.3 Potential Oil Supply and CO2 Demand from CO2 Enhanced Oil Recovery in the United States

David Morgan, Travis Warner, Donald Remson, National Energy Technology Laboratory, USA

The capture of carbon dioxide (CO_2) from industrial sources of CO_2 combustion, such as coal and natural gas fired power plants, and the injection of this captured CO_2 into deep subsurface formations is an important tool for reducing the emission of CO_2 to the atmosphere. There are two methods of injecting large volume of CO_2 into the subsurface: 1) injection of CO_2 into deep saline formations (CO_2 saline storage) and 2) CO_2 enhanced oil recovery (EOR). When CO_2 is injected deep enough into the subsurface, the CO_2 becomes supercritical and supercritical CO_2 is miscible with many crude oils. The mixing of CO_2 with oil can facilitate the production of additional oil after water flooding can no longer produce economically viable levels of oil. During CO_2 EOR, some of the injected CO_2 is eventually produced with oil and brine, but this CO_2 is separated and recycled. Consequently, almost all the purchased CO_2 remains in the subsurface at the end of CO_2 EOR operations. From the perspective of a source of CO_2, CO_2 EOR is a more attractive option for storing CO_2 because a CO_2 EOR operation will pay for CO_2 while a CO_2 saline storage operation must be paid to store CO_2. The recently enacted 45Q tax incentives for CO_2 storage improve the situation marginally for CO_2 saline storage, but CO_2 EOR is almost always a more attractive option for a CO_2 source. As such, it is important to understand the potential to produce oil and utilize CO_2 for CO_2 EOR in the United States (US). This paper presents the results of a study where the potential to implement CO_2 EOR in oil fields in the US was assessed. The Energy Information Agency (EIA), which is part of the US Department of Energy (USDOE), maintains a dataset of conventional oil fields in the US. The National Energy Technology Laboratory (NETL), which is within the Office of Fossil Energy (FE) in

USDOE, recently finalized two tools for analyzing CO_2 EOR: 1) the FE/NETL CO_2 Prophet Model, which is a streamline/stream tube model for simulating oil production from CO_2 EOR, and 2) the FE/NETL Onshore CO_2 EOR Cost Model which uses input and output fluid flows generated by the FE/NETL CO_2 Prophet Model for a pattern (such as a five-spot pattern), implements patterns over time across the oil field and calculates cash flows for revenues and costs for the oil field. A critical cash flow is net earnings which is defined as revenues from oil sales minus costs, which includes capital costs, operations and maintenance (O&M) costs, royalties, state and local taxes, and federal income taxes. When discounted and summed the result is total present value net earnings (TPVNE). If TPVNE exceed zero, then the CO_2 EOR operation covers all costs and meets the minimum desired return on equity for the project. The FE/NETL Onshore CO_2 EOR Cost Model can calculate the first-year break-even price of oil, which is the lowest price of oil in the first-year of the project such that the TPVNE equals (or slightly exceeds) zero. The FE/NETL Onshore CO_2 EOR Cost Model can also calculate the first-year break-even price of CO_2, which is the highest price of CO_2 in the first-year of the project such that the TPVNE equals zero. The first-year break-even oil price was calculated for all the oil fields in the EIA oil field dataset where the oil is amenable to CO_2 EOR. These results were used to generate oil supply curves as a function of CO_2 price for the US. As the price of oil increases, the potential volume of oil that can be produced economically increases. Conversely, as the price of CO_2 increases, the volume of oil that can be produced economically decreases since CO_2 is a cost to the CO_2 EOR operation. The first-year break-even CO_2 price was also calculated for these same oil fields. These results were used to generate CO_2 demand curves as a function of oil price for the US. As the price of oil increases, the demand for CO_2 increases since CO_2 EOR becomes economically more attractive as the price of oil increases. Because the produced oil is eventually combusted, which forms CO_2, the storage of CO_2 as a function of oil price is shown along with the net CO_2 stored (i.e., CO_2 stored minus the CO_2 emitted to the atmosphere when the oil is combusted). While the current price of oil is low relative to historic oil prices, the Coronavirus pandemic will not last forever. The EIA projects that oil prices will rise over the next 30 years to about $100/STB in constant 2019 dollars. If oil prices rise like this, the opportunities for economically viable CO_2 EOR will increase and the demand for captured CO_2 for CO_2 EOR will likely increase.

10.4 Technoeconomic and Life Cycle Analysis of Bio-Energy with Carbon Capture and Storage (BECCS) Baseline

Timothy Fout, Timothy J. Skone, National Energy Technology Laboratory; Kyle Buchheit, Engineer, KeyLogic, Inc.; Eric Lewis, Engineer, Deloitte Consulting, LLP; Kishore Mahbubani, Derrick Carlson, KeyLogic, Inc.; USA

Part of the mission of the U. S. Department of Energy (DOE) is committed to clean coal technology and to reviving America's coal industry. This mission not only focuses on technologies stimulating the economy and providing a boost in domestic energy production, it also requires these technologies provide a responsible stewardship of the environment. Protecting clean air and clean water, conserving our natural habitats, and preserving our natural reserves and resources remains a high priority. In order to pursue this mission, the U.S. DOE Office of Fossil Energy, in conjunction with its National Energy Technology Laboratory (NETL), conducts research, development, and demonstration of advanced fossil-based power generation technologies capable of utilizing domestic energy resources in an environmentally-responsible manner.

The co-firing of biomass with coal is an option of increasing importance with respect to CO_2 emissions as biomass regrowth can remove CO_2 from the atmosphere, thereby offsetting the emissions produced through combustion of biomass. When combined with carbon capture and storage (CCS) the overall system has the potential to be carbon negative. This presentation will discuss the application of bio-energy with carbon capture and storage (BECCS) through both technoeconomic (TEA) and life cycle analyses (LCA). LCA is essential to full evaluate any potentially carbon negative technology in order to determine the true impact of the system. Results from the study will be used not only to evaluate the potential of co-firing coal with biomass but also will serve as the basis for evaluating new technologies that can be applied to a BECCS system to further increase performance or decrease cost. The BECCS-pulverized coal systems modeled utilized a high sulfur bituminous coal and a hybrid poplar biomass for the feed due to its ability to be cultivated as a short rotation crop on marginal lands and its characterization as a non-food source. The percentage of biomass in the plant feed was varied up to 49% in the TEA study and supplemented by two 100% biomass cases for the LCA. All cases in the TEA were modeled with and without 90% capture through a state-of-the-art amine-based capture system. Results of the analysis will be focused into 3 primary categories; Performance, Economics and Environmental. System efficiency, direct emissions, LCOE, capital cost, CO_2 breakeven value and total system environmental impacts will all be covered in this presentation.

10.5 Evaluating Capacitive Deionization and Zeolite Dewatering as Effective Treatment Options for CO_2 -Enhanced Water Recovery Streams

Ayokunle Omosebi, Jinwen Wang, Kunlei Liu, University of Kentucky, USA

Enhanced water recovery couples subsurface CO_2 injection and storage with brine displacement, where the produced water can be treated for human consumption or beneficial use in the power generation, industrial or agricultural sectors. [1] However, sub-surface water can vary widely by location, ranging from a few parts-per-million to several parts-per-thousands in their concentration of total dissolved solids (TDS) [2]. Pressure-driven polymeric membrane technologies, including reverse osmosis, are ubiquitous, but cost-effective at brackish (10,000 ppm) to seawater concentrations (35,000 ppm), allowing for more customized and enhanced treatment options outside of those ranges. At low concentrations, significant energy is used in pressure-driven separation to push water relative to the low level of impurities, while at high concentrations, the mechanical stability of the polymer membranes becoming problematic due to high osmotic pressure requirements. Processes, including electrodeionization and multistage flash distillation, are alternatives for treating low and high salt content streams, respectively, but their energy requirement can still be significant.

University of Kentucky's Center for Applied Energy Research (UK CAER) is currently exploring zeolite dewatering (ZDW) and capacitive deionization (CDI) as treatment options for hyper-saline and brackish level TDS streams. The ceramic zeolite membranes are pressure-stable and can leverage mild temperatures (<120 °C) to effectively treat hypersaline streams at low pressures, while CDI employs electricity input to specifically target salt impurities, removing them from solution at a low energy cost requirement. [3]. Coupled together, the CDI downstream of the zeolite unit can further polish the ppm level ZDW effluent stream for TDS sensitive applications. Current results show salt adsorption capacities > 8 mg/g for CDI at 1.2 Volts, while ZDW provides a water flux of ~ 5 kg/[m²-hr] at 80 psig. Progress on the stability and limitations of these systems will be discussed.

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SESSION 11
CLEAN COAL AND GAS TO FUELS – 1
Atsushi Ishihara and Diane Revay Madden

11.1 Hydrodeoxygenation of Dibenzofuran Over Boron-promoted Ni/SiO₂ Catalysts

Di Liu, Zhen-yi Du, Jie Feng, Wen-ying Li, Taiyuan University of Technology, CHINA

Dibenzofuran (DBF) is a typical representative of furan compounds in coal tar due to its high content and low reactivity. Hydrodeoxygenation (HDO) of dibenzofuran produces hydrocarbon compounds with high H/C ratio, which can be used as fuel oil products. This work aimed to design efficient and promising noble-metal-free catalysts. In this work, Ni/SiO₂ catalysts with different B addition contents were prepared and their catalytic performance was tested in a batch reactor at 280 °C ,6 MPa for 3 h. The Ni-xB/SiO₂ catalysts were synthesized by incipient wetness impregnating SiO₂ support, with different amounts of $Ni(NO_3)_2 \cdot 6H_2O$ and boric acid as the precursors. The catalysts were systematically characterized using XRD, N_2-adsorption desorption, NH_3-TPD techniques. The results showed that the addition of an appropriate amount of B promoted the conversion of DBF and significantly increased the yield of BCHs (including bicyclohexyl and cyclopentylmethyl-cyclohexane). It is particularly remarkable on the catalyst with a Ni/B atomic ratio of 1, and the yield of BCHs can reach 99.2%. Compared with the Ni/SiO₂ catalyst without B addition, the yield of the target product was increased by nearly 50%. Boron oxide loaded on the surface of SiO₂ can generate Lewis acid sites, which are conducive to the adsorption of reactants and promote the breakage of C-O bonds. In addition, the addition of B promotes the dispersion of Ni and exposes more active sites for deoxygenation, promoting the occurrence of the hydrodeoxygenation reaction.

11.2 Phenanthrene Hydrogenation Saturation over Ni/NiAl2O4 Catalyst Prepared by Modified Sol-gel Method

Dao-Cheng Liu, Jie-Ying Jing, Jiu-Zhan Wang, Jie Feng, Wen-Ying Li, Taiyuan University of Technology, CHINA

Hydrogenation of polycyclic aromatic hydrocarbons in coal tar to cycloalkanes added in the jet fuel can significantly enhance the utilization efficiency of coal resource. In this work, phenanthrene, one of the typical polycyclic aromatic hydrocarbons, was served as the model compound to investigate the hydrogenation mechanism. According to thermodynamic analysis, it is found that low temperature and high hydrogen pressure are favorable for the hydrogenation process. However, kinetic analysis indicates that the saturation process from octahydrophenanthrene to perhydrophenanthrene remains a challenge, which is ascribed to the steric hindrance of macromolecular itself and the competitive adsorption among saturated products. Ni-based catalyst, a low-cost alternative to noble metal catalyst, is usually difficult to obtain a fully saturated product because of its lower hydrogenation saturation performance. To improve the activity of Ni-based catalyst, a series of $Ni/NiAl_2O_4$ catalysts with different Ni dosage were synthesized by modified sol-gel method. Compared with the catalysts obtained by impregnation method, the catalyst prepared by modified sol-gel method could efficiently convert phenanthrene into perhydrophenanthrene. Furthermore, as the Ni dosage increased, the catalyst with 15% Ni loading obtain the highest phenanthrene conversion (91%) and perhydrophenanthrene selectivity (60%), which was higher than that of $1.5wt\%Pt/\gamma-Al_2O_3$ (32% perhydrophenanthrene selectivity). The higher hydrogenation saturation performance was closely related to the preparation method. The modified sol-gel method could strengthen the interaction between the Ni nanoparticles and the $NiAl_2O_4$ support, which could favor the formation of Ni nanoparticles in electron-deficient state and consequently facilitate the adsorption and activation of polycyclic aromatic hydrocarbons.

11.3 Effect of Ni2P Loading on the Structure and Phenanthrene Hydrogenation Saturation Performance of Ni2P/ Al2O3 Catalyst

Jiu-Zhan Wang, Dao-Cheng Liu, Jie-Ying Jing, Zhi-Fen Yang, Jie Feng, Wen-Ying Li, Taiyuan University of Technology, CHINA

Phenanthrene, a typical polycyclic aromatic hydrocarbon in coal tar, has an annual output of 900,000 tons. However, it has not been reasonably used due to the absence of the effective approaches. In recent years, phenanthrene hydrogenation was found to be a promising way to use phenanthrene. The perhydrophenanthrene derived from saturated hydrogenation of phenanthrene are ideal components for high-performance jet fuel. The key point to realize the above process is how to develop an efficient catalyst to overcome the steric hindrance in the process of phenanthrene hydrogenation saturation. Due to its special electronic structure and morphology, Ni_2P catalyst has received widespread attention in the field of hydrogenation. The electron-deficient structure of Ni in the Ni_2P catalyst is conducive to the adsorption and hydrogenation of polycyclic aromatic hydrocarbons. In addition, our previous work showed that the Ni_2P/Al_2O_3 catalyst prepared by decomposition of hypophosphite method possessed high active metal dispersion, and the hydrogenation performance is closely related to the content of Ni_2P active phase. In this work, a series of Ni_2P/Al_2O_3 catalysts with different Ni_2P loadings were prepared by decomposition of hypophosphite method and the influence of Ni_2P loading on the structure of Ni_2P/Al_2O_3 catalysts and their phenanthrene hydrogenation saturation performance was investigated. Results show that Ni_2P loading can affect the selectivity of perhydrophenanthrene. When the hydrogenation saturation reaction was performed at 320 ºC, 5 MPa, H_2/oil volume ratio of 600, and a weight hourly space velocity (LHSV) of 50 h^{-1}, 97% phenanthrene conversion and 95% selectivity to perhydrophenanthrene was achieved over Ni_2P/Al_2O_3 catalysts with 10 wt% Ni_2P loading. With the increase of Ni_2P loading, the perhydrophenanthrene selectivity of the catalyst gradually decreased. When the loading reached 25%, the selectivity of perhydrophenanthrene was only 40%, while the conversion of phenanthrene does not change much. It is found that the higher phenanthrene conversion and perhydrophenanthrene selectivity was due to the smaller particle size of the catalyst and lower active metal electron density.

11.4 Hydrothermal Synthesis of Efficient NiMoS/SBA-15 Catalysts for the Hydrodesulfurization

Tian-You Cui, Antony Rajendran, Wen-Ying Li, Taiyuan University of Technology, CHINA

The sulfur containing liquid feedstocks derived from the coal liquefaction emits the SO_x gases which heavily disrupts the environment and the human health. In addition, the presence of sulfur compounds in the feedstocks deactivate the hydrorefining catalysts through catalytic poisoning. Therefore, the ultra-deep removal of sulfur from the coal-derived liquid oils has received a paramount attention to meet stringent rules imposed on the permissible sulfur level in the liquid fuels. The current industrial process (hydrodesulfurization (HDS)), despite its higher efficiency towards the removal of low-boiling sulfur compounds (e.g. sulfides), is not efficient enough to accomplish the complete removal of refractory sulfur (RS) compounds usually represented by the family of dibenzothiophene (DBT) compounds. To attain the efficient removal of RS compounds by HDS, the catalytic design is being considered as the promising strategy. The efficiency of traditional HDS catalysts can be influenced by controlling the factors such as morphology, edge sites, slab length and stacking numbers. In this report, hydrothermal method which uses the chelate precursor ($Ni(acac)_2$) has been attempted to prepare a new type of HDS catalyst (NiMoS/SBA-15). With this method, the active phases are dispersed and especially, the additional sulfidation process is evaded. The used chelating precursor suppresses the formation of nickel-based inactive phases (e.g. Ni_3S_2). The prepared catalyst shows the nanosheet morphology and exhibits the improved efficiency in the removal of DBTs under the optimized reaction conditions.

SESSION 12
POWER PLANTS - 1
Ting Wang and Gary Stiegel

12.1 Direct Injection Carbon Engine (DICE)—The opportunity for Coal in a Renewables World

Louis Wibberley, CSIRO Energy, AUSTRALIA

The power plants for tomorrow's electricity grid must overcome challenges that include higher penetration of renewables, and thus a need for increased flexibility and lower emissions, and water constraints. The direct injection carbon engine, or DICE, combines the superior thermal efficiency, flexibility, and lower capital cost of the diesel engine, with the low cost and availability of coal. DICE is exceptionally matched to the required attributes for the USDOE Coal FIRST Initiative, and readily meets or exceeds all the required attributes of efficiency, scale, response speed, distributed generation, and adaptability.

Overall, DICE allows the novel use of coal to provide the backbone for a nimble, secure, ultra-low emissions power system by underpinning a high penetration of renewables - including the direct use of biomass char and renewable ammonia. It is of fundamental importance to acknowledge that the performance of the overall system is the key, not that of the individual technologies, as neither would likely exist without the other.

Also, once DICE is installed it can utilize a wide range of alternative fuels including crude bio-oils, chars and other niche fuels, etc – giving many other advantages (increased utilization, reduced processing costs and losses, and the use of bioenergy wastes).

There are no major technical barriers in developing DICE to a commercial scale. Rapid development and deployment of this new fuel cycle is possible at a relatively low cost. In particular, DICE provides the ability to leap-frog the traditional high cost development pathway of new technologies, with commercial plant being possible within five years.

The largest challenge facing the development of DICE is a non-technical one:there is no clear owner or champion for the technology, but many interested parties, including the coal industry, technology providers, engine producers, power producers, etc. Although DICE needs considerable development and demonstration, it has an enormous advantage, via the ability to carry out a near-commercial-scale demonstration at a relatively small size (around 10 MW), both quickly and at relatively low cost. This should enable DICE to leapfrog the usual technology development steps, resulting in time to first commercial deployment of five years, and with a cost as low as US$70 million, including fuel processing and logistics.

This paper summarises developments over the last 10 years by CSIRO, including full-scale engine tests in Europe, China, and Australia. It also details recent R&D by the CSIRO focused on derisking the entire fuel cycle, from coal in the ground through to logistics - building on the comprehensive USDOE program of 1978–1992. The work has confirmed the potential of this highly efficient innovative power cycle, using as coal, other carbons, such as from low-temperature processing of biomass, as well as renewable ammonia.

12.2 Particle Size Distribution of Coal in a Pulverized Mixture of Torrefied Biomass

Kiyoshi Sakuragi, MaromuOtaka, Central Research Institute of Electric Power Industry, JAPAN

Co-firing of biomass is conducted in pulverized coal-fired power plants for the purpose of reducing CO2 emissions. Since it is more difficult to pulverize biomass than coal, biomass in the pulverized mixture has a larger particle size than that of coal. Due to higher volatile content and reactivity, biomass does not need to be fine as much as coal. In order to appropriately set the biomass co-firing ratio, it is necessary to separately evaluate the particle size distributions of coal and biomass, and to pulverize each of these into particle sizes corresponding to the combustibility of each. However, evaluation of individual particle distributions of coal as well as biomass in the pulverized mixture using traditional fuel analysis values that are applied to coal, such as ash, fixed carbon, and calorific value is difficult

The current study quantified neutral sugars which are only present in biomass, in order to estimate the coal content in the pulverized torrefied biomass mixture. Individual particle size distributions of coal and torrefied biomass in the pulverized mixture were estimated using the neutral sugar content corresponding to each particle size range. The effect of the difference of species of biomass was clarified for individual particle size distributions of coal and biomass in the pulverized mixture.

12.3 Formation of Agglomerates and Clinkers by Caking Coal in a 550MWe CFB Boiler

Seok-Gi Ahn, Sung-Mook Jung, Korea Southern Power Co., Ltd., SOUTH KOREA

Samcheok plant is one of the largest Circulating Fluidized Bed (CFB) boiler in the world. Samcheok plant consists of 4 CFB boilers of 550MWe Ultra-supercritical and it started operation since the end of 2016. Agglomeration of bed particles in fluidized bed combustion system is considered as a primary operational problem. In the Samcheok plant, agglomeration is mainly generated in the grid of the furnace and the external heat exchanger (EHE). This study introduces the characteristics of agglomeration formed in the Samcheok CFB boiler and describes the causes. Agglomeration is formed by the effect of fuel properties (ash, caking, etc.), facility and operation. The agglomeration is largely classified into two types in Samcheok CFB boiler. The first is the bonding between the bed particles, and the second is the bonding between the coal particles due to the coal caking. We performed X-Ray Fluorescence (XRF), X-Ray Diffraction (XRD), Scanning Electron Microscope-Energy Dispersive X-Ray Spectrometer (SEM-EDS) analysis on the deposit sample. In addition, we sampled EHE internal gas concentration and solid particles during boiler normal operation to analyze the cause of bonding between bed particles. In order to analyze the cause of bonding between coal particles due to coal caking, the expansion as well as the fluidity were considered through the Free-Swelling Index (FSI), Gieseler Plastometer and Dilatometer of coal.

12.4 Mathematical Model to Predict the Behavior of a Supercritical Once-Through Boiler in a Thermal Power Plant

Xuandai Ngo, Byungho Song, Kunsan National University; Jaehyeon Park, Dowon Shun, Jaegoo Lee, Korea Institute of Energy Research; SOUTH KOREA

A mathematical model of a once-through boiler in a power plant has been developed to simulate and analyze the boiler's dynamic behavior. Firstly, a boiler model was developed by the physical laws and properties of internal working fluid inside tubes of the once-through boilers. The properties of water are interpolated from the steam and water data tables. Secondly, the general block model could be established for each compartment unit in the boiler system by mass, energy, and momentum balance equations. After all, the dynamic of the total once-through boiler system can be simulated by the connection of each block model altogether. The block model applied for the water-wall unit is validated with another referential model. The validation revealed that the state variables, including the mass flow rate, the pressure, and the enthalpy, are almost identical, and the temperature describes some small errors. The approach method used in this study could be applied to any supercritical once-through boilers with other configurators. The model can be used to check the safety of new operational scenarios of the boiler before implementing them to the actual power plant. The model also can be further enhanced to simulate special conditions such as the start-up and shut-down process.

12.5 High-precision Modelling of Key Components in Power Plants with Double Reheat

Jianxi Yu, Pei Liu, Zheng Li, Tsinghua University, CHINA

Double reheat is an effective technology for improving power generation efficiency at the current material level, more and more thermal power plants have adopted double reheat technology. However, the thermal system of double reheat units is much more complicated and has a big change compared with single reheat units. There is a lack of modelling research of the thermal system of double reheat units based on actual operation, which hinders system analysis and operation optimization of actual units. A hybrid modelling method of double reheat units is proposed, based on which the models of key components of the thermal system over the full working range are established. First, data reconciliation is applied to reduce the measurement error of operation data and calculate necessary thermal parameters for modelling. Second, the models of key components, including stages of the steam turbine, heat exchangers, and a feedwater pump of the regenerative system, are established by combining physical mechanisms and operation data. Results show that the models are precise over the full working range, further digital twins of key components are developed. Modelling results demonstrate the accuracy and validity of the proposed method, which provides a basis for system analysis and operation optimization of actual double reheat units.

SESSION 13
GASIFICATION TECHNOLOGIES - 4
Johan van Dyk and Rolf Maurer

13.1 R-GAS™ GASIFICATION TECHNOLOGY (A Gasification Technology suitable for high ash content and high ash flow temperature)

J. van Dyk, A. Kramer, D. Stevenson, GTI, USA

The R-GAS™ gasifier is an oxygen-blown, dry-feed, plug-flow entrained reactor able to achieve carbon conversions approaching 100 percent. The gasifier uses GTI proprietary design approaches to enable a compact, long-life, efficient gasifier that increases performance and availability, while decreasing capital costs. An advantage of this gasifier technology is to be able to also gasify high ash and high ash flow temperature feedstocks. The injector design uses a multi-element injection to rapidly mix the coal with oxygen and steam while rapidly dispersing the coal across the reactor's cross-section. Efficient cooling of the injector face plate enables injector life much greater than the two to six months typical of existing water-slurry gasifier injectors, with post-test analysis of injector face erosion indicating potential injector life of two years or more. The liner is also actively cooled, resulting in a solid layer of slag on the gasifier side of the liner. Slag layer formation and retention on the liner surface has been demonstrated over a broad range of feedstocks, from low ash to high ash coals. Post-test inspection of the liner material shows no measurable loss of material due to efficient cooling and effective slag coverage, supporting estimated liner life of three to ten years, or more. The R-GAS™ liner design enables liner life much longer than the six to eighteen month life typically observed for non-cooled refractory brick in existing gasifiers. The dry feed system, rapid mix injector, and cooled liner enable the gasifier to process all ranks of coal, as demonstrated in the pilot plant gasifier testing at GTI.

13.2 Novel Mixed Matrix Membranes for Separation of Oxygen from Air: Structure and Function of Polysulfone-Nanodiamond Composites

Frederick F. Stewart, Idaho National Laboratory; U. (Balu) Balachandran, Argonne National Laboratory; Christopher J. Orme, Idaho National Laboratory; Tae H. Lee, Argonne National Laboratory; John R. Klaehn, Idaho National Laboratory; Andrew P. Han, Pennsylvania State University; Kaitlyn M. Hillery, Fort Hays State University; USA

The US Energy Information Administration's Short-Term Energy Outlook (STEO) provides an interesting recent historical overview of the US energy supply picture as well as predictions for 2021. Although carbon-free renewable energy sources are gaining market share, fossil resources are the dominant fuel for America's economy and economies around the globe. Use of fossil fuels responsibly requires effective capture of environmental contaminants such as carbon dioxide, NOx, and SOx. It has been shown that an enriched oxygen feed to fossil fuel utilization can make the processes more efficient and result in an effluent stream that is easier to manage.

At large industrial scales, cryogenic distillation is the preferred route where longer necessary equilibration times can be accommodated. Membrane-based separations cannot compete economically at large scales. However, the energy production trend in the US is towards a more flexible and resilient arrays of generation. This trend is driven by the increasing penetration of renewables, such as wind and solar, into energy grids.

Flexible generation leads to a dynamic energy market where electricity can vary greatly. Further, there is a drive to reduce the market risks to new plants, which has resulted in the proposition of increased amounts of small modular plants for coal gasification.

Small modular gasification plants, at the 1-5 MWe scales, are not large enough to consume the output of an optimized cryogenic plant for oxygen enrichment. Also, cryogenic plants cannot rapidly respond to changing demand regimes. Alternatives include sorption processes and membranes. Sorption processes to produce oxygen enriched gas operate best at intermediate scales, while the sorption materials can suffer from poor uptake, thus necessitating larger capital expense (CAPEX).

Membranes offer the ability for limited CAPEX and rapid start/stop response times. However, membranes have their disadvantages. Polymer membranes tend to have poor selectivity and throughput, although they can be scaled readily to address the throughput aspect of their performance. To address the performance issues associated with polymer membranes, this paper will discuss the formation of novel mixed matrix membranes (MMM) composed of functionalized detonation nanodiamonds (DNDs) in a polysulfone host.

We have found that nanodiamonds can form roughly homogeneous structures with polysulfone up to about 2% loading, although there can be some polydispersity of loading density. Beyond that we begin to see a degree of porosity being introduced into the membrane material. Characterization of these materials has been performed using a variety of techniques. Gas permeation experiments have revealed that the nanodiamonds can impart a small degree of improvement in oxygen permeability with little loss in selectivity. However, at 5 % and above, we begin to see large increases in oxygen permeability. These increases also come with a loss of selectivity. Observed increases in permeability were as high as two orders of magnitude. For example, polysulfone itself gives a permeance of around 10 GPU where the more porous structure loaded with nanodiamonds can give permeance of over 1000 GPUs. We will also briefly discuss phase inversion of nanodiamond containing polysulfone materials where the oxygen permeance was found to be as high as 10,000 GPU. Additional characterization experiments will be discussed that provide some insight into the nature of the interaction between the nanodiamond and the polysulfone host. Finally, we will provide a discussion of the pathway forward on the development of these mixed matrix membranes as durable commercial membrane modules.

13.3 Developing an Air Separation Reactor: Design from the Carrier to the Reactor

Jonathan W. Lekse, Eric J. Popczun, Sittichai Natesakhawat, Ting Jia, Yuhua Duan, Mary Ann Clarke, Deepthi Chandramouli, Mehrdad Shahnam, William A. Rogers, National Energy Technology Laboratory, USA

There are many industrial processes that can benefit from a pure oxygen stream. For example, in a gasification reaction system, pure oxygen can be used instead of air in a process known as oxygen-blown gasification, which can enable multiple feed sources such as waste plastic, municipal solid waste, or biomass as well as leading to more efficient generation of syngas. In large scale operations, this pure oxygen can be provided by cryogenic separation, but as the size of the system becomes smaller, the large footprint required by cryogenics becomes problematic and costly. One alternative to cryogenically produced oxygen is to use a metal oxide carrier material. Though a wide variety of metal oxides can be used in this air separation process, we have focused on the perovskite family of oxides and, to date, have developed a perovskite oxygen carrier material that has demonstrated rapid, reversible oxygen storage and release over thousands of cycles. In this presentation, we will present data on the synthesis, characterization, computational analysis, and performance testing of the carrier material as well as preliminary computational fluid dynamics modelling of a reactor based on this carrier material.

13.4 Microwave-Assisted Conversion of Low Rank Coal

Victor Abdelsayed, National Energy Technology Laboratory and Leidos Research Support Team; Mark Smith, Dushyant Shekhawa, National Energy Technology Laboratory; USA

Conventional gasification of low rank coal is always associated with many process intensifications challenges due to its high moisture and ash contents and downstream problems due to formation of tars resulting in pipe plugging and shutting down. This is in addition to the big size required of the gasifier and the high cost of operation and maintenance needed. Microwave-assisted gasification reactions for coal/biomass has recently targeted many of these problems via its enhanced reaction conversions and selectivities, modularity, and operational advantages such as rapid shutoff and start-up of the reactor. In this presentation we will present our recent efforts in microwave coal pyrolysis and gasification into syngas and value-added chemicals. The effects of microwave treatment temperature of coal, biomass copyrolysis, reactive gas addition

such as methane and CO_2 will be presented. The correlation between char structure and product distribution will also be given.

13.5 Techno-Economic Analysis of Integrated Gasification Fuel Cell Power Systems

Gregory A. Hackett, National Energy Technology Laboratory, Arun K.S. Iyengar, National Energy Technology Laboratory / KeyLogic, lex A. Noring, National Energy Technology Laboratory / KeyLogic, Dale L. Keairns, National Energy Technology Laboratory / Deloitte, Richard A. Newby, National Energy Technology Laboratory / KeyLogic, USA

Solid oxide fuel cells (SOFC) offer the highest prospective chemical-to-electrical conversion efficiency for any fossil-derived fuel, including coal. The Department of Energy's (DOE) Office of Fossil Energy (FE) SOFC Program coordinates efforts to develop low cost and reliable commercial SOFC systems. Specific technical objectives include system electrical efficiencies of greater than 60% (without carbon capture and storage [CCS]), a SOFC stack cost of $225/kilowatt in high volume production, and lifetime performance degradation of less than 0.2% per 1000 hours over an operating lifetime of 40,000 hours.

This work presents the results of a research and development (R&D) pathway study for coal-based integrated gasification fuel cell (IGFC) power systems with and without CCS. The objective of the study is to provide guidance to DOE-FE's SOFC R&D program.

The IGFC power plant is analogous to an integrated gasification combined cycle (IGCC) power plant, except the gas turbine power island is replaced with a solid oxide fuel cell (SOFC) power island. The SOFC provides for high electric efficiencies associated with the nearly reversible electrochemical conversion of syngas chemical potential to electric power, as compared to a conventional heat engine (Carnot cycle). Essentially, the SOFC serves as a process intensification unit able to reform methane, selectively transport oxygen, and produce electricity. The high conversion rate of the carbonaceous fuel when electrochemically reacted with the transported elemental oxygen results in an increased carbon dioxide content in the effluent (when compared to traditional coal and natural gas plants) which decreases the cost of carbon capture. The heat rejected by the fuel cell system can be recovered further in a combination of Brayton and Rankine cycles, depending on whether the fuel cell system is operating at elevated or atmospheric pressures.

Two parallel developmental scenarios—one with the SOFC operating at atmospheric pressure and one based on a pressurized SOFC operation—were considered as part of the IGFC pathway. From previous studies, which found insignificant cost benefits for pressures higher than three atmospheres, an SOFC operating pressure of three atmospheres has been assumed in the present calculations. Prospective improvements made to gasification technology that result in increased syngas methane content, which has a significant effect on the IGFC system performance, were considered.

The design and cost bases for this pathway study closely follow the bases applied in the NETL Bituminous Baseline report [National Energy Technology Laboratory, "Cost and Performance for Fossil Energy Plants, Volume 1: Bituminous Coal and Natural Gas to Electricity," Revision 4, September 2019] so that direct performance and cost comparisons can be made with the conventional fossil-fuel power plant results estimated in that report. The results show the advantages and disadvantages of IGFC technology compared to other advanced fossil-based electricity generation technologies. Depending on certain external factors, IGFC can be a cost effective and clean method to produce electricity from domestic coal.

SESSION 14
CLEAN COAL AND GAS TO FUELS - 2
Diane Revay Madden and John Duddy

14.1 Hydrodesulfurization of Dibenzothiophene over NiMoS2 Supported on Two-dimensional Metal Oxide Catalysts

Meng Zhang, Huan-Huan Fan, Bao-Xing Wang, Jie Feng, Wen-Ying Li, Taiyuan University of Technology, CHINA

Hydrodesulfurization (HDS) is one of the main processes for the removal of sulfur-containing compounds from coal tars in industry, and the key factor of the HDS technique is to design a catalyst with predominant HDS performance. It has been researched that synthesizing novel support materials, adding modifiers or changing the synthesis method of the support could improve the activity and selectivity of the

supported HDS catalysts. Two-dimensional (2D) materials have attracted extensive attention in the field of catalysis, due to their unique electronic, mechanical and chemical properties. Compared with traditionally catalytic materials, 2D materials have a larger surface area and abundant defect sites, which can provide more active catalytic sites. In our study, a series of graphene-like 2D composite metal oxides TiO_2-Al_2O_3 with different TiO_2 mass contents (2D-TiAl-x) were prepared by using graphene oxide (GO) as the structure directing agent (Figure 1). And the corresponding $NiMoS_2$ catalysts supported on 2D-TiAl-x were prepared by the incipient wetness co-impregnation method. The HDS of dibenzothiophene (DBT) was studied on $NiMoS_2$/2D-TiAl-x, $NiMoS_2$/TiAl-x and $NiMoS_2$/γ-Al_2O_3 catalysts. The support and corresponding catalyst materials were characterized by XRD, N_2-physical adsorption, SEM, H_2-TPR, XPS, Raman, TEM and other test methods. The results show that the graphene-like 2D TiO_2-Al_2O_3 is enrich with oxygen vacancies and larger surface area than the traditional TiO_2-Al_2O_3 composite metal oxide and commercial γ-Al_2O_3. Moreover, graphene-like 2D structure could effectively regulate the metal-support interactions. For all $NiMoS_2$/2D-TiAl-x catalysts, the characterization results clearly showed that metal-support interactions are gradually strengthened with the increasing of the TiO_2 content. Among the three $NiMoS_2$ catalysts, $NiMoS_2$/2D-TiAl-x sulfurized catalyst has higher HDS activity. The results indicated that the graphene-like 2D structure can make the support rich in surface defects, increase the surface area of the support, promote the formation of the catalyst active phase, and further provide more active sites for the reaction, thus promoting the HDS of DBT and improving the activity of the catalyst. It can be seen that the defect sites on the surface of the support and moderate the interaction between the support material and the active metals are critical to the activity of the HDS catalyst.
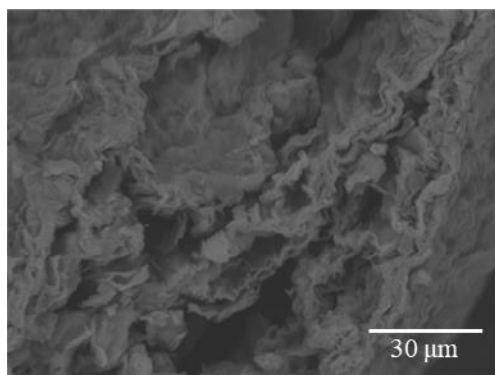
Figure 1. SEM image of graphene-like 2D composite metal oxides TiO_2-Al_2O_3 (2D-TiAl-4)

14.2 A Century of Innovative Coal-To-Liquids Technologies: Where Do We Go from Here?

K. David Lyons, U.S. DOE/National Energy Technology Laboratory; Christopher Munson, Charles Pruss, Henry A. Long, III, Massood Ramezan, KeyLogic Systems, Inc; USA

Coal-to-liquids (CTL) technologies have been a major area of energy research and development for approximately a century. Converting inexpensive and abundant coal into high-quality liquid fuels and chemicals in a reliable, environmentally sound, and cost-effective manner has been a highly coveted goal of the research effort, especially in recent times. Given that many nations throughout the world have little or no natural oil reserves and must rely on foreign imported petroleum and related products for various applications (power generation included), the generation of clean liquid fuels from coal to reduce this dependence is seen as highly attractive. Even in countries like the United States where domestic oil is abundant, CTL technologies increase the diversity of available transportation fuels and increase overall fuel production capacity, leading to greater energy independence. CTL technologies are well-established, mainly based on indirect processes like the well-known Fischer-Tropsch (F-T) process developed in the 1920s and 1930s. In addition, several technologies that directly convert coal and other solid fuels into useful liquid products like gasoline, diesel, wax, jet fuels, methanol, and di-methyl ether (DME) are used throughout the world today.

This paper will provide a brief history of CTL research, beginning in the 1920s, and provide a "how we got here" summary of current CTL technological development, with an emphasis on U.S. Department of Energy (DOE)-led initiatives. This coverage will include an overview of DOE legacy research, CTL economics, environmental issues, and current challenges/research opportunities.

14.3 Development of a Flow Regime Map for Slurry Bubble Column Reactors using Power Spectral Density Function Analysis

Obinna Chiekezi, North Carolina A&T State University; Badie I. Morsi, University of Pittsburgh; and Omar M. Basha, North Carolina A&T State University; USA

In this work, over 400 experimental data points measured in a pilot scale slurry bubble column reactor (SBCR) (0.15 m ID-3 m high) at the University of Pittsburgh [1-9], covering a wide range of operating parameters (T: 320 – 500 K, P: 4 – 31 bar, C_s: 5-15 vol.%, and u_G: 0.05 – 0.3 m/s) and using different gas-liquid-solid systems, were analyzed for the development of a flow regime map for SBCRs. Specifically, pressure fluctuation signals from the dP cells were analyzed using a Fourier transform in order to identify the power spectral density function (PSDF) of each experimental condition. The obtained PSDFs were subsequently used to delineate the effect of gas velocity, catalyst concentration, temperature, pressure, and liquid physical properties on the pressure fluctuations within the column. Flow regime maps were then developed, both by assuming conventional 2-bubble class behavior and a wider bubble-size distribution [10].

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14.4 Assessing the Viability of K-Mo$_2$C for Reverse Water-Gas Shift Scale-Up: Molecular to Laboratory to Pilot-Scale

Marc D. Porosoff, Mitchell Juneau, University of Rochester, USA

Conversion of CO_2 to value-added chemicals and fuels is a potentially valuable route for renewable energy storage and a future CO_2-neutral economy. The first step is CO_2 conversion to CO via the reverse water-gas shift (RWGS) reaction. Effluent CO can then be hydrogenated to chemicals and fuels via Fischer-Tropsch (FT) synthesis over a tandem catalyst or within a second reactor. To implement this process on an industrial scale, low-cost, scalable and highly-selective catalysts are required, prompting investigations into materials that meet these design constraints.

When scaling up a catalyst for RWGS, it is important to synthesize the catalyst with a scalable synthesis method, such as wet impregnation, using low-cost materials. Once synthesized, the catalyst must exhibit high stability over thousands of hours on stream and be easily regenerable to maximize catalyst lifetime[1, 2]. Potassium-promoted molybdenum carbide supported on gamma alumina (K-Mo$_2$C/γ-Al_2O_3) has been previously identified as a low-cost and highly active catalyst for RWGS using DFT

calculations and laboratory-scale experiments; however, to date, there has not been any investigation into the scale-up viability of K-Mo$_2$C/γ-Al$_2$O$_3$, or any TMC-based RWGS catalyst. Therefore, it is necessary to perform a detailed study of catalyst performance across different scales, from molecular to laboratory to pilot, to assess the viability of K-Mo$_2$C/γ-Al$_2$O$_3$ for scale-up.

Although K-Mo$_2$C/γ-Al$_2$O$_3$ is a highly active and selective RWGS catalyst, the viability and performance of K-Mo$_2$C/γ-Al$_2$O$_3$ for scale-up has not yet been determined. In this report, laboratory-scale (~100 mg catalyst) reactor studies are extended to the pilot-scale (~1 kg catalyst), and viability for scale-up is tested further in the laboratory under a range of temperatures (300 – 600 °C) and flow conditions. The pilot-scale experiments illustrate K-Mo$_2$C/γ-Al$_2$O$_3$ is a highly active and selective catalyst (44% CO2 conversion, 98%+ CO selectivity at GHSV = 1.7 L kg-1 s-1 and T = 450 °C), that exhibits no signs of deactivation for over 10 days on stream. Together, experiments across the molecular, pilot and laboratory scales demonstrate that K-Mo$_2$C/γ-Al$_2$O$_3$ is an economically-viable RWGS catalyst with promising future applications in industry.

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14.5 Operating Cost Assurances Through Continuous High Efficiency Treating Chemistry

S Todd Beasley, HTC Purification Corp., CANADA

Carbon Capture from large industrial sources such as Coal Power Plants represent a significant environmental and economic opportunity for mankind. However, these investments typically exceed Hundreds if not Billions of dollars! Capital and Operating cost assurances are crucial!

In most cases these projects utilise specialty chemical formulations (Gas Treating Chemicals – GTC'S) in a continuous absorption / regeneration cycle. Assuming a well-engineered plant and its capital infrastructure - operating challenges and extraordinary operating costs typically result when these chemical formulations become contaminated. The implications of impurities are profoundly negative!

Operating costs spiral and environmental performance becomes severely impaired. If we look at recent operating experiences of large-scale CO2 capture projects, the challenge and significant opportunity of managing the chemistry is a significant lesson learned for our industry.

These systems must be designed to act as an insurance policy for operational integrity.

The challenges in achieving continuous uninterrupted pure chemistry is-multifaceted. Solids, particulates, cations / anions - conversion impurities all of which may have significantly different physical properties and concentrations. Some of these impurities have diminished treating capacity – some have no reactivity at all. Some are corrosive – some cause foaming, but All of them significantly impair the operational stability and operating cost predictability of the CO2 capture system.

This presentation will discuss the latest innovations regarding purification technologies – from impurities encountered, capacity considerations, subsequent waste management and solution analysis.

"Technologies proliferate when their use becomes predictable and economically advantageous"

SESSION 15
POWER PLANTS - 2
Ting Wang and Gary Stiegel

15.1 Condenser Efficiency Improvements Through Nanocomposite Surface Treatment Technology

Vinod Veedu, Matthew Nakatsuka, Erika Brown, Oceanit, USA

In most power plants, the condenser unit is simultaneously indispensable as well as the largest source of thermal heat loss during the steam turbine cycle. Even small changes in thermal heat transfer efficiency due to flow disruption, environmental changes, or biofouling can have significant effects on heat rate and cost per kilowatt-hour. While there are several strategies available to mitigate the effect of fouling, they generally are labor intensive. If left unchecked, repair costs for condenser tubes can be extremely high, owing to the significant opportunity cost associated with taking the entire turbine off-line and breaking the near vacuum seal.

Previous work has shown that a novel in-situ applicable surface treatment consisting of extremely thin nanomaterials was capable of greatly improving the heat transfer properties of shell-and-tube heat exchangers utilizing untreated seawater for cooling. In particular, the ability to have near-equivalent durability as traditional marine epoxies while being applied at 1/10 the thickness allowed for the entire length of the tube to be treated, rather than just protecting tube sheets and pitting within the individual tubes from further erosion and corrosion damage.

This paper goes one step further in detailing the field trial and adaptation of the treatment for a copper-nickel condenser unit with a history of leaks necessitating tube blockage. The surface treatment had dual effects in substantially decreasing the propensity of the exchanger to foul, while also increasing the cold flow rate through the exchanger, due to its hydrophobic nature and complete reduction in surface roughness. Overall reductions in the temperature of the resulting condensate and the cooling water outflow temperatures suggested that the treatment was able to restore the performance of the condenser unit when considering the extended lifetime of the unit, as well as the significant savings by foregoing retubing and repair. Our overall assessment is that the surface treatment provided significant cost savings both over the study period, as well as the projected future lifetime of the treatment.

15.2 Evaluation of High Temperature Distributed Sensing Using Gold-Coated Optical Fiber and OFDR Technique

Juddha Thapa, Jared M. Charley, Leidos Research Support Team; Benjamin T. Chorpening, NETL; USA

Boiler operation and health monitoring could be improved with a higher spatial resolution temperature measurement of key components. To make this possible in a cost-effective manner, NETL is investigating distributed optical fiber sensing for boiler applications, where hundreds of temperature measurements are made along a single optical fiber. To evaluate the likely performance of this approach in the near-term, we employed the optical frequency domain reflectometry (OFDR) technique, with a 5meter long single-mode gold-coated fiber as a sensor. An electric plate-heater apparatus was used to simulate the boiler tubewall air-side environment, with the gold-coated fiber attached in a protective steel tube. The OFDR instrument was calibrated for the gold-coated fiber, and tests performed with the plate-heater operating from room temperature (22°C) to 650°C. The optical fiber temperature readings were compared to thermocouples attached nearby. We also evaluated the effect of the gage lengths and sensor spacings in different tests. Furthermore, we evaluated the performance of the heat-treated and untreated gold-coated fibers. We found that the difference between the thermocouple measured and the optical fiber measured temperatures were less than 10°C, with a 2cm gauge length. The results from our experiments suggest that the gold-coated fiber could be used in boiler applications (such as tubewall monitoring) at steam temperatures to improve boiler operation while load following.

15.3 Vertical Surface Dropwise Condensation Heat Transfer Using Self-Healing Coatings

Sean Hoenig, Richard Bonner, Advanced Cooling Technologies, Inc., USA

In a traditional Rankine cycle, the condenser system for coal-fired power plants uses a pumped cooling water system to reject heat to a wet cooling tower. Heat rejection occurs in a shell and tube heat exchanger by filmwise condensation of low-pressure steam on steel, copper, or titanium. The use of steam surface condensers typically results in low thermal performance on the steam-side due to the filmwise mode of condensation present on common material options. To improve the thermal performance and durability of steam surface condensers, a self-healing, replenishable film-forming amine (FFA) coating deposited on the condenser tubing is proposed. The FFA coating not only promotes efficient dropwise condensation on the condenser tubing but also protects the surface from oxidative corrosion. To measure the thermal performance enhancement of these coatings, a custom test apparatus was used for flat plate condenser surfaces. The initial results suggest improved thermal performance for several condenser materials. Additional findings primarily suggest the affinity of the coating for the condenser material will affect the overall thermal performance enhancement, as well as secondary reasons, including adsorption/desorption kinetics and constriction resistance. A technoeconomic analysis demonstrates the positive value for the power plant user in terms of overall thermal performance, plant process parameters, and total heat exchanger cost.

15.4 Cost and Performance of Bituminous Coal and Natural Gas Plants with Carbon Capture and Storage

Robert E. James III, US DOE NETL; Alex Zoelle, Marc Turner, Norma Kuehn, Leidos Research Support Team; Mark Woods, Key Logic; Travis Shultz, US DOE NETL; USA

The United States Department of Energy Office of Fossil Energy, in conjunction with its National Energy Technology Laboratory (NETL), conducts research, development and demonstration of advanced fossil-based power generation technologies. In the process of identifying research and development (R&D) needs and evaluating the potential for improvement upon state-of-the-art (SOA) technologies, it is often necessary to first establish a comprehensive baseline for performance and cost estimation. To this end, NETL has developed a set of studies titled "Cost and Performance Baselines for Fossil Energy Plants," comprised of four volumes:
- Volume 1: Bituminous Coal and Natural Gas to Electricity
- Volume 2: Coal to Synthetic Natural Gas and Ammonia (Various Coal Ranks)
- Volume 3: Low Rank Coal and Natural Gas to Electricity
- Volume 4: Bituminous Coal to Liquid Fuels

In late 2019, a major update (Revision 4) to Volume 1, "Bituminous Coal and Natural Gas to Electricity," was published. This study consists of an independent assessment of the cost and performance of greenfield integrated gasification combined cycle (IGCC), pulverized coal (PC), and natural gas combined cycle (NGCC) plants – both without and with carbon capture and storage (CCS) - using a systematic and transparent technical and economic approach that reflects current baseload market conditions. Thirteen power plant configurations (cases) were analyzed:
- Seven IGCC configurations – three gasifiers manufacturers with and without 90% CO_2 capture (w/wo CCS)
- Four PC power plant configurations - two subcritical and two supercritical (SC), each w/wo CCS
- Two state-of-the-art 2017 F-Class combustion turbine-based NGCC power plant configurations w/wo CCS

Equipment cost and performance data were compiled from published reports, information obtained from vendor quotes and users of the technology, and data from designing and building utility projects. This update reflects varying degrees of technology vendor input. For IGCC plants, updates included the air separation unit (ASU), steam cycle, syngas scrubber, water gas shift reactors, carbonyl sulfide hydrolysis reactors, low temperature heat recovery process, ammonia scrubber, sour water strippers, syngas humidification, Selexol acid gas removal, CO_2 compressors, and process water treatment systems. PC and NGCC plant updates included the pollution control equipment and process water treatment systems (PC only), CO_2 compression, and steam turbine technology. NGCC plant updates included the combustion turbine technology. However, the final assessment of performance and cost was determined independently and is not endorsed by the individual vendors.

Updated regulatory requirements (e.g., Effluent Limitation Guidelines) were incorporated as appropriate for each technology/case. This study also includes a significant revision to the finance methodology and assumptions, changing to a corporate finance structure.

Thermodynamic and environmental performance, capital and operating/maintenance costs, breakeven CO_2 sales price, and levelized cost of electricity will be presented for each case. This work will serve as a technology baseline against which fossil power generation R&D can be evaluated.

15.5 New Closed Cycle Cryogenic Electric and Coal-Fired Power Production Systems

James Burkhart, NASA Glenn Research Center, USA

The NASA Glenn Research Center participated in the Energy Conversion Alternatives Study (ECAS), which concluded that "topping cycles" such as molten carbonate fuel cells or magneto-hydrodynamic power cycles would greatly increase the combined topping cycle/steam cycle efficiency into the low 50% level. Further independent investigation examined cryogenic bottoming cycles which operate from ambient (300 degrees K) down to absolute zero. These cycles were presented in patent US 10,132,201 B2, which includes cryogenic helium, neon, argon and nitrogen closed cycles with potential cycle efficiencies up to 80%.

These cycles operate as bottoming cycles to conventional steam cycles reaching into the 70% combined cycle range. The potential of these closed cycles operating off of ambient heat alone and generating power appears potentially feasible. To date, prototype electric automobiles and electric freight trucks have been put forth. More detailed analysis of these liquids flowing in piping systems buried in ground surfaces is required, followed by necessary experiments. The best feature of cryogenic fluids is that they act like coolants when in the ground, and thus contribute to climate temperature reduction. These new cryogenic power sources are potentially the key to total climate control, where earth bound sensible heat is converted directly to power without a combustion step. Extended discussion will center on retrofitting coal-fired power plants.

SESSION 16
ENERGY STORAGE - 1
Briggs White and Richard Bajura

16.1 Department of Energy's Advanced Energy Storage Program

Briggs White, NETL, USA

Energy storage is vital to ensuring stability and reliability in a changing grid system in the United States. For fossil energy generation, ramping and cycling frequently can prematurely damage components, which leads to shorter lifetimes for the plants and more expensive electricity overall. With energy storage integration, stresses to the components may be significantly less due to the ability to utilize stored energy when needing to ramp and charge energy when power is in lower demand. This enables plants to operate flexibly, reliably, and sustainably. The National Energy Technology Laboratory's (NETL's) Crosscutting Energy Storage program examines how energy storage can be economically integrated into fossil energy generation to provide long duration energy storage. Preliminary results show promising economic benefits today, but the initial cost of energy storage technologies is prohibitive, even if impacts to plant life and potential recoup of costs are promising. Control systems to integration are also costly. Necessary scaling and manufacturing enhancements will be required to make the technology commonplace with fossil energy generation.

Short term energy storage is available commercially today but yield four or less hours of storage and are in battery form. These options do not utilize byproducts, such as heat, from fossil energy power to make the integration as clean and green as possible. For fossil energy generation, long duration storage is needed; storage options are required to provide power for longer duration (e.g. twelve hours) to provide enough coverage to the generator. However, the current techno-economics behind integration with fossil energy generation are currently unknown.

Beyond the lifetime increases and economic benefits for fossil energy generation, energy storage also makes electricity production significantly greener. Not only does it limit carbon emissions by allowing plants to generate optimally, but it also reduces plant idling and this can be a major contributor to emissions production. With several categories of energy storage technology in research and development stages (thermal, chemical, mechanical, electro-chemical, etc.), NETL examines which of these technologies will be most beneficial to fossil energy generators per region and as a rule of thumb. The study at NETL will better understand the economics behind this energy storage enhancement.

NETL works with universities, industry, and a variety of other collaborators to best evaluate the transient response to various system concepts that minimize the levelized cost of electricity for several storage technologies. Each of the studied storage technologies are long-duration and non-battery due to the needs of fossil energy generation. NETL better understands integration of energy storage through more than techno-economic studies, but also enhances understanding through hands-on experience by collaborating with EPRI to test a pilot scale concrete thermal energy storage system to demonstrate the potential of the technology when directly applied to fossil energy generation. The demonstration will enhance understandings of necessary control systems between plant operations and charging/utilizing methods and engineer through integration challenges.

Results from NETL's projects in energy storage will showcase what is needed to integrate energy storage into fossil energy generators. It is already known that long duration storage is necessary, but the economics and challenges surrounding integration and the potential benefits and synergies are not fully understood. NETL will provide knowledge and solutions to integration of long duration energy storage for fossil energy generators

16.2 Techno-Economic Analysis of the Utility-Scale Energy Storage Concepts Integrated with Fossil Fuel-Based Power Generation

Nenad Sarunac, Professor, EPIC UNC Charlotte; Carlos Romero, Shalinee Kishore, Alberto J. Lamadrid, Mr. Zheng Yao, Energy Research Center, Lehigh University; Rick Mancini, Pramod Kulkarni, John Fernandes, Fu-An Yu, Customized Energy Solutions; Mark D. D'Agostini, Global Combustion Technology Development, Air Products and Chemicals, Inc.; USA

The increasing penetration of the non-dispatchable and variable power supply complicates the load balancing challenge by adding more variability to the dispatchable

power supply side, such as with fossil-fired power generation, resulting in increased and more frequent load cycling. Improving the flexibility of conventional power plants is a key challenge for the transformation of the entire energy system towards a higher share of renewable energies in electricity generation. In addition to other options such as grid and demand-side management, flexible conventional power generation plays a key role for ensuring adequate system stability. Flexible and dispatchable power plants will contribute to this ongoing transformation process as they compensate the fluctuating electricity generation from renewable energy sources such as wind and solar.

Due to the volatile character of the weather-dependent power generation from renewable energies, the need for a stable, secure, and reliable grid operation is rising. In the current energy system, dispatchable power plants based on coal, and natural gas mainly compensate the fluctuating power generation from renewable energies and thereby ensure the stability and reliability of the electrical grid. Considering the expected capacity growth of renewable energy resources, while simultaneously reducing the capacity of conventional power plants, the remaining dispatchable power plant fleet has to meet increasingly higher flexibility and reliability requirements.

An option that is gaining a lot of attention of lately to meet the fossil power plant flexibility challenges is energy storage. Energy storage integrated with a power plant acts as a buffer by absorbing part of the variations in load profile the plant needs to follow, thus reducing cycling, increasing plant flexibility, reducing load ramping, lowering minimum plant load, providing peak power when needed, and time-shifting peak power generation, partially decoupling plant power output and boiler (steam generator) firing rate. This would result in improving the flexibility of the plant, reducing cycling damage, reducing emissions, and improving plant economic performance.

From the perspective of a power plant operator, enhancing flexibility parameters would result in a higher profitability of a specific power plant due to reduced losses at minimum load operation, additional revenues on intraday and control power markets, avoidance of shutdowns, and faster start-ups. From a system perspective, flexible power plants reduce the number of units needed to ensure the stability of the grid. Furthermore, flexible power plants enable the integration of more renewable power, leading to a more efficient interconnected electrical grid system. This is especially the case for power systems characterized by high shares of electricity generation from conventional power plants.

All fossil generating plants have startup costs for on/off-line operation, and inefficiencies in moving though their load operating range. These power generation facilities represent a significant investment in the production of dispatchable electricity but are being phased out as renewable energy resources are entering the energy market, while the remaining units are required to operate at increasingly variable load and conditions they were originally not designed for. As the penetration of renewables increase over the next decades, the efficient, flexible, and reliable operation of the existing fossil resources is critical for a smooth cost-effective decarbonization of the power generation sector.

The main objectives of this project are analysis of the performance and economics of integrated fossil power plant-energy storage options and quantification of projected economic benefits. Four energy storage options were selected for the analysis, including Thermal Energy Storage (TES), Liquid Air Energy Storage (LAES), also referred to as Cryogenic Energy Storage (CES), Battery Energy Storage in combination with Super-Capacitors, and Hydrogen Energy Storage. The analyses will determine their impact on operation and economics of a representative (reference) coal-fired power plant. A coal-fired steam plant was selected as a reference plant because it may provide the greatest benefits from the integration of energy storage and can be used as a foundation for other fossil fuel facilities.

The TES option includes the Ruths steam accumulator, sensible heat storage in pressurized water (condensate and feedwater), molten salt, and solid media. The TES option involving a steam accumulator is conceptually similar to the battery and super-capacitor option, where the capacitor provides a quick dynamic response (power) and the battery provides the energy capacity. LAES or CES, is a long-duration, large-scale energy storage technology that can be deployed in stand-alone mode of operation or integrated with a power plant. The LAES working fluid is liquefied air. The electrolysis version of hydrogen energy storage will be explored, where the produced hydrogen will be compressed and stored. Although the hydrogen storage option is currently challenged by relatively low roundtrip efficiencies, it would integrate well with a steam electric power plant. It is important to note that the proposed energy storage systems can be built in modular fashion providing scalability as demand for energy storage changes in the future.

The project and its results are highly relevant for future advancements of energy storage and its application and integration with power generation assets because: (i) the technical analysis will be performed by using high-fidelity plant models verified against actual operating data and augmented by deep understanding of power plant operation, thus resulting in a realistic Incremental Cost Curve (ICC) for the plant; and (ii) the economic analysis will be performed by using actual grid data and market prices to simulate

operation of the reference plant with and without integrated energy storage, to determine the actual value of storage under realistic grid operating conditions, taking into account revenues due to increases in energy (achieved by reducing inefficiencies due to variable load operation and improved performance) and increased plant participation in the ancillary services market.

16.3 Conceptual Design Study of a Thermal Energy Storage System Using Granular Solids for Coal-fired Boilers

Benjamin T. Chorpening, Pamela Miceus, E. David Huckaby, National Energy Technology Laboratory, USA

As electricity from various renewable energy sources is increasingly supplied to the power grid, the grid's stability will be challenged. Proposed grid-stability solutions will need to address variability of sources, such as solar and wind energy, in order to alleviate problems such as overgeneration and ramping. In regions where increases in solar energy are prominent, such as California, the net power demand curve often referred to as "the Duck Curve," has caused problems for energy dispatchers, due to over-generation and fast ramping demands. In this project, we investigated a conceptual design for a Thermal Energy Storage System (TESS) integrated into a coal-fired power plant to support grid-scale storage. Implementing a TESS into power plants can allow for an increase in renewable sources, increase grid resilience, and allow conventional coal-fired plants to operate more efficiently. For this project, a TESS using granular solids as the energy-storage media is integrated into a conventional coal-fired power plant. The purpose of the TESS is to store energy from the flue gas during low demand periods and transfer the energy to steam during peak demand periods. The storage allows the stabilization of combustion and related boiler components at low loads and provides the opportunity to avoid some shutdowns. This study uses thermodynamic properties of several candidate thermal storage materials to estimate the size of storage system required for several operating scenarios.

16.4 Concrete Thermal Energy Storage Enabling Flexible Operation without Coal Plant Cycling

Scott Hume, Andrew Maxson, Electric Power Research Institute, Inc.; Jennifer Tuey, Bright Energy LLC; Joshua Barron, Research Engineer, Southern Company; Daniel Mardovin, AECOM; USA

Intermittent renewable electricity generation is being added to the power grid at an increasing rate, resulting in many coal plants being pressed to provide flexibility and ancillary services, operation for which they were not originally designed. Today these units are economically disadvantaged with missed opportunities due being unable to turndown far enough and or having inherently slow ramp rates. Moreover, when operating dynamically, results in worse efficiency and higher emissions on per kW basis, and higher maintenance costs due to cycling leading to a shorter life for these units. Providing grid support will be even more important in the future as more intermittent renewable electricity generating units come online. The ability to respond at very short notice to deliver these important grid services and sustained power delivery when renewable supply unexpectedly drops will be essential. This level of flexibility is challenging for coal units, often resulting in the need to operate at minimum generation conditions for protracted periods in uneconomic market conditions to be able to deliver power when needed later.

If large quantities of energy can be stored, the coal units could operate closer to the desired baseload condition without the need for cycling and start-stop operations. Electrochemical batteries have been shown to be capable of meeting some of this need, but at the scale required to balance the future renewable energy ratios (i.e., GWhs) batteries are expensive, require large footprints, struggle with quick frequency response, have relatively short storage durations up to 4 hours and have environmental concerns. Storing energy as heat in a system coupled to a thermal power cycle offers the opportunity to store large quantities of thermal energy in low-cost material, delivering reliable, synchronous generation when needed for extended periods of time. Concrete is a low-cost, readily available, and fully moldable material that is capable of handling the temperatures needed for high efficiency power cycles up to 600°C. Utilizing concrete as a thermal energy storage (TES) media could potentially store energy at up to 4 times lower cost that lithium ion batteries today. Bright Energy, LLC has developed a concrete TES (CTES) system design to capitalize on the storage medium's low cost. To test the capabilities of this system, a team led by the Electric Power Research Institute, Inc. is constructing a CTES pilot plant through funding provided by the U.S. Department of Energy at Alabama Power's coal-fired Plant Gaston in AL, with testing scheduled to be carried out in 2022. A principal goal of the testing will be to expose the CTES blocks to significant thermal cycling to assess its ability to be durable under dynamic operating conditions.

This energy storage will be a steam-in, steam-out arrangement. To charge the system, high-pressure steam from the power plant flows through tubes, heating the concrete modules, which store the thermal energy until needed. When grid demand increases, high-pressure water is introduced to the CTES modules and high-pressure steam is generated and returned to the thermal power plant to generate electricity. The pilot project will test modules similar in size to those expected to be used in larger-scale commercial applications, shown in Figure 1. The inclusion of a CTES system on an existing multi-unit coal plant allows older boiler plant to be retired, while maintaining the capacity of the steam turbines for use with the energy storage system. With the primary energy being sourced from the most efficient unit, that system can operate more closely to the design optimum and can facilitate the application of carbon capture due to the enabling of a consistent full load operation even when the grid demand is highly variable.

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SESSION 17
COMBUSTION TECHNOLOGIES - 4
Rolf Maurer and Andreas Richter

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17.1 Simulation-Based Parametric Study of Operating Conditions for a CLOU Reactor Burning Coal

Zachary Reinking, Kevin J. Whitty, University of Utah; JoAnn S. Lighty, Boise State University; USA

Chemical looping with oxygen uncoupling (CLOU) is an alternate form of chemical looping combustion where the oxygen carrier releases gaseous O_2 in the fuel reactor, which allows for combustion in the fuel reactor to take place in a nitrogen-free environment. CLOU is well-suited for coal, and other solid fuels as the released O_2 readily combusts with solid char. In addition, the heat balances in the system are easier to maintain, as the fuel reactor is exothermic overall due to the combustion reactions.

This study presents several three-dimensional simulations of the University of Utah's dual fluidized bed process unit (PDU), using different initial starting conditions. These include varying air reactor and fuel reactor superficial velocity, lower starting bed mass, decreased coal feed rate, different carrier type, increased metal-oxide loading, and increased fuel particle size. These were performed with the intention of gaining a better understanding of how the PDU will respond to different initial conditions. Simulations are done using CPFD Software's Barracuda-VR™ CFD software. Validation of the drag model used and other hydrodynamic settings for the software were based on experiments using a scaled-down cold-flow unit. Kinetics determined in previous studies were included for oxidation and reduction of cuprous oxide and cupric oxide. A reduced set of rate expressions for the conversion of coal char, based on reported literature data was implemented into the simulations. Literature-based rate data for devolatization, evaporation, steam and CO_2 gasification, methanation, water-gas shift, and other gas-phase reactions were also included. Additionally, reactor wall heat transfer surfaces were implemented at the bottom of the AR to facilitate heat removal.

Results predicted high sensitivity to changes in AR and FR velocity, which caused large shifts in the inventory distribution between reactors. At lower AR velocities, not enough oxygen was supplied to the system to complete coal combustion. Decreasing the coal input from 200 kW to 100 kW caused a sharp temperature drop in both reactors and a decreased utilization of oxygen carrier. Increased coal size caused a larger amount of coal to stay in the fuel reactor instead of being recycled through the cyclone into the loop seal and dipleg. There was not a significant increase in the predicted amount of unreacted coal entering the AR, however. Increased copper loading predicted the lowest amount of unreacted coal in the FR; however, this also caused an excess of gaseous oxygen to exist in the FR cyclone exit stream. Decreasing initial oxygen carrier bed mass predicted much higher amounts of unreacted coal in the FR, and a much lower amount of free gaseous oxygen compared to the base case.

17.2 Performance and Flexibility Improvements of Staged Pressurized Oxy-Combustion

Scott Hume, Electric Power Research Institute, Inc.; Richard L. Axelbaum, Zhiwei Yang, Washington University in St. Louis;Bhupesh Dhungel, Research Scientist, American Air Liquide, Inc., USA; Jonathan D. Slater, Raghbir S. Panesar, Doosan Babcock Limite; UK

Staged Pressurized Oxy-Combustion (SPOC) is a low-carbon coal combustion power technology being developed by Washington University in St. Louis (WUSTL). Oxy-combustion plants enable more straightforward capture of carbon dioxide (CO2) by removing most of the nitrogen in combustion air prior to use, thereby burning fuel in oxygen and flue gas recycle (FGR) instead of air, producing a flue gas containing primarily CO2 and water. CO2 capture at amounts > 90% are possible, using cryogenic

separation. FGR reduces the peak temperature and radiation that would otherwise occur in a fuel/oxygen only flame. SPOC reduces the peak temperatures of combustion by utilizing two or more pressurized boiler modules connected in series to produce fuel staging; hence, only a portion of the fuel is combusted in any given furnace module (the SPOC process is shown in Figure 1). This means that the thermal energy released at each stage can be captured and removed from the gases prior to subsequent stages, when more fuel is introduced. This allows the SPOC process to operate with minimal FGR, avoiding the associated efficiency losses and additional costs. Also, the process operates at an elevated gas-side pressure, reducing boiler size, enhancing heat transfer to achieve a compact boiler configuration as compared to an atmospheric-pressure boiler design, and allowing the recovery of the latent heat of the water from the flue gas at a temperature useful to the steam cycle. The resultant net efficiency of the system is over 3 percentage points greater than traditional atmospheric-pressure oxy-combustion, and 7 percentage points greater than amine-based post-combustion CO2 capture, representing a step-change improvement over first-generation capture technology.
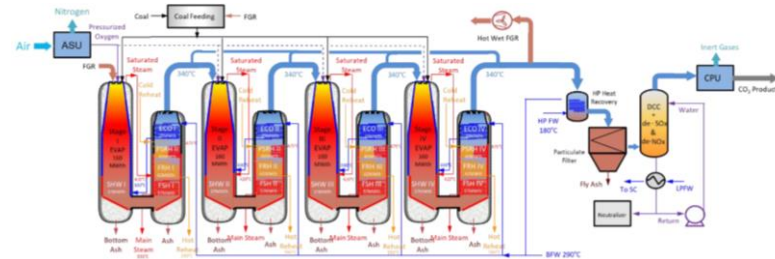

Figure 1: SPOC process

To further develop the concept, WUSTL and the Electric Power Research Institute, Inc., working with leading manufacturers American Air Liquide, Inc. and Doosan Babcock Limited, were awarded funding from the U.S. Department of Energy to investigate a practicable and workable SPOC boiler design. A key finding by the team was the potential for enhanced process flexibility for controlling power generation over a wider load range than is normally available to conventional coal-fired power plants due to the staged nature of the heat release of the SPOC technology. With increasing intermittent renewable generator contribution, on-demand generators need to be highly flexible to participate in the future energy market, requiring extensive operation at reduced load – an operating mode that SPOC appears to be well-suited for.

Conventional coal-fired steam generators typically face challenges in maintaining temperature control of the reheat and main steam at reduced loads. This results in inefficient operation, both in terms of the boiler efficiency and steam turbine heat rate. The results of this project showed that the SPOC process is capable of exceptional turndown, both on a stage basis and with the ability to bypass entire stages. Oxygen supply flexibility was also investigated as this is a key consideration for the overall flexibility of the SPOC process given the operating constraints of conventional air separation units.

A boiler design concept assessment was conducted and focused on delivering a compact and constructible design. The assessment assessed appropriate tube operating metal temperatures at full load and at lower operating loads, balanced against the needs of efficient coal combustion, and the resultant slagging and ash environments. Combustion testing in the 100-kWth pressurized combustion test rig at WUSTL (a photo of the test rig is shown in Figure 2) was carried out to validate the combustion, heat flux profiles, and burnout at multiple loads.
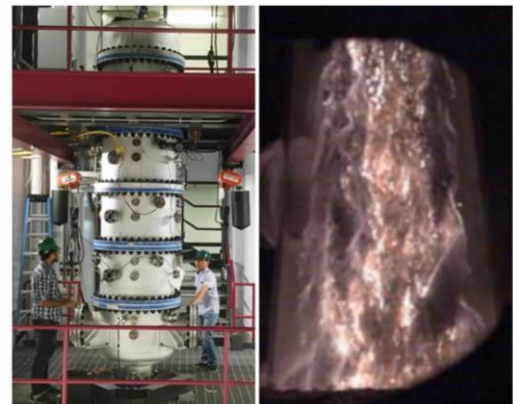

Figure 2: 100-kWth pressurized oxy-combustion unit with 80-kWth coal flame high-speed image

The combustion parameters investigated were flame stability, fuel burnout, ash composition, radiative heat flux, and temperature profiles. The results of these tests, which formed the basis of a full-scale boiler design that encompasses both efficiency and flexibility improvements over conventional oxy-combustion processes, will be presented. The air separation unit flexibility was also investigated, and associated cost implications were addressed. Detailed techno-economic assessment results for a 550-MWe net power block utilizing SPOC will also be provided showing comparison against the baseline U.S. National Energy Technology Laboratory oxy-combustion and post-combustion capture cases.

17.3 Impact of Particle Injection on Gaseous Flow at Elevated Pressure

Ansan Pokharel, Ismail B. Celik, V'yacheslav Akkerman, West Virginia University; Zhiwei Yang, Richard L. Axelbaum, Washington University in Saint Louis, Saint Louis; USA

Optimization of coal injection into a burner can promote efficient and clean coal combustion. To shed light on such injection processes, it is important to understand the flow dynamics and the interplay between the coal and carrier phase. In particular, this is essential for promising new CCUS technologies such as *staged pressurized oxy-combustion* (SPOC), where pulverized coal particles are injected along with a gaseous carrier. The fundamental properties and behavior of such a two-phase flow are scrutinized in the present work by means of comprehensive numerical simulations employing the Ansys FLUENT commercial platform. Specifically, keeping in mind the properties of the SPOC burner, here we consider a coal-air flow in an annular pipe (hollow cylinder) operating at a pressure of 15 bar and a moderate Reynolds number of $\sim 6 \times 10^3$. The influence of the various factors, such as particle loading, the interaction between the phases, and turbulent dispersion, on the flow dynamics is systematically studied. Specifically, particle loading with a volumetric fraction of 1.2 % is defined as high particle loading, while a volumetric fraction of 0.13 % is referred to as low particle loading. In particular, seven different cases for a gas-solid phase flow are investigated, namely:

1) Pure gas flow;
2) Low particle loading two-phase flow with one-way coupling and with turbulence dispersion;
3) Low particle loading two-phase flow with two-way coupling but without turbulence dispersion;
4) Low particle loading two-phase flow with two-way coupling and with turbulence dispersion;
5) High particle loading two-phase flow with one-way coupling and with turbulence dispersion;
6) High particle loading two-phase flow with two-way coupling but without turbulence dispersion;
7) High particle loading two-phase flow with two-way coupling and with turbulence dispersion.

The boundary layer was found to grow *without* fluctuations in turbulent kinetic energy (TKE) for Cases 1, 2, and 5. For Case 4, the TKE fluctuations were observed, but were not as substantial as in Cases 6 and 7. We attribute such a difference in the nature of the fluctuations to the particle loading. In addition, the onset and development of the flow instability have been observed at a random axial distance in Cases 4, 6 and 7. This instability is presumably caused by the two-way coupling with turbulence dispersion in a flow under consideration. It is concluded that the particle loading, one-way or two-way coupling between the phases, and the turbulence dispersion models significantly influence the flow dynamics.

17.4 Mechanism of Methane /Char Chemical Looping Reduction over Calcium-doped Copper Oxide as Oxygen Carrier

Hanjing Tian, Lei Bai, Jarrett Riley, West Virginia University, USA

Chemical looping with oxygen uncoupling (CLOU) is a novel CO2 capture technology by using metal oxides to release gaseous O_2. The advantage of CLOU is the instant oxygen releasing/transfer from the bulk or surface of oxygen carriers, so that the thermodynamic limits for combustion reaction will be overcome. However, fundamental kinetic of surface structure with oxygen transfer, as well as the reduction activity/selectivity has not been established yet. In this study, calcium-doped (1, 2 or 4 wt%) copper oxides based oxygen carriers were prepared by impregnation method and employed in the CLC with Wyodak char and methane as fuels up at 900ºC. Utilizing a combination of XRD and XPS analysis, calcium was confirmed to be dispersed on the surface of CuO. It was claimed that doping Ca improves CuO oxygen uncoupling characteristics. By comparing the chemical looping reduction process of Ca-doped CuO and un-doped CuO, Ca surface-doping increases the lattice oxygen transfers and surface O_2 formation under CLOU conditions. Meanwhile the comparison of decomposition

reactivity of doped and undoped CuO suggested the change of reduction pathway from a sequential (CuO→Cu2O→Cu) to a direct transition (CuO→Cu) during OCs decomposition or once the solid fuel was introduced. Moreover, with the increasing of surface Ca-doping (1, 2 or 4 wt%), char gasification was initiated, which led to enhancing CO production. Periodical density functional theory (DFT) calculations also be reported to clarify the mechanism of gaseous O2 release of Ca-doped CuO.

17.5 Amine Sorbents for Selective Recovery of Heavy Metals from Coal Waste Effluent Streams

Qiuming Wang, Walter C. Wilfong, Brian W. Kail, Fan Shi, Tuo Ji, McMahan L. Gray, National Energy Technology Laboratory, Department of Energy, USA

Toxic heavy metals in water sources have proven to be a major threat to communities throughout the world. Much of the cost of industrial wastewater treatment is driven by the need to remove heavy metals that cannot be discharged to local waterways. To address the problem of heavy metal contamination in wastewater streams, a library of novel patented sorbent materials has been developed at the National Energy Technology Laboratory (NETL) that demonstrates high affinity to heavy metals, such as Se, Cd, Hg, As, Pb and Cr. NETL 53A and PES-0.43-500 showed high capacity and selectivity for toxic (Pb, Cd, Hg, Se, As, Se), and other heavy (Al, Mn, Zn, Cu, etc.) metals removal/recovery from synthetic solutions and high salinity coal waste effluent streams. Initial testing on industrial FGD effluent streams has shown 53A captured 55-96% of Cr, Cd, and Hg and PES-0.43-500 captured 58-86% of the Cr, Cd, Pb and Hg. PES-0.43-500 also achieved superior removal of uranium (U, non-radioactive) and rhenium (Re) down to below their reporting limits. Adsorption of both U and Re suggests that Basic Immobilized Amine Sorbent (BIAS) sorbents could be used for radioactive applications, like cleaning superfund sites. Robust performance and easy scalability of green BIAS materials make them attractive for commercialization.

SESSION 18
CARBON MANAGEMENT - 4
Bingyun Li and Ahmed Aboudheir

18.1 Economic Analysis of Flexible Carbon Capture Systems

Yash Kumar, Pamela Shirley, KeyLogic Systems; Shangmin Lin, Deloitte Consulting LLC; Jeff Hoffmann, Joel Theis, National Energy Technology Laboratory; Arun Iyengar, KeyLogic Systems; USA

The development of variable renewable electric (VRE) power resources in recent years and the possibility of greater amounts being built in the future may require new and existing coal-fired power plants (CFPPs) to operate more flexibly. Continued operation and deployment of CFPPs could also warrant capture of their carbon dioxide (CO_2) emissions considering possible future curbs on greenhouse gas (GHG) emissions. The National Energy Technology Laboratory (NETL) has been actively pursuing the development of high-performance low-cost carbon capture technologies under the Carbon Capture Research and Development (R&D) programs at the Department of Energy (DOE). Carbon capture and storage (CCS) implementation for CFPPs are still at a nascent stage mainly due to the significant investment required combined with the lack of policy drivers. Energy market studies have shown that additional revenue drivers, such as utilization of CO_2 to produce oil through enhanced oil recovery (EOR) operations, along with incentives such as the tax credits from the 45Q program, are likely to be required to enable deployment of CO_2 capture technologies at CFPPs to offset the large capital investment associated with CCS systems.

The present study developed a detailed analysis of viable business models for CCS retrofits at CFPPs that included either selling the CO_2 to EOR operations or sequestering the CO_2 in saline formations with and without the incentives offered by the 45Q program. The existing United States (U.S.) CFPPs that were particularly suited to CCS retrofits in the short-term were identified based on a comprehensive process that considered geospatial restrictions, technological constraints, and regulations. In particular, existing CFPPs were shortlisted for economic dispatch analysis based on presence of emissions control systems; nameplate capacity, CO_2 emissions threshold; and locational and technical constraints relative to EOR fields or Saline Storage basins. A CCS retrofit configuration that included pairing the main plant with a dedicated auxiliary plant to support the CCS loads was analyzed. The impact of the CCS retrofit on the operations of the identified plant, particularly its capacity factor, was investigated using a linear optimization and dispatch (LOAD) model with a special sub-module for modeling the auxiliary CCS plant configuration. The CCS sub-module allows for modeling the closely coupled interaction between the main plant and the auxiliary plant including the complex trade-off between generation of economic value from the sale of the CO_2 captured and the market value of dispatched electricity (from both the main and auxiliary plants). A comprehensive discounted cash flow analysis was carried out to evaluate the internal rate of return (IRR) for a capture project at each unit of the plant

based on the findings of the LOAD model along with electricity revenues from the power systems simulations using the commercial platform PROMOD™.

A total of five plants including 13 units were investigated. Results show a variation in plant profitability depending on the differences in electricity market and EOR CO_2 revenue relative to fuel costs. The results show that with the 45Q tax credit, all 13 units at the 5 plants are financially viable for CO_2 capture projects for *CO_2-EOR* at CO_2 prices greater than \$15/tonne. However, CO_2 prices greater than \$45/tonne are required for the financial viability of EOR projects at all the units considered without the 45Q incentive. Most of the units were also found to be financially viable for *saline storage projects* with the 45Q tax credit when the CO_2 transport and storage project costs were lower than \$10/tonne of CO_2.

18.2 SimCCS: An Open-source Tool for Optimizing CO_2 Capture, Transport, and Storage Infrastructure

Richard S. Middleton, Los Alamos National Laboratory; Kevin M. Ellett, Indiana University; Brendan A. Hoover, Los Alamos National Laboratory; Xiaochun Li, Ning Wei, Chinese Academy of Sciences; Sean P. Yaw, Montana State University; USA

Carbon capture and storage (CCS) is a key technology for reducing CO_2 emissions from coal-related industries including coal-fired electricity generation, coal liquefaction, and hydrogen production. CCS will enable coal to remain a central part of the global economy for power and fuel production while minimizing the carbon footprint. Commercial-scale CCS technology will involve deploying infrastructure on a massive and costly scale. In the US, this could mean deploying CCS infrastructure on a similar scale as natural gas infrastructure. This effort will require careful and comprehensive planning to ensure that capture locations, storage sites, and the dedicated CO_2 distribution pipelines are selected in a robust and cost-effective manner. *SimCCS* (https://*SimCCS*.com/) is an optimization model that employs an open-access system framework to enable researchers, stakeholders, and policymakers to design CCS infrastructure networks. It is a portable software package, useable and shareable by the CCS research, industrial, policy, and public communities. Accessing user-provided CO_2 source, sink, and transportation data, *SimCCS* creates candidate transportation routes and formalizes an optimization problem that determines the most cost-effective CCS system design. This optimization problem is then solved either through a high-performance computing interface or through third-party software on a local desktop computing platform. *SimCCS* is written in Java and is publicly available via GitHub to encourage collaboration, modification, and community development. *SimCCS* won two R&D 100 Awards in 2019.

SimCCS is a central tool for the US-China Clean Energy Research Center (CERC) Advanced Coal Technologies Consortium (ACTC; https://cerc-actc.wvu.edu/). It has been used collaboratively by US and China partners in the CERC-ACTC to address large-scale CCS problems in key areas in both the US and China. Here, we demonstrate *SimCCS* using examples from the CERC-ACTC project including coal-based infrastructure for the US' Illinois basin (focusing on coal-fired electricity generation) and China's Ordos basin (focusing on coal use for electricity, fuels, and chemicals). We illustrate how *SimCCS* develops end-to-end CCS infrastructure solutions including identifying optimal CO_2 capture points, geospatial deploys a realistic CO_2 pipeline network, technoeconomic analysis, and CO_2 storage and utilization. Further, we show how *SimCCS*' economic assessment integrates CO_2 incentives such as the US' 45Q CO_2 credits and CO_2 revenues such as enhanced oil recovery. Overall, *SimCCS* is an important tool to help understand how coal can continue to play a central role in the global economy while minimizing the environmental impact.

18.3 Microwave-Assisted Sorbent Regeneration for Post-Combustion CO2 Capture from a Humidified Flue Gas

Candice Ellison, James Hoffman, Dushyant Shekhawat, DOE/National Energy Technology Laboratory; USA

In a typical post-combustion CO_2 capture process, sorbent regeneration accounts for a significant energy penalty on the overall process. For hygroscopic (i.e. hydrophilic) sorbents in particular, competitive adsorption of H_2O on the surface limits the CO_2 adsorption capacity of the sorbent, which reduces the cycling productivity and increases the regeneration energy penalty. The effect of flue gas moisture on CO_2 adsorption has been widely studied on type X zeolites, including 13X, and several authors have suggested rapid cycling as one solution to overcoming the limited CO_2 adsorption capacity during TSA processes from a humidified flue gas. To achieve rapid cycling, this study uses microwave energy for sorbent regeneration under both dry and humidified conditions. Our previous work showed that microwaves significantly increase regeneration rates under dry CO_2 conditions leading to increased cycling productivity. For this study, microwave heating is investigated as a technique for rapid co-desorption of CO_2 and H_2O from zeolite 13X, a hygroscopic sorbent that particularly suffers from adsorption of moisture. Cyclic adsorption/desorption testing with a humidified CO_2 gas in a fixed bed microwave and conventional reactor was carried out. It was found that while adsorption capacity decreases as a result of competitive moisture adsorption, application of microwaves during the regeneration step made it possible to increase desorption rates of co-adsorbed CO_2 and H_2O compared to conventional thermal regeneration resulting in improved cycling productivity. The rapid desorption is mainly attributed to the strong microwave interaction with water molecules due to E-field induced dipolar rotation during microwave irradiation. Further analysis of the CO_2 desorption curves will be presented.

18.4 Carbon Capture Program at DOE/NETL: Overview

Dan Hancu, DOE/NETL, USA

The U.S. Department of Energy's (DOE) Fossil Energy Program has adopted a comprehensive, multi-pronged approach to the research and development (R&D) of advanced carbon dioxide (CO2) capture technologies for today's fossil fuel-based power platforms as well as for industrial systems. The National Energy Technology Laboratory (NETL) is implementing the Carbon Capture R&D Program to develop the next generation of advanced CO2 capture concepts. The success of this research will enable cost-effective implementation of carbon capture and storage (CCS) technologies throughout the power generation sector and ensure the United States will continue to have access to safe, reliable, and affordable energy from fossil fuels.

The Carbon Capture program consists of two core research areas, Post-Combustion Capture and Pre-Combustion Capture, composed of projects with technology readiness levels (TRL) ranging from conceptual engineering and materials design (i.e., TRL 2) to 25 MW-electrical (MWe) equivalent pilot testing (i.e., TRL 5-7). These two core areas are focused on creating technological improvements providing a step-change in both cost and performance as compared to current state-of-the-art solvent-based capture systems. Post-combustion systems separate CO2 from the flue gas stream produced by conventional fossil fuel-fired power plants after fuel combustion in air. In this approach, CO2 is separated from nitrogen (N2), the primary constituent of the flue gas. Pre-combustion systems are designed to separate CO2 and hydrogen (H2) from the syngas stream produced by the gasifier in integrated gasification combined cycle (IGCC) power plants. In both cases, R&D is underway to develop technologies based on advanced solvents, sorbents, membranes, hybrid systems, and other novel concepts. Additionally, the program advances technologies in emerging research areas of Carbon Capture from Industrial Sources and Negative Emissions Technologies such as Direct Air Capture (DAC) and biomass-coal co-firing with Carbon Capture (BECCS).

The talk will provide a technical overview of the DOE/NETL's Carbon Capture Program.

18.5 Electrocatalytic Conversion of CO_2 and Water into Industrially Relevant Chemicals

Douglas R. Kauffman, National Energy Technology Laboratory, USA

The electrochemical CO_2 reduction reaction (CO$_2$RR) is a promising carbon mitigation strategy uses excess electrons to convert CO_2 and water into carbon-neutral chemicals and fuels. The oxygen evolution reaction (OER), also referred to as "water oxidation", is an equally important reaction that represents the anodic process in CO_2 electrolyzers. Large overpotentials and costly state-of-the-art catalysts for both reactions introduce substantial cost-barriers that hinder large-scale deployment of electrochemical systems, and further catalyst improvements are needed. This talk will highlight NETL's recent catalyst development efforts for both CO$_2$RR and OER, with an emphasis on: (1) improving activity, product selectivity and Faradaic efficiency, (2) reducing precious

metal requirements, and (3) developing atomic-level understanding of catalyst performance.

CO₂RR catalyst development efforts will highlight well-defined nanoalloys that reduce or eliminate precious metal content while improving overall performance. In particular, we developed synthetic strategies to produce ~2 nm diameter gold-copper nanocatalysts that reduced precious metal requirements by 50% while retaining excellent activity and product selectivity. We will also describe recent efforts to control product selectivity by tuning the 3D surface structure of transition metal oxides. This approach allowed us to completely eliminate the need for precious metals while retaining product selectivity that rivals state-of-the-art silver and gold. OER catalyst development efforts will describe our recent "applied surface science" approach that combines ultra-high vacuum synthesis and characterization techniques with aqueous electrochemistry. These efforts allowed atomic-level imaging of well-defined catalysts, precise identification of important catalytic reaction centers, and the ability to assign *site specific* turnover frequency values, and we demonstrate that edge effects can boost the OER activity of inexpensive iron oxide over that of state-of-the-art IrO₂ catalysts. In all cases, the use of synchrotron and laboratory characterization techniques, coupled with complementary computational modeling, allowed us to formulate atomic-level understanding of the catalytic process. The combined efforts provide catalyst design strategies for lowering the cost and improving the energy efficiency of electrochemical CO₂ conversion technologies.

SESSION 19
COAL SCIENCE - 1
Allan Kolker and Francis Lau

19.1 Analysis of Thermal Behavior of Crystalline Minerals in Argonne Premium Coals Under Air and Argon Atmospheres

Atsushi Ishihara, Mie University; Kentarou Takai, Tadanori Hashimoto; USA

Coal is mainly used as a raw material for coal-fired power generation fuel and iron-making coke. Ash components in coal have problems of affecting the high temperature corrosion of gas turbine blades in thermal power generation and the production and property of coke used in iron making. For the reasons, it is important to know the change in behavior of ash components with treating temperature and heating rate. In this study, the thermal behavior of ash components of Upper Freeport (UF) coal, one of bituminous coal with medium volatile matter, Illinois No.6 (IL) coal, one of bituminous coal with high volatile matter and Beulah-Zap, one of brown coal (BZ), among Argonne Premium Coals under air and argon atmospheres were investigated using XRD, TEM-EDS and TG-DTA.

UF, IL and BZ coals were purchased from Argonne National Laboratory. Chemical composition of UF is C 85.50%, H 4.70%, N 1.55%, S 0.74%, O 7.51%, that of IL is C 77.67%, H 5.00%, N 1.32%, S 2.38%, O 13.51%, and that of BZ is C 72.94%, H 4.83%, N 1.15%, S 0.70%, O 20.34%, respectively. Thermal gravimetric (TG) and differential thermal analyses (DTA) using Shimadzu DTG60AH were performed under the conditions, air or argon atmospheres, the flow rate 100 ml/min, the temperature 800℃, 900℃, 1000℃, 1100℃ or 1200℃, the heating rate 10℃/min. Further, TG-DTA measurement of coal samples treated by TG-DTA at 800℃, 900℃, 1000℃, 1100℃ or 1200℃ under an argon atmosphere was also performed at 800℃ under air atmosphere. In order to obtain samples for X-ray diffraction (XRD) measurement, 0.7 g of Upper Freeport was treated in 100 ml/min under air or argon atmosphere at 800℃, 900℃, 1000℃, 1100℃, 1200℃ at a heating rate of 10℃/min. XRD patterns were measured in order to examine the crystal structures of ash components in coal samples treated under air or argon atmosphere using Ultima IV. Transmission electron microscopy (TEM) measurement of samples treated by TG-DTA measurement under air or argon atmosphere was performed using JEM-1011 (JEOL Co. Ltd.). STEM-EDS was measured by JEM-2100F/HK in Nagoya University.

In this study, the changes in the behavior of ash components in UF, IL and BZ coals with changing the treating atmosphere and temperature were investigated using TG-DTA, XRD and TEM measurements. Quartz, hematite, andalusite (Al₂O₃·SiO₂) and anhydride (CaSO₄) existed under all heat-treatment conditions. Calcite (CaCO₃) existed after heat-treatment at 800℃ under air atmosphere, however, it disappeared at higher than 800℃. From the TEM observation, needle-like crystals, which were not seen in the raw sample, were observed in UF heat-treated under air atmosphere, although such crystals were not seen in IL heat-treated under air atmosphere. When IL sample was heat-treated under air atmosphere after heat-treated under Ar, however, needle-like crystals appeared. When TEM-EDS of these samples was measured, it was shown that these needle-like crystals were composed of Al₂O₃ and SiO₂. In IL treatment under air atmosphere, lime (CaO) was observed while oldhamite (CaS) was observed under Ar atmosphere. Further, in BZ treatment under air atmosphere, quartz (SiO₂), calcite (CaCO₃) and anhydride (CaSO₄)

were observed at 800℃ but disappeared at 1200℃. Instead of these minerals, mullite (Al₆Si₂O₁₃), gehlenite (Ca₂Al₂SiO₇) and Ca₃Al₂O₆ appeared at 1000℃ and remained even at 1200℃.

19.2 Molecular Dynamics Simulation of Methane Adsorption on High-Rank Coal

Zhiyuan Yang, Yinyan Li, Xue wenying, Xiaoyu Song, Zhiqiang Yin, Xi'an University of Science and Technology, CHINA

Abstract: The adsorption characteristics of coalbed methane have an important pole on the adsorption properties of coal. By Fourier transform infrared spectroscopy (FTIR), ¹³C solid-state nuclear magnetic resonance (¹³C NMR), X-ray diffractometry (XRD), and high-resolution transmission electron microscopy (HETEM), the model of Yangquan macromolecule for anthractice coal could be constructed. The simulation was conducted by the Forcite and Sorption modules in the 2017Accelrys Materials Studio (MS), which was used to simulate the molecular mechanics and molecular dynamics of the constructed configurations, and the minimum energy configurations were obtained. Then the density of configuration is explored and the density of the constructed coal is about 1.44g/cm³, which is taken as the real density of Yangquan coal. On this basis, the interaction mechanism between coal macromolecule and methane was explored. The results show that temperature and pressure have an important influence on methane adsorption by coal molecules. With the increase of temperature, the amount of methane adsorption decreases. With the increase of pressure, the amount of methane adsorption increases, and finally approaches a critical value. The relative error of Langmuir adsorption constant (a) between the simulated and experimental isothermal adsorption results at 303.15k is 15.1%, which indicates that it is feasible to study methane adsorption behavior by constructing coal macromolecules. In the saturated adsorption, the saturated adsorption amount of methane molecules adsorbed by coal macromolecular structure is 8, and the adsorption is accumulated in coal. In the macromolecular structure of coal, carbonyl has the strongest adsorption capacity for methane. The order of functional groups on the surface of coal macromolecules is carbonyl > hydroxyl > methyl > ether bond.

19.3 Beneficiation of Coal Using Supercritical Water and Carbon Dioxide Extraction: Sulfur Removal

Matthew J. DeCuir, Virginia Commonwealth University; Ram B. Gupta, Virginia Commonwealth University; Bhima Sastri, U.S. Department of Energy; USA

This work explores the use of carbon dioxide, water, and their mixtures as solvent for the precombustion beneficiation of raw coal without using any toxic mineral acids in the temperature range of 200–400 °C. The fluid polarity, ionic constant, and supercritical point can be adjusted by H2O/CO2 ratio and temperature. Adding carbon dioxide to hydrothermal fluid also increases the ionization by forming carbonic acid. Extractions with supercritical fluids have several benefits including enhanced mass transport, ease of separation and recycle, wide range of extractive capability and tunability, better inherent safety, and in the case of carbon dioxide and water–low cost. A semi-continuous extraction system was designed and built in which pressure, temperature and the relative flow rates of CO2 and H2O can be controlled. Coal powder is kept in a packed bed and the extraction is carried out at 143 bar pressure. Using sulfur as a model heteroatom, extractive efficiency is examined as a function of the temperature, fluid composition, fluid flow, and extraction time. The results indicate that carbon dioxide, water, and supercritical water-carbon dioxide (ScWC) all can effectively extract about 50% of total sulfur from bituminous coal in 1 h. Extraction above 350 °C decreased effectiveness, and extraction above the supercritical point of pure water caused hydrothermal carbonization. ScWC extraction may provide necessary control to prevent organic dissolution while removing sulfur.

19.4 Design of a Pilot Scale Spouted Bed Reactor for Thermal Desorption of Contaminants from Coal

Gerrit Botha, Quang Truong, Srujan Rokkam, Advanced Cooling Technologies, Inc.; Carlos Romero, Lehigh University; Zheng Yao, Energy Research Center, Lehigh University; Bhima Sastri, U.S. Department of Energy; USA

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. Most of these pollutants are persistent and accumulates in food chains and the environment. One of the main drawbacks in using coal for electricity generation, is the presence of these contaminants and the additional steps/cost needed to remove these contaminants. This research aims to develop a means to remove coal contaminants using a suitable thermal desorption processes that provides an economical option for small modular plants.

Thermal desorption is the process of forcing hot air through pulverized coal. To increase the efficiency, the coal is agitated, this is usually achieved by means of using a rotating

drum. Raising the temperature to above 300°C had shown that Mercury, Sulphur, Arsenic, and Lead compounds can be removed from coal. Although this method works, it is energy intensive, as external heat and agitation must be supplied. To optimize and increase the efficiency of the thermal desorption process, a custom spouted bed reactor (ACT's design with modified internal geometry) was investigated. The main advantage if the spouting bed is that the coal can be agitated without using any moving mechanical components and the custom design improves overall mixing of the coal.

A DEM/CFD analysis was done with MFiX to investigate the flow path for a simple and ACT design, lab-scale, spouted bed reactor in 2D. The design considerations were then used and verified with a lab-scale experiment. From the lab-scale experiment, it was found that up to 65% of Mercury, 28% of Sulphur, 43% of Arsenic, and 45% of Lead compounds where removed from bituminous coal via thermal desorption [Ref. 1].

Using MFiX for a 3D simulation of the custom spouted bed design caused issues, as the internal structures of the 3D geometry could not be properly meshed with the native MFiX mesher. After investigating different DEM software packages, EDEM coupled with Ansys Fluent proved adequate for the 3D pilot scale design. The lab-scale experimental results were used to calibrate a lab-scale spouted-bed in EDEM. The calibrated EDEM simulation was then used to optimize the design for the pilot-scale spouted bed reactor. The DEM/CFD results show that the optimized custom-spouted bed can reduce the energy requirements by 25%. Subsequently, the scalability of ACT's custom spouted bed and thermal desorption on Lignite and Anthracite were investigated. This work was funded by Department of Energy SBIR program, Award Number DE-SC0017232, awarded to Advanced Cooling Technologies, Inc.

Ref 1: Truong, Q., Rokkam, S. and Romero C. et. al., Spouted Bed Reactor Designs for Thermal Desorption of Mercury Compounds, DOE Phase I Final Report, DOE-ACT-17232, Dec 2017. https://www.osti.gov/biblio/1411122.

19.5 Development of A Unified and Comprehensive American Coal Database (acd) to Support Source to End Coal Resource Analytics

Devin Justman, Leidos Research Support Team; Kelly Rose, National Energy Technology Laboratory (NETL); Randall (Burt) Thomas, Scientist, Leidos Research Support Team; USA

Significant information and data exists on domestic US coal resources from numerous open-source datasets. However, at present these are found in disparate, multivariate, multiple source, multi-format files, including historical documents that are poorly searchable. In their current format these data offer little utility to end-users including buyers, researchers, and government entities. Moreover, current coal databases are often missing key information, such as proximate/ultimate analyses and contextual data which are often needed for intelligent analytics to support a range of end-user needs. Tackling the challenge of big-data analytics for coal resources and carbon management requires a unified American Coal Database (ACD) to improve efficiency, environmental stewardship and data-driven technology breakthroughs. The ACD was developed through an approach incorporating a series of online searching, cataloging, and processing to integrate the complex, disparate but relevant data resources spanning spatio-temporal, coal quality, and end-use attributes and characteristics. Additionally, we present opportunities to enhance this approach using a novel, machine learning, natural language processing algorithm. This work specifically addresses data-needs for models that will target pairing coals of different compositions and qualities with compatible boilers at power production facilities to ensure maximum efficiency, fuel flexibility, power production, and economic outcomes. Currently, the ACD contains more than 60 datasets related to coal resource geology, infrastructure, and geochemistry including over 47,000 coal sample records that can facilitate science-driven data analytics to offer insights for optimization on both the pairing of coals with appropriate power production facilities and to determine efficiencies that benefit both the post-combustion materials and power industries in the US and export market. Future analyses utilizing the ACD may also benefit the penetration of new technologies, including those related to the beneficiation and co-production of critical minerals and other materials. Ultimately, this user friendly machine-readable database provides a useful and important foundation for future coal research initiatives including efforts at improving production efficiency, infrastructure, coal transport network efficiency, and foster the development of new markets for coal as a carbon nanomaterial feedstock.

20.1 Utilization of Fly Ash Generated by Pulverized Coal Combustion Boiler Dumped in a Coastal Landfill Site

Hirokazu Murata, Shimizu Corporation, JAPAN

In FY 2018, coal-fired thermal power plants in Japan supplied 287.2 billion kWh of power and generated nearly 12.8 million tons of coal ash from raw coal. Eighty percent of this coal ash was used effectively, mostly as raw materials in cement and as civil engineering construction materials. The remaining 20% was buried in a landfill site, 8% of which was in a landfill reclamation area and 12% of which was in a coastal reclamation area. If the coal ash buried in the landfill site can be safely and effectively used as recycled material that replace natural resources, the landfill site could potentially supply a large amount of recycled material at one time and function as a stock yard. As a result, this scenario could contribute to the formation of a recycling-oriented society and reduce the natural environmental load.

We reported previously (1) that fresh water can be added to fly ash (dry matter) from a pulverized coal combustion boiler to simulate the conditions of fly ash stored in a landfill site. Tests were conducted to confirm the presence of an aging effect on the buried fly ash (aging ash). As a result of the aging effect, the concentrations of heavy metals in the leachate from the buried fly ash were lower than from the unburied fly ash and decreased over time. On the other hand, the leachate concentrations in the aging ash buried in the coastal reclamation area are unknown. In this study, in order to understand the effect of seawater on coal ash during the aging period, seawater was added to fly ash samples and changes in heavy metal elution were observed. We also evaluated how differences in the length of the aging period affects the subsequent materialization.

Simulated aging fly ash (SAFA) was used in this study because, compared to using a core sample of aging ash buried in an actual landfill site, more accurate burial durations can be determined. By using the SAFA, it was possible to understand how the elution of heavy metals changed over time. The coal ash used in this experiment was fly ash collected from electrostatic precipitators in 13 coal-fired thermal power plants in Japan. In addition, the amount of seawater added to the prepared fly ash samples was mixed at an optimal moisture content that maximized the degree of compaction for each fly ash sample. The characteristics of fly ash in Japan are dependent upon the coal types imported from overseas, and so the characteristics of generated fly ash vary.

Using SAFA that was cured in a closed container in a wet state, hexavalent chromium (Cr (VI)), arsenic (As), selenium (Se), fluorine (F), and boron (B) were measured by periodically testing changes in heavy metal concentrations of the elution. Furthermore, effects on materials created using SAFA due to differences in the aging period were determined by preparing a sample in which a small amount of cement (3% blast furnace slag cement B type) was added to the SAFA for different aging periods (90 days, 180 days, and 360 days). We then evaluated any changes in the dissolution behavior that resulted from this difference. Since physical requirements such as strength changes depend on the intended use of the fly ash, the material can conform to a wide range of physical requirements by reducing the amount of added cement to the extent possible. Therefore, considering the minimum amount of cement that can be uniformly mixed, 3% cement was added.

The elution tests were performed once every recycling period (at 7 days, 28 days, and 91 days). As a result, in the experiment using seawater, the heavy metal concentrations in the elution, except for Cr (VI) decreased as the aging period lengthened, similar to the results obtained in the experiment using freshwater. In addition, in materials created using aging ash with an aging period of 90 days or longer, the heavy metal concentrations in the elution, except for that of Cr (VI), were reduced below Japanese environmental quality standard values for soil regardless of the length of the aging period. The aging effects of seawater on the fly ash are summarized below.

1) Due to seawater aging, the concentrations of As, Se, F, and B decreased with longer aging periods.

2) Adding 3% cement to aging ash with an aging period of >90 days can suppress heavy metal concentrations (except for Cr (VI)) below the Japanese environmental quality standard values for soil.

As a result, risks associated with Cr (VI) in the elution still remain, so it is necessary to take additional measures to mitigate it. However, due to the aging effects of seawater, the elution of many heavy metals contained in fly ash were successfully suppressed.

Reference

(1)Hirokazu Murata, Motoyuki Asada, Masato Kawaguchi, "Fundamental Study on Leaching Characteristics of Heavy Metals from Landfilled Coal Ash", 2017 International Pittsburgh Coal Conference, Pittsburgh, PA, USA, 2017

20.2 Effect of Temperature and Ash Composition on Sodium Release and Occurrence Modes Transition in High-Alkali Coals

Zishun Li, Tai Zhang, Zhaohui Liu, Huazhong University of Science and Technology, CHINA

Burning a coal containing a high alkali yield can cause severe fouling issues. Studies have shown that occurrence modes of alkali metals can greatly influence the fouling tendency. In this study, sodium releasing character of two typical high-alkali coals with different ash composition were investigated in a horizontal tube furnace. Sequential chemical extraction, ICP-MS, XRD were used to explore the occurrence modes and crystal forms of sodium in residual ash. The focus is on the effect of the interaction between ash and sodium on the volatilization and migration conversion of sodium as temperature increases. The results show that sodium is released rapidly with the increase of temperature, and it mainly occurs before 1100 K. Most of the released sodium is originated from H_2O-soluble sodium. Ash components also have an important influence on the release of sodium, and there is a clear negative correlation between the sodium release rate and the molar ratio of [(Al+Si)-(Ca+Mg)] and Na in ash. The occurrence modes variation of sodium can be divided into three stages according to the increase in temperature: NH_4Ac-soluble sodium is transformed into HCl-soluble sodium from room temperature up to 700 K, considerable amount of H_2O-soluble sodium is transformed into insoluble sodium at 700-1000 K, part of the HCl-soluble sodium is transformed into insoluble sodium at 1000-1300 K. In addition, XRD analysis shows that NaCl and Na_2SO_4 are the main form of sodium at low temperature. While as the temperature rises, sodium reacts with other minerals in the ash, transforming to more complex minerals in the higher element series. At high temperatures, sodium mainly exists in the form of insoluble aluminosilicates.

20.3 Continuous, Real-Time TSS Monitoring Verifies Effluent Quality and Coal Ash Management Performance While Reducing Compliance Costs

Dave Fraley, YSI Incorporated; Chris Bauman, Dave Donahue, Xylem Inc.; USA

Reducing the cost and compliance burden associated with meeting final remediation effluent requirements continues to be a key driver to technical innovation. As many power plants continue to struggle with the critical last step in their coal ash remediation processes – the final testing phase – some plants have successfully adopted the use of recently advanced sensor technology to measure real-time total suspended solids (TSS) to verify their discharge water is meeting specified requirements. Accurate on-line TSS monitoring helps ensure and verify the remediation process is performing as intended at all times, regardless of variability in upstream influent. The sensing probe uses optical methods that detect the intensity of scattered light and digitally reports TSS concentrations in mg/L, which is effective and useful for calculating mass balances, a critical component of upstream treatment process control. Power plants traditionally rely on laboratories (including mobile labs) for TSS analysis, and testing often requires extensive manpower for attaining samples in remote locations, sometimes multiple times a day. On-line TSS monitoring significantly reduces this effort. The sensor's two measurement methods provide TSS readings that are accurate at extremely low concentrations (0.1 mg/L), with repeatability of <0.015% or >0.0006 FNU. Having the ability to monitor TSS real time, and obtain accurate results that are repeatable and verifiable with random lab tests, allows for users to automate functions such as controlling pumps transporting effluent, or start and stop pretreatment processes designed to keep effluent within permit guidelines.

20.4 Measurement of Heat Work Through Viscous Deformation During Coal Ash Fusibility Testing

Peter Y. Hsieh, US DOE/NETL, USA

Critical temperatures obtained during coal ash fusibility testing are important criteria for evaluating coal quality and for managing coal ash and slag. Coal ash is a complex mixture of incombustible oxides derived from sedimentary minerals. Because pyrometric cones are made from the same minerals that are major components of coal ash, the deformation of coal ash cones during ash fusibility testing is more similar to the deformation of pyrometric cones in the firing of traditional ceramics than the melting of a pure substance in a melting point apparatus. Recent work has shown that pyrometric cone deformation is likely to be viscoplastic in nature, with end-point temperatures strongly correlated with Littleton softening point temperatures, as calculated through thermophysical and slag viscosity models. If viscoplastic deformation in pyrometric cones measures heat work (i.e., the combined effect of temperature and time), then coal ash fusibility tests (AFTs) also measure heat work. Measured AFT critical temperatures depend not only on the initial coal ash

composition, but also on the processing history of the ash sample and the heating rate used during the test.

Using thermophysical and slag viscosity modeling, 4,726 coal ash records from the U.S. Geological Survey Coal Quality (COALQUAL) database were evaluated to estimate their solid phase fraction and effective viscosity values at AFT critical temperatures. The findings suggest two-phase viscous flow plays an important role in the deformation of coal ash cones. Moreover, strong positive linear correlations between AFT critical temperatures and respective liquidus temperatures help to explain the spurious correlation previously reported between AFT critical temperatures and the critical viscosity temperature in molten coal ash slags. Lastly, the correlation between AFT critical temperatures and the liquidus temperature provides a firm thermodynamic basis for all models that predict AFT critical temperatures based on coal ash composition. In contrast, a weak linear correlation between the initial deformation temperature and the solidus temperature suggests either equilibrium thermophysical modeling is not suitable where a large clay-derived amorphous phase may be present, or initial cone deformation is not caused directly by a percolation structure breakdown or a capillary-slurry state transition.

AFT temperature values, which measure heat work on coal ash, are likely to be helpful where long coal ash residence times and high operating temperatures are encountered: stoker furnaces, fluidized-bed combustion systems, and slagging gasifiers. Where coal ash residence times are short, as in pulverized coal combustion systems, AFT critical temperatures are less likely to reflect actual coal ash melting behavior. Further work on the effect of heating rate and rate of change in effective viscosity during AFT is needed to explain AFT critical temperature variability and improve repeatability and reproducibility under standardized testing conditions.

Figure: Pyrometric cones after firing.

SESSION 21
VALUE-ADDED PRODUCTS FROM COAL – 1
Zhiyuan Yang and Johan Duddy

21.1 Study On Controllable Synthesis of 9- Fluorenylmethanol by 9-Hydroxymethylation of Fluorene with Two-Step Method

Mei-Xin Guo, Taiyuan University of Technology; Cui-Ping Ye, Taiyuan University of Technology and Training Base of State Key Laboratory of Coal Science and Technology Jointly Constructed by Shanxi Province and Ministry of Science and Technology; Tian-Tian Shi, Rui-Nan Wang, Ya-Fei Qiao, Mei-Sheng Liang, Taiyuan University of Technology; CHINA

Anthracene residue is the remains after extracting anthracene and carbazole of the anthracene oil fraction with boiling point of 280-360℃. It is mainly rich in phenanthrene, fluorene and other high value-added components. It is a typical industrial organic solid waste. As important chemical intermediates, phenanthrene and fluorene are widely used in materials, medicine, pesticides and other fields. Due to the similar properties of phenanthrene and fluorene, it is difficult to achieve effective extraction by conventional physical separation methods. We used reaction separation coupling technology to separate fluorene and phenanthrene in anthracene residue. However, 9-fluorenylmethanol, the downstream of fluorene is an important chemical raw material. If fluorene is converted into 9-fluorenylmethanol through hydroxylmethylation, the difference in solubility between phenanthrene and 9-fluorenylmethanol is further enlarged, making the extraction of phenanthrene easier. Using fluorene as a raw material, two-step synthesis of 9-fluorenylmethanol was adopted. Under the catalysis of a base, the fluorene is first acylated to 9-formylfluorene, and then reduced to 9-fluorenylmethanol without separating the intermediate products. Elimination of conjugated bases (E1cb) can easily dehydrate 9-fluorenylmethanol to form ene-rich compounds under alkaline conditions, which could polymerize to form viscous by-products, and affecting the yield of product separation and purification in turn. Therefore, how to control the reaction conditions to reduce the formation of by-products is the focus and difficulty of this research. The experiment investigated the influencing

factors for 9-fluorenylmethanol synthesis by changing the types of acylating reagents and reducing reagents, reaction temperature and time, or adding auxiliary agents. The use of polar aprotic solvents shortens the acylation reaction time, and keeping the reduction system at a sufficiently low temperature can slow down the dehydration rate of 9-fluorenylmethanol. Furthermore, the addition of appropriate Lewis acid auxiliaries can improve the selectivity of the reduction reaction, reduce the formation of by-products and improve the yield of the target products. Adding the inorganic salt, such as barium chloride or calcium chloride before sodium borohydride addition, 9-formylfluorene can be highly selectively reduced to 9-fluorenylmethanol, and the yield can reach up to 76.27%. Meanwhile, the separation process of subsequent products can be simplified.

21.2 Medium-Low-Temperature Coal Tar Refining System for Co-production of Naphthenic Oil and Phenolic Compounds

Yi Huang, Wen-Ying Li, Jie Feng, Professor, Taiyuan University of Technology, CHINA

Abstract:
The conversion of medium- low-temperature coal tar into high performance fuel and value-added chemicals is a main approach to address the current global energy challenges. Due to the higher content heteroatom compounds and the higher price of coal tar with respect to petroleum feedstocks the profit associated with coal-based diesel is about half compared to that of the traditional petrol-diesel, which limits its competitiveness on the market. To this aim, a newly coal tar process has been developed that enable the efficient transformation. It is suggested to produce phenolic compounds and naphthenic oil of the system. Since the complex compounds and reactions involved during the hydrogenation process, a systematic matrix of model compounds was presented to represent the coal tar and product after the quality and quantity analysis. Kinetics modeling of the coal tar hydrogenation was proposed to optimize the process parameter and predict the characteristics of the products. The whole process energy efficiency, carbon, hydrogen, and oxygen element utilization efficiency are calculated, which value are 81.62 %, 88.21 %, 87.13 %, 31.25%, respectively. Life cycle assessment shows that the energy use, greenhouse gas emission and production cost of the system is 9.39 MJ/kg-product, 2.7 t CO_2-eq/t-product, and 3141.2 CNY/t-product. The newly process should be a good choice for energy safe strategy technology, and it is suggested that more efforts are needed to develop efficient and low-cost coal tar production technology to reduce energy consumption, investment and pollutant emissions.

21.3 A Brief History of Coal-To-Olefins Technologies

Dave Lyons, U.S. DOE/National Energy Technology Laboratory; Michael Angyus, Henry A. Long, III, Massood Ramezan, KeyLogic Systems, Inc; USA
Olefins represent a major component of the petroleum chemicals industry with collective markets summing to more than $300 billion. The 1973 oil embargo ignited research on coal-to-olefins (CTO) technology in order to secure the domestic production of these important chemicals. In the last 50 years, significant progress has been made, both technologically and commercially, to make synthesis of olefins from coal a reality. China is the primary commercial player, producing around one-tenth the global market for petroleum-based olefins, while the United States has made, and continues to make, a large impact on research and demonstration of CTO technology. The general process of CTO employs gasification of coal to create syngas, subsequent production of methanol from syngas, and methanol-to-olefins (MTO) technology. While coal is a domestic and abundant feedstock, gasification of coal leads to the production of greenhouse gasses (GHGs) and wastewater, presenting a major challenge for the CTO industry in light of increasing environmental awareness. As restrictions on emissions increase, it is paramount that economic carbon capture and/or carbon capture and utilization technologies, as well as wastewater treatment techniques, be developed for economically competitive production of olefins from coal. This paper provides an overview of the technology for synthesizing olefins from coal, a history of developments in the later 20th century up until the present, its costs and environmental impacts, and current challenges and opportunities with particular reference to the United States.

21.4 Development of X-MAT® Coal Core Composites for Roofing Materials and Lithium Ion Battery Anode Applications

William Easter, Semplastics, 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 roof tiles 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 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. The current status of the coal-based roof tile project will be discussed.

In addition, Semplastics set up a battery lab in February 2019 to develop anodic materials for lithium battery applications. Several of the experimental battery anode formulations also use coal particles combined with proprietary chemical formulations. Experimental results indicate that these coal core composites have higher specific capacities than graphite which is the current anodic material of choice for lithium ion batteries. Up-to-date results of the coal-based anode materials will be presented.

This talk will highlight the continued progress and challenges experienced in the roof tile project as well as initial results of the coal core composite anodic experimental results.

21.5 Overview of NETL Advanced Coal Processing Program

Joseph Stoffa, National Energy Technology Laboratory, USA

The Advanced Coal Processing Program, conducted under the U.S. Department of Energy's Office of Fossil Energy (FE) and National Energy Technology Laboratory (NETL), is developing advanced technologies to produce high-performance, high-value carbon materials from coal. Laboratory- and pilot-scale projects within the program promise to elevate the value of U.S. coal and transform its use for the future. Research and development (R&D) activities within the Advanced Coal Processing Program have made significant progress in transforming coal into carbon products for applications such as building materials, carbon fiber, battery anodes, conductive inks, computer memory devices, and more. The program has recently sought R&D focused on coal-derived components for building, infrastructure, and high-value applications. This talk will highlight the recent progress and accomplishments and the future direction of the NETL Advanced Coal Processing Program.

SESSION 22
CLEAN COAL DEMONSTRATION AND COMMERCIAL PROJECTS – 1
Venkat Venkataraman and Thomas Sarkus

22.1 Application of Clean Coal Technologies for Development of Thar Coal in Pakistan

Farid A Malik, FC College, A Chartered University, PAKISTAN

After ignoring for over 30 years the 175 billion tons of black gold at Thar, Pakistan is now moving towards a coal based energy system. Two mouth of mine coal fired power plants of 330-megawatt capacity each are on line. Focus remains on the application of clean coal technologies.

Ever since the recovery of huge gas reserves (12TCF) in 1952, the country has developed an extensive state of the art gas transmission and distribution network spread over 1000 KM. As the reserves are now depleted there is a serious shortfall (2000 mm cfd) which is now being met by imported and expensive Liquified Natural Gas (LNG).

Being an agricultural country Pakistan produces about 6 million tons of Urea fertilizer every year from natural gas whose resource is now depleted. There is also a thriving Compressed Natural Gas (CNG) sector that requires 200 mm cfd of natural gas. Studies are being carried out for production of Syngas as a feed stock for Urea and Synthetic Natural Gas (SNG) for the CNG sector. Using Thar coal replacement of imported LNG by locally produced SNG is also being evaluated. Now that mining has started at Thar, Pakistan faces a challenge to build a 21st century environment friendly clean coal based energy system. Several state of the art technologies are being considered (IGCC, SNG, GTL, CTL etc.).

22.2 Long Term Performance Evaluation & Commercial Plant Design for CO_2 Capture from Coal Flue Gases Using a Novel Catalyst-promoted Solvent

Ahmed Aboudheir, Aboudheir Consulting Ltd, CANADA; Maohong Fan, University of Wyoming, USA

Post-combustion carbon dioxide (CO_2) capture from gaseous mixtures using liquid absorbents has been and will continue to be one of the leading industrial techniques for CO_2 capture and there remains opportunity for significant further innovation to improve the cost and performance of these proven technologies. Amine-based solvents, have been deployed at several coal-fired generation facilities, where CO_2 recovered from flue gases - ranging from 130 to 5,000 short tons per day (STPD), has been subsequently used for food processing, making added value products in industrial applications, and as a motive in enhanced oil recovery operations.

To improve the efficiency and the productivity of liquid absorbent CO_2 capture from coal flue gases, the University of Wyoming (UW) has developed a nanostructured $TiO(OH)_2$ catalyst additive for amine-based solvents, which increases the rate of CO_2 stripping from the rich CO_2 solvent stream, reducing the reboiler energy requirements. On new capital projects, the addition of this novel catalyst additive in high reactive solvents for CO_2 absorption allows the size of the absorption column to be reduced significantly.

The laboratory CO_2 absorption/desorption behavior using catalyst-promoted monoethanolamine (MEA) has been shown to be enhanced, with a noted marked reduction in striping temperature compared to the baseline condition, representing the non-catalyzed MEA solvent alone within the existing commercial CO_2 capture plant operation.

In this paper, the long-term performance evaluation and commercial plant design for a large-scale CO_2 capture plant from coal flue gases incorporating the UW catalyst-promoted solvent is presented. The presentation covers: reporting the enhanced kinetics of reaction and enhancement factors to the CO_2 absorption/desorption process of the novel catalyst-promoted solvent, obtained through laboratory experiments at UW and the University of Regina (UR). These new data and parameters are integrated into a rate-based model to simulate the behavior of existing pilot plant measurements and used to design a large-scale CO_2 capture plant.

The catalyst degradation characteristics were quantified in a Solvent Recirculation System, which showed that the additive does not mechanically disintegrate and is stable. The design of a new catalyst promoted absorption/desorption amine capture system is offered, Forward plans to further scale up the catalyst manufacture and undertake long term performance rests in a semi-commercial application at the InnoTech 6.6 STPD CO_2 capture demo plant located in Calgary, AB, Canada is described. This program will be used to verify the performance of the novel catalyst-promoted MEA solvent solution. Assuming these scaleup evaluations are successful, pre-commercial demonstration will follow at the National Carbon capture center (NCCC) 10 STPD CO_2 capture facility, located in Wilsonville, Al, USA. This later test program will determine the scaleup parameters for the design and operation of catalyst-promoted amine CO_2 capture systems, including needed changes in operational practice that capture the beneficial use of the technology. To predict the impact of potential saving on the capital and operation expenditures (CAPEX and OPEX) of commercial application in large CO_2 capture plants, a rate-based modelling approach will be used to design a 5,000 STPD CO_2 capture plant based on coal-fired flue gas streams and a 90% CO_2 recovery rate.

In conclusion, the experimental and modeling results that describe the performance attributes of the UW catalyst-promoted MEA solvent reveal that there are significant CAPEX/OPEX reductions foreseeable, namely: (1) smaller absorption columns because the catalyst promoted amine-based solution allows the use of highly reactive solvents; (2) simple process flowsheet by eliminating any need for heat integrations within the CO_2 capture process and eliminating the need to use intercoolers/liquid redistributors within the absorption column; (3) lower heat duty requirement to strip CO_2 from the rich solvent because of the use of the nanostructured $TiO(OH)_2$ as a catalyst.

22.3 Modeling and Simulation of the Pilot Solvent Test Unit at the National Carbon Capture Center

Ahmed Aboudheir, Aboudheir Consulting Ltd, CANADA; Justin Anthony, Southern Company Services Inc., USA

Accurate commercial plant design for CO_2 capture from coal flue gases can be achieved using a rate-based modeling approach. To demonstrate the rate-based modeling capability, a modeling and simulation study has been conducted on the Pilot Solvent Test Unit (PSTU) at the National Carbon Capture Center (NCCC) located at Wilsonville, Alabama.

The 10 ton per day (tpd) Pilot Solvent Test Unit uses a slipstream flue gas from a commercially dispatched base-loaded 880-MW coal-fired boiler to demonstrate the post-combustion CO_2 capture technologies from coal flue gases. The PSTU is a 0.5 MWe solvent-based CO_2 capture absorber/stripper system designed to process 5000 pounds per hour (pph) of coal derived flue gas. The unit requires a nominal solvent inventory of 4000 gallons (gal) and can provide critical data in support of scale-up to commercial demonstrations. The design for the PSTU is based on 30-40 wt.% monoethanolamine (MEA) to achieve an overall CO_2 removal rate of 90%, This design provides the flexibility to accommodate a variety of operating conditions and solvents.

A rate-based modelling approach is used to simulate the performance of the PSTU using actual plant process flow-sheet and operating parameters. The average absolute deviation of the main predicted parameters from the measured parameters is less than 4%. Based on the results obtained from the modeling and simulation of the PSTU, it is possible with confidence to scale up and design a commercial CO_2 capture plant from coal flue gases with reactive chemical solvents using a rate-based modeling approach.

22.4 Coal-Based Power Plants of the Future: Electricity and Ammonia Polygeneration

Howard Bugg, Jesse Goellner, Allegheny Science and Technology, USA

Team AST developed a coal-based power system for application in the evolving bulk power system. Specifically, the design is a polygeneration plant for the co-production of electricity and ammonia from coal in a flexible system that can adapt to complex and shifting realities inherent in a modern electrical grid with significant renewable penetration.

The general business philosophy of the polygeneration design centers on offering multiple potential revenue streams, including (1) commercial electricity available for sale to the grid, (2) salable ancillary services (e.g., capacity markets, frequency stability, voltage regulation, etc.), (3) and NH_3 for commercial delivery at or near retail (as opposed to wholesale) prices. By combining these three different revenue streams in a polygeneration facility that offers high operational flexibility, it is possible to modulate plant operations on a very short time scale to meet emerging market signals and opportunities. This ability to correctly match production to market demand will allow for optimization of plant profitability.

At a high level, the plant consists of two gasifier trains, a power island and two ammonia loops. This coal-based system functions at a smaller scale than traditional baseload coal and natural gas power plants to provide both distributed, dispatchable power and ancillary services to power systems that are stressed due to lower inertia and a more complex, geographically disjointed topology.

To do so, the system's optimal scale must be centered on a design philosophy that values operational response, adaptability, and resiliency in addition to the standard concerns of availability and efficiency. Rather than relying on significant technological innovation that can be both risky and costly, the approach to meet the objectives of the Coal FIRST Initiative (CFI) is centered on intelligent and purposeful application of solid engineering and process development.

22.5 U.S. Department of Energy National Carbon Capture Center, Supporting Technology Scale-up and International Collaboration

Doug McCarty, Southern Company, 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 fossil energy technology solutions. Bridging the gap between laboratory research and large-scale demonstrations, the center works to accelerate the development of technologies to reduce greenhouse gas emissions from natural gas- and coal-based power plants. The facility evaluates next-generation carbon dioxide (CO_2) capture processes from third-party developers, focusing on the early-stage development of the most promising, cost-effective technologies for future commercial deployment. 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 by approximately one-third.

Since its creation in 2009, the NCCC has performed more than 100,000 hours of technology testing, with research through mid-2017 focused on post-combustion CO_2 capture, gasification, and pre-combustion CO_2 capture technologies. After completing more than 20 projects in the gasification and pre-combustion capture areas, the center concluded this work as the scope of DOE-sponsored fossil energy R&D programs evolved. As the demand for post-combustion CO_2 capture options grows, work in this area continues to reduce the cost of carbon capture and bring new technologies closer to the marketplace. Evaluation of developing technologies using actual flue gas under industrial conditions provides critical information on material and process suitability for scale-up to commercial applications.

The center is broadening 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, future testing at the NCCC will support of research and development (R&D) of CO_2 utilization technologies that will efficiently, economically and cleanly transform CO_2 into value-added products.

Because reduction of CO_2 emissions is an international issue, the NCCC provides worldwide technology leadership – it co-founded the International Test Center Network, 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 15 test facilities that are members.

The NCCC has also been active in establishing test collaborations with international groups. The NCCC has successfully tested technologies from seven different countries. Establishing relationships to secure funding, gain management support, meet test goals and satisfy legal requirements of both the international organization and the NCCC is a significant achievement and forms a strong basis for future partnerships for larger-scale development. Oil and gas companies have joined the NCCC and have a strong international CCUS partnership that will further support international collaboration.

Unanticipated additional benefits to NCCC international collaboration have emerged in addition to 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 value of input into studies, roadmaps and policy development by including international perspective, (3) attenuation of inconsistent support of CCUS R&D among individual countries, and (4) encouragement to passionate participants in CCUS R&D to stay in the field by expanding interest from new, international funders. The NCCC hopes to build on the international relationships that have been established in order to contribute to the important step of moving from early-stage R&D projects to a commercial product.

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 CO_2 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 carbon capture technologies. This presentation will detail the center's capabilities, role in supporting international collaboration, and future plans.

SESSION 23
COAL ASH MANAGEMENT – 2
Peter Hsieh and Jinichiro Nakano

23.1 Navigating the U.S. Coal Ash Market

Mark Rokoff, AECOM; Dave Cox, FirmoGraphs; John Priebe, AECOM; USA

Owners of U.S. coal ash management units navigate a rapidly-changing landscape of regulations, legal and PUC decisions, shareholder concerns, and ENGO pressures. Relevant data and trends include regulatory drivers, closure approaches, and approved management and treatment technologies. This presentation will share market trends, including implications for operators, construction and engineering firms, and technology providers seeking to optimize public benefit and effectively serve industry.

23.2 Concentration of Rare Earth Elements into a Single Compound in Molten Coal Ash

Jinichiro Nakano, Anna Nakano, U.S. Department of Energy National Energy Technology Laboratory, and Leidos Research Support Team; Jack Widmer, U.S. Department of Energy National Energy Technology Laboratory, and Oak Ridge Institute for Science and Education; USA

Rare earth elements (REEs) are finding increased use as critical components especially in clean technologies including electric/hybrid vehicles, energy generation, and energy/electric storages. The scarcity and high costs of beneficiated REEs have caused high production costs, negatively impacting the development and implementation of clean technologies. While mining REEs has slowed in the U.S., reflecting environmental restrictions and the lack of REE processing facilities, coal byproducts hold potential as a REE resource. Coal byproducts, such as ash and solidified slag generated by power plants, gasification facilities, and steelmaking plants, contain a few hundreds to thousands of ppm of REEs. The key technological challenge to recover REEs lies in how the REEs exist in the coal byproducts. REEs can be present in various chemical and physical forms (chars, glass, and mineral particles); each with different properties, challenges that burden conventional beneficiation techniques such as leaching. NETL's fusion based technology mitigates this by transforming the whole material into a molten state, then concentrating the REEs into a single compound form, which then allows subsequent extraction of the REEs using existing beneficiation methods. In this work, the overall technology of such a process is described. An exemplified case is discussed with a fused synthetic coal ash bearing 560 ppm europium where subsequent crystal evolutions were examined for europium concentrations. Six mineral phases were identified in the melt while europium was only present in phosphate, suggesting REEs may be preferentially segregated to a single compound. In this exemplified case, europium concentrations in the phosphate was found as high as 11,000 ppm, a 20-fold increase from the initial concentration in the ash.

23.4 Experimental Investigation on The Effect of Using a Ponded Ash on The Mechanical Properties and Durability of OPC and Geopolymer Concrete

Omar Alsanusi Amer, Prasad Rangaraju, Weiqi Wang,Clemson University, USA

Vast quantities of ashes produced by burning coal in power plants are disposed-off in long-term storage facilities known as storage ponds, and the stored ash is referred to as ponded ash. Ponded ash has negatively affected the environment in several instances, including groundwater contamination through leaching of hazardous heavy metals, which necessitates an immediate need to find beneficial applications for these ashes. Ponded ash often fails to meet the limit on the loss on ignition (LOI), which determines the content of unburnt carbon. A high LOI ash usually increases the water-demand and negatively impacts the durability of concrete, affecting mainly the quality and the quantity of air entrainment meant for freeze-thaw protection of concrete.

The objective of this study is to investigate the possibility of making beneficial use of ponded ash in ordinary Portland cement (OPC) and geopolymer concrete by blending it with another pozzolan that can alleviate its negative impacts. In this study, blends of high LOI fly ash with ground glass fibers (GGF) were investigated. For this purpose, the experimental work encompassed four stages — first, the characterization of the selected ponded ash for the chemical and mineralogical composition and physical properties. Second, investigation of the pozzolanic activity of the chosen ponded ash individually and in combination with GGF. Third, the evaluation of properties of fresh and hardened mortar and concrete with binary and ternary blends of cementitious materials in both OPC and geopolymer systems. The final step included testing the durability of OPC and geopolymer concrete, prepared using the optimum combinations from the previous stage, against freeze-thaw durability, alkali-silica reaction (ASR), and rapid chloride permeability test (RCPT). The results from this study thus far prove the effectiveness of using GGF with high LOI fly ash to improve the performance of ponded ash in both OPC and geopolymer systems.

SESSION 24
VALUE-ADDED PRODUCTS FROM COAL - 2
John Duddy and Evan Granite

24.1 Bespoke, High-Purity Coal Tar with Microwave Plasma Pyrolysis

Vignesh Viswanathan, Aayush Mantri, George Skoptsov, H Quest Vanguard, Inc., USA

Coal tar is a dark, viscous liquid comprised primarily of polyaromatic hydrocarbons. Today, it is manufactured exclusively as a by-product of metallurgical coal coking in high-temperature coking ovens. In the 19th century, coal tar was the principal source of organic chemicals and synthetic materials, providing raw materials for industrial production of dyes, pigments, solvents, analgesics, platform chemicals, as well as paving

and waterproofing materials; and ultimately giving rise to the petrochemical industry of the 20th century.

Today, the lighter components of coal tar are used in the wood treatment industry, as a source of chemicals (most notably naphthalene), and as an alternative feedstock for production of carbon black. The primary use of coal tar pitch is in production of anodes for aluminum smelting. In Asia, coal tar pitch also increasingly serves synthetic graphite, needle coke, and ultra-high performance carbon fiber manufacturing industries, as the global demand for these high-value end products is growing. Presently, China currently dominates coal tar production (20 million ton/yr) accounting for 72 % of the global supply.

In North America, however, coking capacities have been in decline since the 1980s, owing to decline of the steelmaking industry, growth of the EAF mini-mills, and to the by-product coke ovens' grave environmental impact. Furthermore, very high capital investment requirements (8.3 USD/kg-liq-year), long residence time (12-36 hours), and poor liquid yields (5-15 wt%) make conventional coking non-viable for production of coal tar as the primary product. Finally, the resulting tar has high concentrations of quinoline insolubles (QI), sulfur and other impurities which necessitate expensive post-processing before the tar can be used in the production of high-performance materials.

H Quest Vanguard, Inc is developing microwave plasma driven ultra-rapid (100-500 ms residence times) coal pyrolysis. In this innovative process, entrained in an oxygen-free gas stream, the coal particles enter a non-thermal plasma and are rapidly heated ($\sim 10^5$ K/sec), resulting in a carbonized exterior and electrically conductive coal particles. Microwave radiation can then directly couple to entrained particles creating localized high energy regions. Aromatic and polyaromatic tar components are stripped from the macromolecular structure of coal and ejected into the gas stream leaving behind porous char particles.

Non-equilibrium nature of plasma conversion allows bulk temperature to remain below pyrolytic temperatures (500 ºC), suppressing carbonization of hydrocarbons and thus enabling exceptionally high liquid yields (> 50 wt%) at low energy inputs. The electrically driven process has sub-second startup time, and zero process CO_2 emissions when powered with carbon-neutral electricity sources.

Previous tests with a major commercial coal tar distiller have shown that microwave plasma derived coal tar may be drop-in compatible with the existing distillation processes even when derived from high-sulfur thermal coals. Reduction of S% (from 5% in parent coal to < 1% in both char and tar) owes to reaction of co-fed hydrogen with pyritic as well as organically bound sulfur. Furthermore, petrographic analysis of pitches indicated absence of QI impurities, which may be explained by very low residence times and the lower bulk temperature. Conversion in methane atmosphere results in aromatic hydrocarbon species terminated with methyl and carboxylic groups, which are expected to improve crosslinking during carbonization and graphitization (synthetic graphite and carbon fiber production). Recent tests were conducted at high coal throughputs and microwave powers (>5 kW). Tests on coals ranging from subbituminous (PRB) to high- and low-volatile bituminous thermal and metallurgical (e.g. Pocahontas #3, Blind Canyon, others) coals were conducted. The study of effects of coal grade, particle size, energy input, and process gas composition on conversion rate, product yield, energy requirements, and aromatic product distribution will be presented.

24.2 Incorporation of Lightweight CFOAM® Carbon Foam Aggregates into Concrete

Rudolph Olson III, CFOAM LLC; Dan Connell, CONSOL Energy; USA

CFOAM LLC has been manufacturing vitreous carbon foam from coal in panel form for several years. The primary application has been as a tooling board use in the manufacture of carbon fiber composites. Standard CFOAM® carbon foam products are usually manufactured in panel form, but it can also be produced in aggregate form ranging roughly from 0.4 to 25 millimeters in size. These very lightweight aggregates have unique properties and performance characteristics relative to conventional silicate based aggregates that could add value to new concrete designs, such as better insulation, fire ratings, freeze/thaw durability, blast resistance, shock and sound absorption, skid resistance, and placement via improved concrete pumping. Examples of specific applications include parking garages, manufactured stone veneer, and heat insulation for roofs, water pipes, and walls. Some additional performance benefits for use in concrete include: 1) the resultant structure would be impervious to alkali silica reaction induced by aggregate given carbon composition, 2) the porous nature of the aggregate could be used for internal curing purposes to enhance concrete hydration, 3) its low friability

versus other forms of light weight aggregate like pumice would limit generation of fines during transport and processing, and 4) the high strength-to-weight ratio of the aggregate would translate to a high strength-to-weight ratio for the concrete. A discussion on the processing, microstructure, properties and performance will be provided.

24.3 Incorporation of Graphite into Coal-Based CFOAM® Carbon Foam

Rudolph Olson III, CFOAM LLC; Dan Connell, CONSOL Energy; USA

CFOAM LLC has been manufacturing vitreous, open-cell CFOAM® carbon foam from coal for several years. The primary application has been as a tooling board for use in the manufacture of carbon fiber composites. Its light weight, machinability, and low coefficient of thermal expansion lends itself to this application. CFOAM® carbon foam has also been used as a heat exchanger for fluid given its inertness, high surface area, and open-cell characteristics. For these applications, one desire has been for higher thermal conductivity to speed heat transfer rates. For these reasons, we have developed a method to incorporate graphite into the CFOAM structure, offering a new carbon composite material with increased thermal conductivity. This product will enable greater efficiency for heat exchangers at manageable cost, enabling the design of smaller and more cost effective units, as well as increased heat up and cool down rates for carbon fiber composite tools, reducing manufacturing costs with shorter cure cycles and increasing the capacity of tool shops via greater throughput. A discussion on the processing, microstructure, properties and performance will be provided.

24.4 Economic and Environmental Impacts of High-Value Pitch Carbon Fiber Manufacturing

Sujit Das, Prashant Nagapurkar, Oak Ridge National Laboratory, USA

U.S. demand of coal for power generation has declined because of a shift to natural gas, due to lower natural gas prices, and to renewable energy sources. This decline is causing significant economic impacts to the US coal industry. The complex, dense carbon chemical structure of coal, abundant domestic supply, and stable, low price gives it a great potential for use in a wide range of value-added non-fuel coal products (e.g., nanomaterials at 20,000–100,000 $/kg and commercial-grade carbon fiber at 22–33 $/kg), as well as in upgraded coal fuels. Of several potential new non-fuel coal product markets, global carbon fiber demand is projected to increase more than two-fold from the 2019 level of ~ 100,000 metric tonnes during this decade. Cost as well as embodied energy of carbon fiber composites manufacturing (i.e., in terms of $/kg and MJ/kg) will be critical factors affecting the uptake of CFRP composites in three projected non-traditional growing carbon fiber markets, i.e., wind energy, automotive, and pressure vessels. which combined contributed to 40%-45% of total 2019 market, significantly higher than the traditional premium aerospace market share of 20%.

Alternative potential of pitch carbon fiber manufacturing through direct raw coal liquefaction conversion route of raw coal to coal tar pitch as the carbon fiber precursor may offer both economic and environmental challenges for the carbon fiber market. An updated technoeconomic analysis of pitch carbon fiber manufacturing in collaboration with the industry shows the pitch carbon fiber could potentially be a low-cost carbon fiber source to meet the growing demand for carbon fiber reinforced polymer composite applications. A significantly higher conversion yield using low cost and abundance of domestic raw coal supply in addition to integration potential of a few fiber conversion process steps have the significant final carbon fiber cost reduction opportunity compared to the conventional petroleum-based fiber manufacturing pathway. Environmental impacts of pitch carbon fiber manufacturing will be presented whether benefits of dense carbon in coal resulting in a significantly lower precursor amount requirements outweighs higher likely emissions during the raw coal conversion of coal tar pitch precursor for carbon fiber manufacturing.

24.5 On Understanding the Effectiveness of Coal Feedstock as Composite Filler

Madhusudhan R. Pallaka, Sarah D. Burton, John C. Linehan, Keerti S. Kappagantula, Pacific Northwest National Lab, USA

Abstract:
In pursuit of finding sustainable end uses for coal to develop value-added coal products, the research on coal-based polymer composites with applications in building materials has gained traction in the recent years. Research to date largely focused on the development of coal plastic composites (CPCs) with dry coal feedstock used as reinforcement/fillers in thermoplastic substrates such as high-density polyethylene, or polypropylene with potential application as a building material. Previous work demonstrated that dry coal is an optimal feedstock material for making polyethylene-based CPCs with thermal, mechanical, and environmental performance on par with or better than existing market standard wood plastic composites used for making decking, floors, railings and other building applications. An interesting question to consider at

this stage of application development is how coal, in particulate form is outperforming wood fibers. This is even more intriguing since traditional composite performance theories predict otherwise based on the reinforcement aspect ratio features. It is well known that polymer matrix composite properties are dependent on the polymer/reinforcement interface, with special significance given to filler particle surface chemistry and filler-polymer matrix interfacial interaction. Therefore, to understand the effectiveness of dry coal as optimal filler material in polymer composites, the interfacial properties of polyethylene-based CPCs with two different coals, namely Pittsburgh # 8 and Powder River Basin will be presented in this talk. Surface chemistry of the coal varieties, investigated using ^{13}C solid state nuclear magnetic resonance spectroscopy, will be discussed. In addition, coal/polyethylene interfacial elastic modulus determined using nanoindentation testing, will be evaluated. Finally, reasons for effective bulk scale CPC properties will be scrutinized in the context of coal surface chemistry and filler content to identify strategies for manufacturing commercial coal composites with enhanced performance.

SESSION 25
CLEAN COAL DEMONSTRATION AND COMMERCIAL PROJECTS – 2
Thomas Sarkus and Venkat Venkataraman

25.1 Flameless Pressurized Oxy-fuel (FPO) Technology Update, Scale-up and Commercialization Objectives

Richard Horner, University of Wyoming, USA; Massimo Malavasi ITEA S.p.a., ITALY

With increasing recognition that coal can have a deliberate and necessary role in the production of stationary power in the future, the need to ensure strict compliance with current and emerging environmental legislation - notable the release and utilization of produced anthropogenic carbon dioxide from the combustion of coal is imperative. Clear key performance attributes for next generation clean-coal combustion technology include ability to produce "near-zero" airborne pollution emission while delivering a competitive levelised cost of electricity (LCOE) compared to super critical pulverized coal (SC-PC) air firing solutions. Further attributes of emerging combustion technology must include the ability to respond to fluctuating demand for power (load following) – notably so as increasing renewable energy supply, which by nature is fluctuating, enters the grid. Fuel flexibility and suitability to function in smaller scale distributed power generation schemes are further desirable features. If technology solutions can be found to achieve these laudable performance requirements, then coal remains an option to fulfill a strategic role in the US. stationary energy production sector that leverages its abundance of reliable domestic supply at low cost.

This presentation provides an update on technology advances, the scale up and commercialization objectives of Flameless Pressurized Oxy-Combustion (FPO) technology of ITEA S.p.a. FPO offers key proven performance that matches these aforementioned headline requirements. Further, FPO offers an attractive and realistic retrofit option for supporting the continued use of the existing – and aging coal fired generation fleet. The simplicity of the technology also reduces engineering complexity (and therefore capital cost) to achieve efficient energy production, based upon lower-rank coal and other solid fuels, reducing the historic recent need associated with advancing super critical air-combustion solutions, the invention of new high-performance alloys that can tolerate very high temperatures.

FPO provides integrated carbon capture which does not suffer the parasitic energy penalties associated with bolt on post carbon capture solutions. Suffice for water vapor removal, the carbon dioxide generated as a direct result of flameless combustion is of a quality that is utilization ready as it does not contain other pollutants, whether for the food industry, for below ground storage or in enhanced oil recovery applications or to make value added products. Dependent upon feedstock quality, only neutralization of this CO2 post combustion flue gas stream is necessary together with compression - if needed, to facilitate pipeline transport. This integrated nature and approach to combust and capture CO2 together, means that an FPO electricity generation scheme (combustion + turbo machinery) has an extremely high operating efficiency (ca 42%).

To date, FPO technology has been extensively evaluated and proven at a scale of 5MWth. At this time a DOE funded front-end engineering design (FEED) study for a 25MWth (minimum) pilot demonstration is in hand in the US. This first of a kind technology demonstration is – subject to further award of funding in 2021, scheduled to be constructed at a small central energy plant on the University of Wyoming (UW) campus in Laramie, Wyoming.

One of the features of flameless oxy-fired combustion, is that non-combustible species such as mineral matter and heavy metals migrate into the combustor bottom ash where the heat of combustion forms benign vitrified beads, which do not leach. The non-

leaching characteristics of the vitrified slag produced, means that it can be recovered and used to make construction materials.

Flameless firing is able to provide high levels of power generation performance across the combustor full utilization range - from standby to full load, with operating efficiency differences of only <5%, with ability to rapidly respond to rapid fluctuations in grid power demand. This achievement is largely due to the recent development by ITEA S.p.a. of Once-through-steam-Generator (OTSG), constant control logic technology. Coupled with combustor, and advanced software control, this proprietary solution allows the entire pressurized firing loop ramp up to load in less than ½ hour. The further validation of this 'fast response' operating performance characteristic will be included in the planned large pilot demonstrating scheduled to be constructed and operational in Wyoming.

At this time, R&D activity continues to better characterize FPO combustor performance when fed with lower oxygen quality. Early laboratory evidence suggests that lowering O$_2$ quality may still yield similar performance benefits, to the high quality (typically 92%) historically used in oxy-fuel combustion; thereby significantly reducing the cost of oxygen supply and thus the LCOE.

Another (often neglected) fundamental FPO attribute is that the combustion technology platform firing loop, is simple and very small. Not only does this mean the technology has a small construction footprint, the simple engineering truly favors existing coal fleet retrofit, with appealing economic returns, and with existing unit maintained in operation up to the very last moment, minimal impact on plant operation. This very small FPO technology platform footprint, affords application to modularization too- essential for keeping power cost low at small scale.

Most recent advances of FPO has included the experimental demonstration of the "flexible fuel" capability, on waste and natural gas. Still required is further ancillary equipment development to optimize operation on solid waste (e.g. solid fuel preparation such as milling and water slurry formation). Once sufficiently developed is conceivable that FPO can accommodate multi-solid fuel feedstocks – even biomass, which co-fired with coal offers a pathway to carbon negativity, assuming the produced CO2 is responsibly utilized.

Finally, it is worth noting that industry is seeking to move increasingly to low rank and inferior quality coal types, including those containing high mineral matter. Early evidence from mathematical modeling, suggests that FPO offers an attractive techno-economic solution to permit firing of these inferior solid fuels too.

Even at this stage of its evolution, FPO has demonstrated that it is a flexible and innovative technology solution that can truly address most of the challenges that are confronting the future of coal as a fuel source in stationary power generation.

25.2 DOE Transformative Power Generation Program: Coal FIRST, Existing Plants and Advanced Technologies

John Rockey, DOE/NETL, USA

In 2018 the DOE initiated the Transformative Power Generation (TPG) program. The goal of the TPG program is to enable generation of efficient, cost-effective electricity from coal with near-zero atmospheric emissions and the potential for net-negative carbon dioxide emissions. Transformative Power Generation R&D focuses on development of impactful near-term technologies to improve the existing fleet and transformational technologies that will modernize the coal-fired fleet. Research efforts are focused in three areas: **Coal Plants of the Future – Coal FIRST**, **Improvements for Existing Plants**, and **Advanced Combustion Technologies**. The Transformative Power Generation program uses a multi-pronged and coordinated approach to identify and perform R&D through in-house research and cost-shared R&D with external partners in academia, industry, and other national laboratories.

The Transformative Power Generation program is funding a research and development initiative to advance the small-scale, modular coal-based power plant of the future. This effort—the **Coal FIRST** (Flexible, Innovative, Resilient, Small, Transformative) initiative—will develop the coal plants of the future needed to provide secure, stable, and reliable power. This R&D will underpin coal-fired power plants that are capable of *flexible* operations to meet the needs of the grid; use *innovative* and cutting-edge components that improve efficiency and reduce emissions; provide *resilient* power to Americans; are *small* compared to today's conventional utility-scale coal; and will *transform* how coal technologies are designed and manufactured.

Through Coal FIRST, the Transformative Power Generation program is seeking to enable U.S. manufacturers to create the cleanest (including systems that are capable of net-negative carbon dioxide emissions), highest performing, and most cost-effective coal-based power plants in the world. The goal of this area is to develop mid-term technology options (2030's timeframe) that will help even today's best coal power plants improve efficiency and flexibility over the next decade.

Through R&D for **Improvements to Existing Plants**, the Transformative Power Generation program is supporting near-term research to improve the efficiency, flexibility, and reliability of existing coal fueled plants. The existing coal power generating fleet plays a critical role providing reliable on-demand power generation required for power grid stability, and it is important that these existing units can continue to operate in an efficient and reliable manner. The Transformational Power Generation program is pursuing R&D that focuses on the identification of impactful, near-term opportunities applicable to the needs of the existing fleet.

The goal of Improvements to Existing Plants is to characterize potential, emerging, or current approaches with "market pull" for advanced coal combustion systems and identify near-term commercial opportunities applicable to the needs of the existing fleet. Projects in this area of research are expected to bring about near-term benefits for incorporation into commercial plants that will continue to operate on coal into the future. The current research is concentrating on existing fleet characterization and assessment; dynamic performance and reliability; materials; sensors, controls, and diagnostics; and power plant component improvements.

The **Advanced Combustion Technologies** R&D area is developing chemical looping and pressurized oxy-combustion technologies that will enable combustion-based, coal-fueled power plants to capture carbon dioxide at higher efficiency and reduced cost compared to today's state-of-the-art post-combustion capture technologies.

25.3 Collaboration and Knowledge Sharing on the Ordos CCS project: Updates from the US-China Clean Energy Research Center – Advanced Coal Technology Consortium

Philip H. Stauffer, Los Alamos National Laboratory, USA; Xiaochun Li, Liwei Zhang, Chinese Academy of Sciences, CHINA; Minh Nguyen, U. of Wyoming, USA; Manguang Gan, Jun Li, Ning Wei, Chinese Academy of Sciences, CHINA; X. Zhang, Schlumberger Software Integrated Solutions; Anthony Ku, NICE America Research, USA and National Institute of Clean and low carbon Energy, CHINA

US-China Clean Energy Research Center – Advanced Coal Technology Consortium (CERC - ACTC) has a platform to advance the technologies needed to utilize coal resources in an environmentally friendly manner and to explore the challenges of clean coal power generation. As part of this 10 year effort, a subset of the research portfolio (Theme 2) is tasked with assisting the US and China in expediting our understanding of existing large demonstration projects and their associated research through effective knowledge sharing among participants. The project aims to collaborate on large demos facilitating collaboration and knowledge sharing on existing and planned CCUS demonstrations in both US and China. Theme 2 has several focus areas, including knowledge sharing on large scale IGCC systems and post-combustion amine performance with data sharing between Huaneng and Southern Company/CERI.

A second major thrust of Theme 2, the topic of our presentation, is the Ordos Carbon Capture and Storage (CCS) project, implemented by Shenhua Group. This ambitious demonstration project, the first of its kind in Asia, captured carbon dioxide (CO_2) from a coal to liquids facility in Erdos City, China. A total of 300,000 metric tons of CO2 were captured from the facility over three years (2011-2014) and trucked to Shenbei Slope injection site in North Yulin. Injection occurred into Mesozoic sandstones and Paleozoic carbonates and was marked by very little pressure build up. Our US-China CERC-ACTC team began to study this project in 2015 soon after the injection period stopped. Personnel exchanges between the US (U. of Wyoming and Los Alamos National Laboratory) and China (Chinese Academy of Sciences) fostered a collaborative environment and the team published several papers that have led to a deeper understanding of the flow system at the injection site. Further input from Shenhua Group kept the research well connected to site data and details of events at the injection site. Building on the reservoir simulations work, the team has spent the last year applying the National Risk Assessment Partnership (NRAP) Integrated Assessment Model (IAM) for Carbon Storage (CS). We present the first application of the NRAP-IAM-CS at a site in China, driving the model with underlying ECLIPSE simulations to explore the potential for wellbore leakage at the site. Results indicate that leakage risk is low. However, continued monitoring is suggested because coal mining activities directly over the injected CO_2 plume put miners in the path of low probability leakage risk through the existing injection borehole and two monitoring boreholes.

25.4 Conceptual Design and Pre-FEED Study of a Supercritical Pressurized Fluidized Bed Combustion Power Plant with CO_2 Capture

Daniel P. Connell, CONSOL Energy Inc.; Harvey Goldstein, David Stauffer, Esko Polvi, Worley Group, Inc.; Tom Porterfield, Farnham & Pfile Engineering, Inc.; Evan Blumer, OsoMono LTD; Barbara Arnold, PrepTech, Inc.; USA

As part of the U.S. Department of Energy's Coal FIRST program, CONSOL Energy, Worley Group, and Farnham & Pfile Engineering completed conceptual design and pre-

FEED (front end engineering and design) studies for an advanced coal-based power plant utilizing pressurized fluidized bed combustion (PFBC) technology. A base version of the PFBC technology has already been commercialized, with units currently in operation in Sweden, Germany, and Japan. These installations provide proof of certain key features of the technology, including high efficiency, low emissions, byproduct reuse, modular construction, and fuel flexibility. The concept evaluated under the Coal FIRST program builds upon the base PFBC platform to create an advanced, state-of-the-art coal-based power generation system. Novel aspects of this advanced PFBC technology include: (1) integration of the smaller P200 PFBC modules with a supercritical steam cycle to maximize modular construction capabilities while maintaining high efficiency, (2) optimizing the steam cycle, turbomachine, and heat integration, and taking advantage of advances in materials and digital control technologies to realize improvements in operating flexibility and efficiency, (3) integrating carbon dioxide capture and storage, and (4) incorporating a new gas turbomachine and hot gas filter to replace the earlier ABB GT35P machine. In addition, the business case evaluated under the Coal FIRST project takes advantage of the fuel flexibility of the PFBC to use fine, wet waste coal and wet biomass as fuel sources. The waste coal, which is a byproduct of the coal preparation process, can be obtained either by reclaiming tailings from existing slurry impoundments or by diverting the thickener underflow stream (before it is sent for disposal) from actively operating coal preparation plants. There is broad availability of this material; CONSOL's Pennsylvania Mining Complex (PAMC) in southwestern PA alone produces close to 3 million tons/year of fine coal refuse with a higher heating value of ~7,000-8,000 Btu/lb (dry basis), which is more-than sufficient to fuel a 300 MW net advanced PFBC power plant with CO_2 capture. This slurry is currently disposed of at a cost, so it has the potential to provide a low- or zero-cost fuel source, and using it eliminates an environmental liability, improving the sustainability of the coal supply chain. The biomass, when co-fed with the waste fuel at a modest rate (5-10% of the total fuel input) and coupled with reasonably deep CO_2 capture (~97%), provides an opportunity for the overall power plant to achieve CO_2-negative operation through BECCS (bioenergy with carbon capture and storage). The PFBC provides an advantage in enabling the biomass to be fired without pre-drying, resulting in a streamlined supply chain and lower cost. This presentation summarizes the results of the pre-FEED study, including preliminary power plant design, performance and cost results, and discusses key technical and economic considerations for further development of the technology, based on a commercial demonstration plant envisioned to be sited at PAMC.

25.5 Coal-Based Power Plants of the Future – Hybrid Coal and Gas Boiler and Turbine Concept with Post Combustion Carbon Capture (HGCC)

Nicole Nguyen, Barr Engineering Co.; Rob Broglio, Doosan Heavy Industries and Construction; Bruce Browers, Chad Haugen, Barr Engineering Co.; USA; Kihyun Lee, Sung-Gju Kang, Doosan Heavy Industries and Construction, SOUTH KOREA; Srivats Srinivasachar, Envergex LLC; Steve Benson, Microbeam Technologies Inc.; Mike Jones, MLJ Consulting, LLC; Junior Nasah, University of North Dakota; USA

The proposed plant focuses on achieving power generation with high-efficiency and load cycling capability that integrates with increased use of renewable generation. The system combines a state-of-the-art ultra-supercritical (USC) coal power plant with a natural gas combustion turbine and energy storage system (ESS), to achieve ultra-low emissions and waste reduction, including carbon capture (CC). We term this concept as the Hybrid Gas/Coal Concept (HGCC). The typical role of the heat recovery steam generator (HRSG) in a normal natural gas firing combined cycle (NGCC) power plant will be replaced by a coal boiler (hot windbox repowering).

26.1 A New Rock Mass Cuttability Classification for Roadheaders

Sair Kahraman, Behnaz Dibavar, Masoud Rostami, Hacettepe University; Mustafa Fener, Ankara University; TURKEY

Roadheaders have been widely used in mining for gallery drivages and in civil engineering for tunnel excavations. The correct estimation of the roadheader performance is important especially for determining the job duration and the cost estimation. In this study, a new rock mass cuttability classification (RMCC) system was developed for the estimation of roadheader performances in the excavation of coal and coal measure rocks.

The RMCC system includes six parameters: the uniaxial compressive strength (UCS), the volumetric joint count (J_v, joint/m^3), the strike and dip of joints, the joint aperture, the Cerchar abrasivity index (CAI), and the water ingress. The UCS parameter is divided into five categories: < 20 MPa, 20–40 MPa, 40–60 MPa, 60–120 MPa, > 120 MPa. Because coals have cleat systems, their J_v values are higher than 150 joint/m^3. In addition, since the coal measure rocks are sedimentary weak rocks, they have bedding planes and frequent joint systems. Considering these situations, the J_v is divided into five categories: > 150 joint/m^3, 150–100 joint/m^3, 100–75 joint/m^3, 75–50 joint/m^3, < 50 joint/m^3. The parameter of the strike and dip of joints is divided into three categories: Strike vertical to tunnel axis, strike parallel to tunnel axis, and strike oblique to tunnel axis. The first category has two sub-categories: Drive with dip and drive against dip. The dip angle for each category are divided into three ranges: 0º-30º, 30º-60º, and 60º-90º. Since the joints with too large aperture are not generally encountered in underground excavations, the parameter of the joint aperture is started from 5 mm and divided into five categories: Very open (>5mm), open (5-1mm), tight (1.0 - 0.1mm), very tight (< 0.1mm), and hard cemented filling. The parameter of the CAI is divided into three categories: < 0.5, 0.5-1, 1-2, 2-4, and > 4. The parameter of the ground water is divided into five categories: Flowing, dripping, wet, damp, dry. The total rating for the RMCC system ranges from 0 to 100. As the total rating value increases, the cuttability becomes easier.

The performance measurements of roadheaders were carried out in a coal mine and the net cutting rates (NCR) were determined for the validation of the RMCC system. A very strong linear correlation was found between the NCR and the RMCC index, suggesting the RMCC system is valid. It can be said that the suggested RMCC system can be used reliably for the assessment of the roadheader performances in coal mines

26.2 Predictive Coal-Methane-Air Fire Scenario in a Cylindrical Obstructed Mining Passage

Samuel Ogunfuye, Furkan Kodakoglu, Co-Author: Lateef Kareem, V'yacheslav Akkerman, West Virginia University, USA

Historically, accidental gaseous and dusty explosions represented a hazard to both personnel and equipment in the coalmining industry. To attain an acceptable level of risks against these disasters, novel preventive mining safety strategies such as rigorous predictive scenarios of accidental coalmining fires are critically needed. In the present work, the previous efforts of the authors towards the development of a theoretical model of a coalmining scenario are extended to the configuration of a cylindrical mining passage, with the obstacles attached to the walls. Such an extension is motivated by the fact that obstructions (such as mining equipment, belt conveyor systems, and piles of rubbles) are inevitably present in a coalmine passage, blocking a noticeable segment of the passage. Specifically, the theories of globally-spherical, self-accelerating premixed expanding flames, of finger flame acceleration, and of ultrafast flame acceleration in obstructed conduits are combined into a novel, in-situ developed, unified analytical formulation. The formulation is then validated by a comparison with the experimental measurements and the numerical simulations from the literature, with good agreement observed. Specifically, we have identified and scrutinized the keys stages of the premixed flame front evolution and quantified its major characteristics such as the flame tip position, its velocity, acceleration rate, and the run-up distance. Starting with gaseous burning, the formulation is subsequently extended to the gaseous-dusty environments, with combustible (coal) and inert (sand) dust as well as their mixture studied. Specifically, the impacts of the equivalence ratio, the dust size and concentration on the flame evolution are systematically investigated. It is shown that the entire acceleration scenario may promote the total burning rate up to a near-sonic value, and with a potential of detonation triggering by an accelerating flame. Moreover, staring with an incompressible approach, in this particular work we extend it to account for gas compressibility, because the latter cannot be ignored as soon as the flame velocity starts approaching the sound threshold. Overall, it is shown that gas compressibility generally

moderates flame acceleration and such an impact depends strongly on various thermal-chemical properties. In particular, the role of compressibility is relatively small for very lean and rich flames, thereby justifying an applicability of the incompressible formulation in that case. In contrast, compressibility appears of crucial importance for near-stoichiometric combustion, thereby making the present analysis viable.

26.3 Evaluating CFD and Modeling Techniques for a Multi-Nodal Sensor Network Designed for the Detection and Control of Methane in Longwall Coal Mines

Brian Cappellini, Amber Barr, Derek Johnson, Nigel Clark, West Virginia University, USA

Machine automation and atmospheric monitoring are used by many industries to improve safety and productivity in the workplace. The underground Methane Watchdog System (MWS) is a multi-nodal network of sensors currently under development. The MWS aims to improve safety and productivity by continuously monitoring methane emissions and other atmospheric parameters. These parameters include wind speed, temperature, pressure, and relative humidity and are found within each of the ten sampling nodes that make up the MWS. A design goal of the MWS consists of the ability for easy integration within current shields used as part of the longwall section. A remote central processing hub (CPH) collects nodal signals, converts them to useful engineering units, records data for historical analysis, and provides control capabilities. This work examines various modeling and simulation approaches to realize full system effectiveness and potential in identifying high methane concentration zones and recognizing scenarios that imply explosion danger. These models couple historical production data with characterized methane emissions for development of control algorithms. Computational fluid dynamics (CFD) models allow greater insight into the prediction of hazardous scenarios but require significant computational power. One-dimensional (1-D) modeling provides examination of linkages between ventilation flow rate, methane emissions, and shearer location along the face. Modeling results show that variations in ventilation flow dominate methane concentration especially near the tailgate; with lesser impacts from coal production (shearer velocity) and methane desorption rates. These results highlight the need for a spatially distributed monitoring network that measures both methane concentration and ventilation velocity. Since the shearer represents a primary ignition source, the 1-D model also tracks shearer location with respect to MWS monitoring nodes. This capability enables development of nearly real time methane profiles across the entire face; an advantage for avoiding dangerous events, decreasing downtime, or managing shearer speed in closed loop with methane concentration. An extension of this approach can also examine predictive capabilities using both temporal and spatial derivatives to further increase safety.

26.4 Design and Development of Multi-Nodal Methane Monitoring System for Improved Mine Safety

Amber Barr, Brian Cappellini, Derek Johnson, Nigel Clark, West Virginia University, USA

Explosions initiated by methane combustion pose significant dangers in longwall mining that may lead to injuries and fatalities. Safety is improved through diligent monitoring of methane concentration. Currently, regulations require a methane monitor be placed on the shearer and downwind of the cutting head. Handheld monitor measurements must be taken at various times and locations. If any methane monitor measures a concentration greater than 1%, a warning signal must be given. Based on previous research and the location of the methane monitor mounted on the shearer (closest monitor to the face), if 1% methane is measured, the concentration at the face may be higher, and may be already be at the lower explosive limit (5%). If any monitor measures a concentration greater than 2%, production is halted. However, there are gaps in measurements (spatially and temporally) where a dangerous methane-air mixture may develop and go unnoticed. This poses a risk if shearers or work activity ignite the dangerous mixture. A multi-nodal methane watchdog system (MWS) has been designed and developed to improve detection of methane clouds or plumes. The prototype consists of ten sampling nodes distributed along the longwall. Each node has a sampling location near the face and near the gob. The units are connected in series and communicated with a central processing hub (CPH). Each node consists of an explosion proof box which houses sensors and necessary components. All sensors (2 methane, 1 temperature, 1 pressure, and 1 relative humidity) are mounted in a custom aluminum sampling block. Two sampling tubes draw from relevant locations and carry the gas to the sampling block at the node. The units can sample continuously, alternating between each location. The

sampling for each unit is powered using a customized water ejector. Pressurized water, already powering spray nozzles, provides an inherently explosion proof motive energy source for active sampling. The MWS nodes are powered by low voltage direct current power common among shields. The system has been tested at a mock mine facility to gain additional insight for further refinement. It is proposed that an optimized MWS be integrated into mining operations to improve both safety and efficiency.

SESSION 27
RARE EARTH ELEMENTS - 1
Brian Shaffer and Allan Kolker

27.1 Rare Earth Elements from Coal and Related Materials: An Overview of Research at the National Energy Technology Laboratory

Thomas J. Tarka, National Energy Technology Laboratory, 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 coal and related materials. The RIC REE research portfolio is focused on identifying novel and low-cost pathways to reduce the cost of REE 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 a look at the program moving forward, including potential opportunities for partner on NETL RIC-related efforts.

27.2 Entry Points into a Domestic Rare Earth Element Supply Chain: Understanding the Opportunity for Coal-Derived Products

W. Morgan Summers, Thomas J. Tarka, P. E., Senior Engineer, National Energy Technology Laboratory; Alison Fritz, Stanford University/ National Energy Technology Laboratory; Dennis Harkreader, National Energy Technology Laboratory; USA

The Department of Energy's program to produce Rare Earth Elements (REE) and Critical Minerals (CM) from coal and related materials was created to alleviate concerns over U.S. dependence on foreign supplies and to provide domestic industry a secure supply of the materials they need to participate in evolving markets. The lack of a mature domestic REE supply chain, however, presents two questions: (1) who will purchase these materials once they are produced, and (2) what product, particularly what purity, is industry looking for? The diversity of coal related feedstocks and myriad of extraction and enrichment pathways adds to the dilemma, as REE materials could be produced at a variety of purities and forms. Engineers in the National Energy Technology Laboratory (NETL)'s Research and Innovation Center (RIC) have conducted numerous market and techno-economic analyses on domestic REE needs and pathways, as well as extensive interviews with industry leaders, all with the goal of investigating the opportunities for coal-derived REE and CM products. This talk will provide an overview of their findings.

NETL's RIC conducts research to support the creation of a domestic supply of Rare Earth Elements (REE) and Critical Minerals (CM) from coal and related materials. The RIC REE research portfolio is focused on identifying novel and low-cost pathways to reduce the cost of REE 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.

27.3 Recovery of Rare Earth Elements and Critical Minerals from Coal-Based Resources

Mary Anne Alvin, National Energy Technology Laboratory, USA

DOE-NETL's Rare Earth Element and Critical Minerals (REE-CM) Program has demonstrated the technical feasibility of recovering REEs from coal and coal-based materials, and has recently achieved production of small quantities of 80-90% pure, mixed rare earth oxide concentrates, in first-of-a-kind, domestic bench/pilot-scale extraction, separation and recovery facilities. Technology development is now focused on addressing system scale-up with process optimization and efficiency improvements, with improved economics and recovery of critical minerals, ultimately targeting production of salable rare earth oxides and metals, as well as critical minerals for incorporation into commodity and national defense intermediate and end products. Accomplishments in each of these areas will be discussed.

27.4 Completed Testing of Bench-Scale Rare Earth Element Extraction from North Dakota Lignites and Implications for Pilot-Scale Extraction

Nolan Theaker, University of North Dakota, USA

Coal has been identified as a promising unconventional resource for rare earth elements (REE) and critical minerals (CM). The University of North Dakota has developed a technology targeting extraction of REE/CM from low rank coals, such as lignite. The lignite-bound REE/CM are bound in an easily extractible, organic binding (rather than as mineral forms), and a technology and bench-scale process for extracting and recovering the REE/CM is presented. Implications of the completed testing on the bench unit and how this affects further testing, including at the pilot scale, is also discussed.

27.5 Visible & Near Infrared (VNIR), Short-Wavelength Infrared (SWIR) and Thermal Infrared (TIR) Spectroscopy of Coal Fly Ash: Implications for Remote Sensing Detection of Rare Earth Elements

Bernard E. Hubbard, Allan Kolker, U.S. Geological Survey; James C. Hower, University of Kentucky; Clint Scott, U.S. Geological Survey; USA

Fly ash has long been considered a potential resource for extraction of rare earth elements (REEs). For field sampling at close range, hand-held X-Ray fluorescence is increasingly popular for semi-quantitative REE determination. In the present study, we investigated remote sensing approaches that are potentially applicable at a much greater range of scales, including detection by airborne or spaceborne instruments. Visible & Near Infrared (VNIR) and Short-Wavelength Infrared (SWIR) spectral reflectance data (400 – 2,500 nm) are useful tools for possible detection of spectrally active REEs (e.g., Neodymium, Nd) in these and other coal and coal waste materials. Thermal Infrared (TIR) emissivity data (8,000 – 14,000 nm) are complementary to VNIR and SWIR. TIR is useful for detecting the presence of host aluminosilicate glasses, which are both abundant in coal fly ash and in which most of the REEs are contained. In order to determine if individual REEs and/or aluminosilicate glasses can be detected in coal fly ash using remote sensing data with sufficient spectral and spatial resolution, we measured VNIR-SWIR reflectance and TIR emissivity spectra for 19 coal fly ash samples having known REE contents. The samples include fly ash from U.S. power stations that burn bituminous coal from the central Appalachian basin, the Illinois basin, and subbituminous coal from the Powder River basin. The remaining samples include four U.S. fly ash samples having mixed or unspecified sources and three samples of fly ash obtained from a Chinese powerplant burning bituminous coal. Fly ash samples from the U.S. central Appalachian basin include four samples of ash from the Fire Clay coal of eastern Kentucky, which is known for its REE enrichment (>500 ppm; up to 1,409 ppm for our samples). Past studies have placed minimum detection limits for REEs with the strongest absorption features at above 300 ppm, for samples containing minimal amounts of dark or opaque minerals.

VNIR-SWIR spectral measurements were done using a Perkin Elmer Lambda 950 laboratory spectrometer, which measures direct hemispherical reflectance (DHR) from 250 to 2,500 nm. Results of spectral analysis in the VNIR-SWIR wavelengths show that all but two samples yield overall reflectance values less than 40%. The two remaining samples that are both visually and spectrally the brightest, are from the Powder River basin, but these have some of the lowest REE concentrations (< 300 ppm) among the sample suite. All 19 spectra display no discernible REE-related absorption features but are all dominated by a broad absorption feature at SWIR wavelengths between 2,136 and 2,346 nm. The latter feature is related to hydrated aluminosilicate glasses and is markedly reduced in absorption band intensity (i.e., quenched) to varying degrees due to the presence of unburned carbon in the samples. Spectral quenching effects reduce the overall reflectance of several of these samples to as low as <10%, likely complicating remote sensing detection of REEs in coal fly ash using VNIR-SWIR.

TIR spectral measurements were done using a Nicolet 670 FTIR Spectrometer, which measures DHR from 2,000 to 15,000 nm. At TIR wavelengths, 18 out of 19 coal fly ash samples display spectral emissivity features (i.e., hemispherical reflectance peaks) at around 9,300 nm due to the presence of aluminosilicate glasses, which subtly shifts depending on the composition of the glass. By comparison, artificial silica glass and natural rhyolitic obsidian glass spectra from the JPL ECOSTRESS spectral library display similar features at around 9,450 and 9,180 nm, respectively. Unlike VNIR-SWIR reflectance data, unburned carbon is spectrally featureless at the TIR wavelengths studied. However, two of the 19 samples (i.e., the Powder River basin samples) are extremely fine-grained and display additional spectral features (7,182 nm and 7,262 nm) that may be related to volume scattering as is well documented in prior studies. The relative depth of the ~9,300 nm feature was plotted against REE concentrations for each sample and a visually striking trend resulted using fits to either linear, second order, and third order polynomial equations. However, R^2 values were rather low (i.e., < 0.18) due to the small sample size, even with the removal of three outliers. The results suggest that TIR emissivity data acquired from airborne or spaceborne instruments can be used successfully to quantify the abundances of aluminosilicate glasses in coal fly ash materials, and potentially, with measurements on a larger library of samples, their REE contents.

POSTER SESSION 1
Francis Lau

P1.1 Mercury Adsorption Characteristics for Waste Material Sorbents

Jeongmin Park, Sang-Sup Lee, Chungbuk National University, SOUTH KOREA

In combustion system, mercury is first released in three forms. It is first emitted as elemental mercury (Hg^0), and converted to oxidized mercury (Hg^{2+}) and particulate mercury (Hg_P). Among them, elemental mercury is difficult to remove with conventional air pollution control devices, and thus additional sorbent injection is needed. Therefore, many studies have been conducted to develop efficient low-cost adsorbents. Especially, the use of waste materials as adsorbents can contribute not only to recycling of waste but also to elemental mercury removal. Mercury adsorption of adsorbents with low surface area and pore volume are also known to be affected by chemical impregnation and acid gas composition. Therefore, in this study, activated carbon manufactured from sewage sludge, unburned carbon and coal activated carbon were used. In order to investigate the effect of $FeCl_3$ impregnation and HCl on mercury adsorption, sorbents and $FeCl_3$-impregnated sorbents were tested using two simulated flue gas conditions: 12% CO_2, 5% O_2, 7% H_2O, 60 - 70 $\mu g/m^3$ Hg^0, 200 ppm SO_2, 200 ppm NO, 0 ppm or 20 ppm HCl.

P1.2 Flow Uniformization in an Electrostatic Precipitator with Perforated Plates

Dong-Uk Kim, Sang-Sup Lee, Chungbuk National University, SOUTH KOREA

An Electrostatic Precipitator (ESP) is a widely used to reduce particulate matters emitted from coal power plants, incinerators, and coal boilers. A wide-angel diffuser located at the entrance of the ESP causes a non-uniform flow distribution due to boundary layer separation. Because a non-uniform flow distribution deteriorates the efficiency of an ESP, it is important to operate under the uniform flow condition. In this study, we investigated the effect of location and number of perforated plates installed in the wide-angle diffuser on the flow distribution in the body of the ESP. To do this, experiment and CFD simulation were conducted for the lab-scale ESP model. One perforated plate installed in the diffuser did not uniformize the flow distribution in the body of the ESP. Although two perforated plates highly improved the flow uniformity, stalled flow regions still existed at the top and bottom of the ESP body. With 3 perforated plates, a wall-jet flow was found in the body of the ESP with the depleted flow in the central region. In both experiment and simulation, a uniform flow distribution was obtained by placing 2 perforated plates on the inlet side and 1 perforated plate on the outlet side to prevent flow deflection.

P1.3 A One-dimensional Steady-state Model of Transport Bed Coal Gasification with in-situ CO_2 Capture using CaO Sorbent

Zaya Li, Bo Wang, Xiaojin Guo, Lifeng Zhao, CAS Key Laboratory of Advanced Energy and Power, Institute of Engineering Thermophysics, Chinese Academy of Sciences and University of Chinese Academy of Sciences, CHINA

In coal gasification with in-situ CO_2 capture technologies such as Hypr-RING, one of the key issues is to transport heat between the gasifier and regenerator. Higher capacity on heat transfer permit wider range for operating. Transport bed gasifier is considered as a kind of reactor with high capacity on heat transfer. However, a steady-state model is needed prior to test on pilot scale. A one-dimensional steady-state model composed of four sub-models, including reaction kinetics, thermodynamic, and hydrodynamic, are proposed in this work to simulate the steady-state process of coal gasification with in-situ CO_2 capture using transport bed performed as gasifier. As the similar one-dimensional steady-state model without carbonation and calcination of CaO accord well with the experimental data of common transport bed coal gasification in literatures, it is believed that it can also be adopted to coal gasification with in-situ CO_2 capture process. The effects of steam-to-coal ratio, Ca-looping/C ratio and superficial gas velocity are simulated, and sensitivity analyses based on different operating parameters are also carried out. Comprehensive comparisons of simulation results with further experimental data in bench-scale can help to improve the precision and range of the model.

P1.4 Study On the Coal Pyrolysis and Simi-Char Combustion Behavior During the Poly Generation Process for Power Generation

Shuaidan Li, Hougang Wang, Lei Zhang, China Huadian Electric Power Research Institute Co., LTD., CHINA

Poly-generation for power generation could produce high added value product such as tar and gas. The low added value simi-char are sent to the boiler and combust for power generation. This technology could improve the benefit of coal-fired power plant. However, simi-char is hard to combust and may limit the utilization of poly-generation technology. In order to improve the operation parameters and increase the benefit of poly-generation power plant, coal pyrolysis and simi-char combustion behavior of two different coal were studied in this paper.

Both pyrolysis behaviors and simi-char combustion behavior were studied in a TGA. For the coal pyrolysis behavior study, samples were heated up to 1000°C at 5 different heating rates. The results show that with the increasing of heating rate, simi-char yield would decrease slightly at the same temperature. Residence time of pyrolysis process would not affect to the simi-char yield significantly. Pyrolysis temperature may have more affect to simi-char yield. For the simi-char combustion behavior study, coal was heated up to 550°C-650°C under N_2 atmosphere, then hold for 1min-10min and transform into simi-char. Simi-char were then heated up to 850°C-950°C and combusted in the air and N_2 atmosphere. The results show that the simi-char which is generated by long residence time (5min and 10min) are more active than that of short residence time (1min and 2min).

P1.5 Construction of Micropore Structures in Macromolecule of Buertai Coal

Zhiyuan Yang, Zhiqiang Yin, Wenying Xue, Zhuoyue Meng, Yinyan Li, Anning Zhou, Xi'an University of Science and Technology, CHINA

China is a major coal resource country, understanding its structural parameters and influencing factors of methane adsorption are effective way of realizing the efficient and clean conversion of such coal. Pore structure affects many properties of coal, the pores in the coal macromolecular structure are mainly micropores (<2nm), these pores have a great influence on methane adsorption. To study these pore structures, the Atom Volumes & Surfaces tools in the Materials Studio (MS) software was used. 8 different gas molecules were as probes to obtain the surface area, pore volume and void fraction of the Buertai coal macromolecule, when He molecule used as the probe, the value of surface area, pore volume and void fraction are the maximum, which can reach $90m^2/g$, $0.1cm^3/g$ and 1.2%, respectively. As the probe radius increases, both pore volume and void fraction decrease evenly, but the surface area decreases rapidly when the probe radius is 1.73 Å. The same result is also confirmed in the pore size distribution (PSD) curve, the value of the PSD curve reaches its maximum when the probe molecular radius is 1.3 Å, and when the probe molecular radius is greater than 1.9 Å, the PSD curve becomes smooth soon, which indicates that the radius of the most micropores in coal are less than 1.9 Å.

POSTER SESSION 2
Omar Basha

P2.1 Design Optimization, Thermal Management and Scale-Up of Microchannel Reactors for the Conversion of CO_2 Rich Syngas

Chiemeka Chukwudoro, Nafeezuddin Mohammad, Shyam Aravamudhan, Debasish Kuila, Omar M. Basha, North Carolina A & T State University, USA

Microchannel reactors have attracted significant attention in recent years, due to their ability to leverage reduced heat and mass length scales to maximize process intensification, which has the potential to deliver major benefits to the chemical process industry, by accelerating the response to market changes, simplifying scaleup and providing the basis for rapid development of new products and processes.
However, there remain significant improvements to be made in the design of the microchannel reactors, specifically in the areas of maximizing catalyst utilization, improving heat management both within the reactor and in a scaled-up unit consisting of multiple reactors, and overall scale-up strategies to enhance market viability.

Therefore, this work will present detailed computational fluid dynamics (CFD) simulations to optimize the design of a microchannel reactor (50 $\mu m \times 100$ $\mu m \times 1.3$ cm, with 118 microchannels) currently being used at North Carolina A&T State University for the catalytic conversion of CO_2 rich syngas to hydrocarbons using Fischer-Tropsch synthesis. Various reactor designs are considered by optimizing the reactor inlet, gas distribution and channel design, and are compared based on their potential to maximize catalyst utilization, optimize heat management and enhance overall reactor liquid products yield. Moreover, strategies for unit scale-up, which is achieved by geometric stacking of multiple microchannel reactor units, will be presented, with the objective of minimizing productivity losses with increasing number of microchannel reactor.

P2.2 Theoretical Modeling of Mixed-Solids as High-Performance CO₂ Sorbents Operating Under Desired Conditions

Yuhua Duan, US Department of Energy, National Energy Technology Laboratory, USA

CO₂ is one of the major combustion products which once released into the air can contribute to global climate change. It is generally accepted that current technologies for capturing CO₂ are still too energy intensive and thus cost prohibitive for implementation on coal based power plants. Hence, there is a critical need for development of new materials that can capture CO₂ reversibly with acceptable energy costs. Accordingly, solid sorbents have been reported in several previous studies to be promising candidates for CO₂ sorbent applications through a reversible chemical transformation due to their high CO₂ absorption capacities at moderate working temperatures. Molecular modeling can play a role in identifying optimal sorbents.

By combining thermodynamic database mining with first principles density functional theory and phonon lattice dynamics calculations, a theoretical screening methodology to identify the most promising CO₂ sorbent candidates from the vast array of possible solid materials have been proposed and validated at the National Energy Technology Laboratory (NETL). The advantage of this method is that it identifies the thermodynamic properties of the CO₂ capture reaction as a function of temperature and pressure without any experimental input beyond crystallographic structural information of the solid phases involved. The calculated thermodynamic properties of different classes of solid materials versus temperature and pressure changes were further used to evaluate the equilibrium properties for the CO₂ adsorption/desorption cycles. According to the requirements imposed by the pre- and post- combustion technologies and based on our calculated thermodynamic properties for the CO₂ capture reactions by the solids of interest, we were able to identify only those solid materials for which lower capture energy costs are expected at the desired pressure and temperature conditions. These CO₂ sorbent candidates were further considered for experimental validations.

However, at a given CO₂ pressure, the turnover temperature (T_t) of an individual solid capture CO₂ reaction is fixed and may be outside the operating temperature range (ΔT_o) for a particularly capture technology. In order to shift such T_t of a solid into the range of ΔT_o, its corresponding thermodynamic property must be changed by changing its molecular structure by mixing with other materials or doping with other elements. In this study, through investigating several mixed sorbent materials, we demonstrate that by mixing/doping different types of solids it's possible for a sorbent to shift its T_t to the range of practical operating temperature conditions.

P2.3 A Novel Microwave-Accelerated Regeneration Process for Post-Combustion Carbon Capture

Tuo Ji, Fan Shi, Walter C. Wilfong, Qiuming Wang, Brian W. Kail, McMahan L. Gray, Department of Energy, National Energy Technology Laboratory, USA

Aqueous amine-scrubbing carbon capture process has gained widespread acceptance as a viable route for post-combustion capture of carbon dioxide (CO2). However, it often requires a large amount of superheated steam to raise the bulk temperature typically above 120 C for reactive regeneration. In this work, NETL amine-based sorbent mixed with silicone oil as a slurry sorbent has been developed for CO2 adsorption/desorption process aided by the Microwave (MW)- Accelerated Regeneration. Using non-aqueous silicone oil can minimize water use and also reduce the energy penalty for slurry regeneration because silicone oil has a much lower heat capacity but a higher boiling point than water. Moreover, selective MW heating of CO2-adsorbed BIAS can accelerate the CO2 desorption flux by 10 times in comparison with thermal heating and consume much less energy for CO2 desorption, even at process temperatures of 65-85°C. These results indicated that the MW-accelerated swing method is of high energy efficiency. A conceptual process techno-economic assessment (TEA) was conducted by using the Integrated Environmental Control Model (IECM). The resulting cost of CO2 avoided by MARS-based capture technology (excluding CO2 transport and storage) at a 650 MW-gross coal-fired power plant is estimated to be as low as $35/ton CO2, which is much less than that ($55/ton CO2) by amine-based carbon capture. This MARS-based carbon capture provides a potential affordable pathway for large-scale applications to existing industrial facilities, such as steel, cement, and chemical plants, which are also major sources of CO2 emissions.

P2.4 Development of a Continuous Nanotechnology Process for Converting Carbon Dioxide to Valuable Products

Rui Wang, Husain E. Ashkanani, University of Pittsburgh; Bingyun Li, West Virginia University; and Badie I. Morsi, University of Pittsburgh; USA

A unique nanotechnological process, employing aqueous amino acids (AA) to capture CO₂ from flue gas in postcombustion applications with the aim to produce commercially valuable products (sodium bicarbonate nanoparticles), is being developed in Aspen Plus

v.10. Our previous modeling studies in Matlab and Aspen Plus [1, 2] have validated the feasibility of this unique process, and our parametric studies have demonstrated its potential high CO₂ capture efficiency and high sodium bicarbonate nanoparticles yield in small and large-scale absorbers. In the present study, a continuous nanotechnological process is being developed in Aspen Plus v.10. This process is designed for high CO₂ capture efficiency from a typical raw flue gas streams to produce pure sodium bicarbonate nanoparticles. The typical flue gas used contains gaseous impurities, such as SO₂, SO₃, HCl and NO_x [3], which could derail the production of pure sodium bicarbonate nanoparticles. The continuous process includes 3 main units: (1) gaseous impurities removal unit, (2) CO₂ capture unit, and (3) sodium bicarbonate nanoparticles separation unit.

In the gaseous impurities' removal unit, water is used to dissolve the impurities from the raw flue gas in a countercurrent packed-bed, containing structured packing. The raw flue gas enters from the bottom, whereas water enters from the top of the packed-bed. The impurities-free flue gas exiting from the top of the packed-bed is sent to the CO₂ capture unit, whereas the water stream containing the dissolved impurities exiting from the bottom of the packed-bed is sent to a reverse osmosis unit (ROU) which consists of 3-stages provided with special membranes. The clean water stream (permeate) from the ROU is recycled back to the packed-bed for reuse, while the water stream loaded with dissolved impurities (retentate) is sent for further processing or disposal.

In the CO₂ capture unit, an aqueous stream of glycine/sodium hydroxide is used to react with CO₂ of the impurities-free flue gas in a countercurrent packed-bed absorber. The exiting gas stream at the top of the absorber is vented to the atmosphere, whereas the exiting liquid solution at the bottom of the absorber consisting of an aqueous solution of glycine, negligible amount of unreacted sodium glycinate, and sodium bicarbonate nanoparticles is sent to the sodium bicarbonate nanoparticles separation unit. In this unit, known also as the ultrafiltration unit (UFU), the sodium bicarbonate nanoparticles are separated from the solution using special membranes, whereas the liquid solution is further mixed with a metered amount of NaOH and recycled back to the absorber.

This paper discusses detailed modeling and optimization of the unique nanotechnological continuous process in Aspen Plus v.10 to achieve over 98% CO₂ capture from a typical flue gas stream and produce a stoichiometric amount of pure sodium bicarbonate nanoparticles.

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P2.5 Evolution of Basic Immobilized Amine Sorbent Pellets for Post-Combustion CO₂ Capture

W. Chris Wilfong, Leidos Research Support Team, National Energy Technology Laboratory; McMahan L. Gray, Physical Scientist, National Energy Technology Laboratory; Brian Kail, Qiuming Wang, Tuo Ji, Fan Shi, Victor Kusuma, Leidos Research Support Team, National Energy Technology Laboratory, U.S. Department of Energy; Parag Shah, Nicholas Fusco, PQ Corporation; USA

Basic immobilized amine sorbents (BIAS) are one of the most promising technologies for post-combustion CO₂ capture, reversibly binding the greenhouse gas through acid-base chemistry. While the bulk of BIAS-based CO₂ capture focuses on particle development, a growing portion of the studies investigates more practical sorbent forms into which the particles are incorporated. These forms include 3D-printed monoliths, solid/hollow fibers, but moreover pellets. The most viable pelletization method involves the extrusion of wet BIAS (or support)/polymer binder pastes followed by drying into solid rods or shaping them during drying into spheres. The objective of this work is to highlight the evolution of our BIAS pellet material, beginning from g-scale screening for the optimum formulation to kg-scale production of the final recipe, using commercial pilot-scale equipment.

Initial pelletization efforts screened different polymer binders like polyvinyl alcohol, polyvinyl acetate, polystyrene, and polyvinyl chloride for the CO₂ capture capacity behavior and mechanical strength they imparted to their polyamine/silica/fly ash/binder pellet rods. While PVC gave the highest mechanical strength, stability testing revealed a 31% degradation in CO₂ capture after 10 adsorption (55 ºC)-desorption (105 ºC) cycles, 7-8 hours, due to reaction of PVC with the BIAS amine groups. Incompatibility of the amine-binder system and use of a toxic tetrahydrofuran binder solvent (to dissolve PVC) predicated the need to find a more stable polymer.

For the second iteration of pellets *(advancement 1)*, the polychloroprene (PC) polymer was explored. Contrasting the reactive PVC-based pellet, this PC-based pellet displayed only a 4% loss in CO_2 capacity after 11 hours of combined dry/humid CO_2 capture cycle testing. Yet, because the raw PC chunks required milling before use of a toxic 1,4-dioxane solvent, an aqueous latex-based analogue was required.

Latex polychloroprene *(advancement 2)* was instrumental towards scaling pellet production because of its lower toxicity and the avoided polymer processing. We further attempted to enhance CO_2 uptake kinetics and thermal stability by preparing silica/FA pellet supports then post-functionalizing with a cross-linked mixture of polyethylenimine (MW=800, PEI_{800}) and N-N-diglycidyl-4-glycidyloxyaniline (E3) *(advancement 3)*. A <15% drop in the ~1.5 mmol CO_2/g capacity after 27 hours of dry adsorption-desorption cycling plus 48 hours of steam treatment (105 ºC, 7.2% H_2O/He) prompted us to scale pellet synthesis, first utilizing a commercially available lab-scale pelletizer then pilot scale equipment afforded through an industrial partner *(advancement 4)*.

Key goals of pelletizing FA/silica pellet supports with a lab-scale mixer (twin paddle)-extruder (single-screw) machine were to understand the effects of different operating variables/parameters on the viscoelastic properties of the wet binder/powder extrudate via storage (G') and loss (G") moduli, and the CO_2 capture and mechanical strength of the solid pellet support and sorbent. An optimally thick and extrudable paste having a G'≥9.5 x 10^5 was fully extrudable and gave viable amine-functionalized pellet sorbents with similar CO_2 capture capacity as the by-hand pellets. Production of a 5 kg batch of supports by PQ Corporation was accomplished using a pilot-scale, single-screw extruder to form the thick paste (high G' value; by planetary mixer) into adhesive ropes that were dried into strong distinct rods. Future impregnation and CO_2 capture tests of the resulting sorbents are in progress. This work paves the way for a future large-scale demonstration.

POSTER SESSION 3
Massood Ramezan

P3.1 Study on Ultra-Low Emission (ULE) Reduction Effects of SO_2 and NO_x in Coal-Fired Power Plants

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This paper we use satellite data from five isolated power plants to explore how local emissions levels change in the immediate vicinity of the power plant before and after ultra-low emissions (ULE) retrofitted. Sulphur dioxide (SO_2) and nitrogen dioxide (NO_2) observations from Ozone monitoring Instrument (OMI) satellite data were used to evaluate the emission changes of five isolate power plants retrofitted by ULE technology. The results show that all five isolated power plants show obvious point source characteristics. The SO_2 reduction ratios of actual emission and satellite observation for five power plant are 58.7% (10.0%),39.8% (21.1%),36.5% (27.2%),49.8% (54.5%),32.6% (47.5%), respectively. The NO_2 reduction ratios of actual emission and satellite observation for five power plant are 46.4% (10.1%), 58.3% (39.9%),34.0% (28.2%),23.1% (16.4%), respectively. The trend of emission reduction before and after the ULE retrofitted of SO_2 and NO_2 point column concentration by satellite observation is consistent with the calculated trend of emission reduction.

P3.2 Economic Study on Plasma Gasification of Municipal Solid Waste Coupled with Coal-Fired Power Plant Project

Shuaidan Li, Lei Zhang, Hougang Wang, Xiaojiang Li, China Huadian Electric Power Research Institute Co., LTD., CHINA

Plasma gasification for municipal solid waste (MSW) technology could decompose some of the pollutant such as dioxin, furan, and so on. However, due to the high cost of investment, this technology is still not widely use in China. On the other hand, plasma gasification of MSW and coupled with coal-fired power plant may reduce the investment of the project. Besides, it could also provide a new way for the transformation of Chinese coal-fired power plant. In general, this technology needs to build a plasma gasifier before the coal-fired boiler. MSW turn into syngas a plasma gasifier at first, then syngas is sent into the coal-fired boiler for power generation.

This paper studied the economic of a plasma gasifier of municipal solid waste and coupled with coal-fired power plant project. Three different electricity prices were calculated. The result shows that policy allowance would significantly affect to the benefit. The project would have a considerable rate of return if the electricity price is 650 Yuan/MWh and the garbage disposal allowance is about 40 Yuan/t. Otherwise, the

project would have financial loss if electricity price is equal to that of coal-fired power generation. Sensitivity analysis shows that compared with the investment cost, utilization hours and electricity price would have more affect to the benefit.

P3.3 Performance of Graphene-Based Composite Porous Carbon for Adsorption and Separation of Methane

Zhiyuan Yang, Xiaoqian Ju, Hongbin Liao, Zhiqiang Yin, Xi'an University of Science and Technology, CHINA

In order to realize the separation and enrichment of methane in coalbed methane (CBM), this paper used coal based activated carbon (CbAC) and graphene oxide (GO) to prepare graphene based composite porous carbon (GCPC) by KOH activation. The pore structure of the composite material is more developed. The specific surface area of the sample is 2695.22 m^2/g and the average pore size is 3.24 nm. At 303k, 3 MPa, the equilibrium adsorption capacity of methane is 7.76 mmol/g. The separation coefficient of CH_4: N_2 is 2.72 at 298 k (the volume flow rate of N_2 and CH_4 is 4:1). The results show that adding a small amount of graphene oxide can greatly enrich the pore structure of CbAC and improve its adsorption capacity. This method provides a way to effectively separate methane from nitrogen in low concentration coalbed methane and realize the resource utilization of methane.

P3.4 Analysis of Liquefaction Recycle Solvent by Comprehensive Two-dimensional Gas Chromatography

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The recycle solvent is an important index in direct coal liquefaction (DCL) technology. Clarifying the composition and structure of the recycle solvent is helpful to improve the products quality of DCL. The composition of the recycle solvent is very complex, which could include hundreds of hydrogenated aromatic hydrocarbons. Due to the limited peak capacity, gas-mass spectrometry (GC-MS) analysis is insufficient to clarify the detailed of solvent composition. The comprehensive two-dimensional gas chromatography-mass spectrometry/hydrogen flame ionization detector (GC×GC-MS/FID) has high resolution, large peak capacity, and high sensitivity. It can effectively separate complex composition. In our study, qualitative and quantitative analysis of the recycle solvent was performed by using GC×GC-MS/FID. The qualitative analysis was performed by NIST library search, standard mass spectrum comparison, and two-dimensional spectral features. The composition of recycle solvent was broadly divided into six categories such as alkanes (A), monocyclic (B), bicyclic (C), tricyclic (E), tetracyclic (F), and other aromatic hydrocarbons (D) (Figure 1). While paraffins are mainly present as alkanes, phenol and cresol are the major compounds in monocyclic compounds. Naphthalene, tetralin, and decalin are the major components in bicyclic compounds whereas anthracene, phenanthrene, dihydrophenanthrene, and octahydroanthracene are mainly identified in tricyclic compounds. Tetracyclic compounds mainly include pyrene, dihydropyrene, and tetrahydropyrene. Indene and biphenyl are identified as other aromatic hydrocarbons. These compounds were quantified by the peak area normalization method. The results showed that tetralin and its derivatives have the highest content, followed by naphthalene and its derivatives, followed by tricyclic anthracene series, of which octahydroanthracene has the highest content.
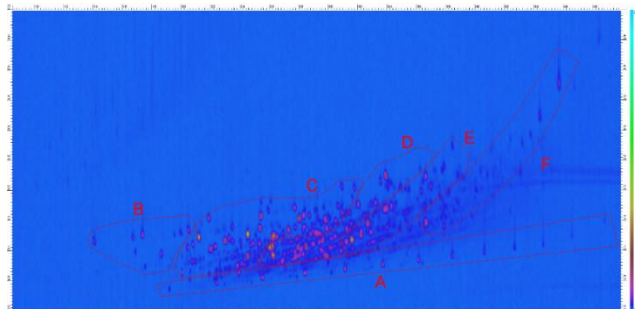

Figure 1. Analysis of the recycle solvent by two-dimensional GC×GC-MS/FID. A: alkanes, B: monocyclic, C: bicyclic, D: other aromatic hydrocarbons, E: tricyclic and F: tetracyclic.

P3.5 Testing of Several Industrial Methods for Extracting Rare-Earth Elements from Ash and Slag Waste of the Primorskaya Hydroelectric Power Plant

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The extraction of rare earth elements from coal burning wastes is advisable in the integrated treatment of such wastes to reduce their negative impact on the environment and obtain commercial benefits. It is proved that rare earth elements (REE) are present in ash and slag waste of power plants in concentrations sufficient for industrial extraction. REE extraction ratio depends on the chosen method, reagents used, "liquid – solid phase" ratio, and temperature and time of leaching. The preliminary preparation of ash and slag increases the extraction efficiency. In this study, we tested the industrial methods for extracting rare-earth elements on ash and slag waste from the Primorskaya hydroelectric power plant (Primorsky Krai, Russia). The REE content in these ash and slag samples largely correlates with global data, which shows the fundamental possibility of their application as raw materials. Using the concentration table and magnetic separator, ash and slag materials were separated into fractions that differed in their magnetic properties, particle size, and mass. This procedure concentrated scattered elements in certain fractions. The directed application of a strong magnetic field created by neodymium magnets further concentrated REE in one of the fractions. Some elements were enriched by $2 - 7$ times. The effect of various acids and their mixtures on the REE extraction ratio from ash was estimated. For most REEs, the extraction ratio varied from 60 to 80 %, while it was shown that the type of acid and its concentration do not significantly affect the amount of rare and trace metals extracted. High recoverability of REE is ensured even when using molar solution of nitric acid at $1 : 1$ mass ratio with the studied sample. The fusion of ash and slag with alkaline components as one of the stages of sample preparation makes it possible to recover 100% of some REE. Using this method, one can obtain a by-product – highly dispersed silicon dioxide powder (concentration of about 98%) with the surface area of SiO_2 particles of more than 450 m^2/g and average pore diameter of 6.1 nm. The reported study was funded by RFBR according to the research project № 18-29-24138.

POSTER SESSION 4
Leslie Ruppert

P4.1 Effect of Power Plant Capacity on the CAPEX, OPEX, and LCOC of the CO_2 Capture Process in Pre-Combustion Applications

Husain E. Ashkanani, Rui Wang, U.S. Department of Energy, National Energy Technology Laboratory and University of Pittsburgh; Wei Shi, U.S. Department of Energy, National Energy Technology Laboratory and Leidos Research Support Team, National Energy Technology Laboratory; Nicholas S. Siefert, U.S. Department of Energy, National Energy Technology Laboratory; Robert L. Thompson, U.S. Department of Energy, National Energy Technology Laboratory and Leidos Research Support Team, National Energy Technology Laboratory; Kathryn Smith, U.S. Department of Energy, National Energy Technology Laboratory and University of Pittsburgh; Janice A. Steckel, Isaac K. Gamwo, David Hopkinson, U.S. Department of Energy, National Energy Technology Laboratory; Kevin Resnik, U.S. Department of Energy, National Energy Technology Laboratory and Leidos Research Support Team, National Energy Technology Laboratory; Badie I. Morsi, U.S. Department of Energy, National Energy Technology Laboratory and University of Pittsburgh; USA

Aspen Plus v8.8 was used to simulate the pre-combustion CO_2 capture process from a typical fuel gas stream at different power plant capacities ranging from 54.3 to 543 MW. Polyethylene glycol polydimethyl siloxane (PEGPDMS-1) was used as a physical solvent to capture CO_2 in a countercurrent packed-bed absorber containing a structured packing (Mellapak 250Y). The process pressure was 51.4 bar and the solvent temperature was varied from 10 to 40 oC. The internal diameter of the absorber ranged from 1.9 to 7 m and the packing height from 13.9 to 45.5 m. The physico-chemical properties were obtained and modeled using the Perturbed Chain-Statistical Associating Fluid Theory (PC-SAFT) Equation-of-State (EOS).

Four process constraints were imposed in Aspen Plus: (1) no flooding in the absorber, (2) the absorber height to diameter ratio (H/D) is greater than or equal 6, (3) at least 90 mol% of the CO_2 capture from the fuel gas stream, and (4) the CO_2 stream destined to sequestration sites should contain less than 600 ppm water concentration and less than or equal 0.5 mol% of fuel gases (H2, CO, CH$_4$). The plant lifetime was assumed to be 30 years with an annual discount rate of 10% and an annual maintenance cost of 4% of the total capital expenses.

Seven power plants with different capacities were used and for each plant, the corresponding CO_2 capture process was simulated. The absorber flooding was checked

using the generalized pressure drop correlation (GPDC) by Leva [1] and the capital expenditure (CAPEX), operating expenditure (OPEX), and levelized costs per ton of CO_2 captured (LCOC) were calculated [2-5]. Normalized by the largest power plant capacity (543 MW) used in the simulation, the results indicated that the capital and operating

expenditures increased, however, the LCOC decreased with increasing plant capacity. This behavior was due to the increased annual tonnage of the CO_2 captured with plant capacity as shown in Figure 1. The calculated CAPEX, OPEX, LCOC and the tonnage of CO_2 captured for the 543 MW power plant were about 52 MM$, 22 MM$/year, 7.46 $/ton and 4 MM ton/year.

P4.2 The Omnis Separation Plant; Transforming Coal Waste into High-Value Products for Agriculture, Power and Industry

Greg Smith, Omnis Energy LLC, USA

Over 70% of the world's topsoil has been lost in the last 150 years and demand for clean, low-cost energy is exponentially increasing. As we look towards 2050, energy, food security and jobs are key challenges facing the United States and the rest of the world.

Omnis Energy have developed a technology to transform coal waste into high-grade energy and agricultural products to meet these challenges. The Omnis Separation Plant cost-effectively separates coal waste, from both underflow generated by ongoing operations and waste sites subject to reclamation, into ultrafine carbon, mineral and water fractions. This facilitates the production of ultra-pure carbon products for energy and industrial markets in addition to a mineral product that can be used to restructure and rebalance damaged soil, revitalizing farmland and boosting plant growth.

Patented milling, micro-particle separation and dewatering process steps are incorporated into this process and products can be engineered to meet customer and logistical needs. Through the utilization of coal waste as a feedstock, Omnis Energy is also addressing the environmental and financial liabilities associated with coal waste for past, current and future land users.

Following several years of laboratory and pilot-scale research and development, including successful trials conducted by purchasers, the first plant in the United States is nearing completion at CONSOL's Bailey operation in Pennsylvania. Additional plants are also being scheduled for completion in China through Fenix Technologies, a "sister" company to Omnis Energy.

P4.3 Investigation of Air Extraction Integration and Carbon Capture in IGCC

Shisir Acharya, Ting Wang, University of New Orleans, USA

Coal is one of the major sources of energy currently used worldwide. It provides up to 996 Billion KWh of electricity in the United States, which is approximately 23.5% of the total electricity produced. Despite the vast usage of coal as a source of energy, it is considered by many people to be a "dirty" source of energy. Substances such as Carbon dioxide (CO_2), Nitrogen Oxides (NO_x), Sulfur oxide (SO_x), Mercury (Hg) are produced when coal is burned to produce energy. These substances contribute to climate change, environmental pollution, health problems etc. Therefore, it is our obligation to utilize coal in a cleaner way. Cleaner coal energy can be produced by using an ultra-supercritical Pulverized Coal (PC) power plant or by employing the Integrated Gasification Combined Cycle (IGCC). Since the 1970s, the IGCC technology has been developed and demonstrated, but it has still not been widely commercialized. The objectives of this study are to investigate integrations of air extraction between gas turbine and Air Separation Units (ASU) and implementation of carbon capture. Five different cases of IGCC are investigated and their performance and emissions are compared with the U.S. Department of Energy's benchmarked subcritical PC, ultra-supercritical PC, and NGCC plants. The five IGCC cases include Air-Blown IGCC, Slurry-fed IGCC, and different degrees of air integration between ASU and the Gas Turbine. The results show that a moderate air integration of about 17% of ASU air input is the most effective when compared to 50% and 0% compressed air extraction from the gas turbine. The results also show about a difference of 5.6 point in efficiency when CO_2 capture and storage (CCS) is considered in IGCC. The cases were simulated using the Thermoflex® software.

P4.4 The Allam Cycles for Fossil Fueled Power Plants

Richard Dennis, National Energy Technology Laboratory (NETL), USA

The US Department of Energy is investing in the development of power cycles based on supercritical carbon dioxide (sCO_2) as the working fluid. Power plants based on these cycles have the potential for a lower COE with better efficiency in many heat source

applications including fossil fuels, concentrated solar power, nuclear energy and waste heat recovery. The DOE is investing in all of these applications. The DOE Office of Fossil Energy manages R&D projects supporting the Recompression Brayton cycle, the Allam cycle with carbon capture and cycles optimized for waste heat recovery. This presentation will present an overview of research activity in sCO_2 based power cycles in the DOE Office of Fossil Energy.

The presentation will discuss two primary sCO_2 cycles: the recompression Brayton cycle and the Allam Cycle. The RCB cycle uses SCO_2 as the working fluid and can be seen to replace steam-based Rankin cycles in thermally heated applications like coal combustors, concentrated solar power and nuclear energy. The Allam cycle is a semi-closed cycle that is directly fired with pure oxygen and gaseous carbon-based fuels producing high turbine inlet temperatures, the working fluid is SCO_2. Both cycles offer a line of sight to lower cost and higher efficiency applications. The Allam cycle is designed for 95 % CO_2 capture. The benefits and technical challenges of these cycles will be discussed. A relevant project portfolio will be presented including the world's largest and most advanced demonstration of a Recompression Brayton cycle.

POSTER SESSION 5
Evan Granite

P5.1 Technoeconomic Assessment for Extraction of Rare Earth Elements from Acid Mine Drainage

Alison Fritz, Stanford University/ National Energy Technology Laboratory; Thomas Tarka, National Energy Technology Laboratory; USA

The Department of Energy National Energy Technology Laboratory Rare Earth Elements (REE) Program has identified multiple pathways for REE extraction from coal feedstocks, which are currently undergoing technoeconomic screening. The goal of this paper is to ascertain the economic viability for scale-up of one of these feedstocks, a novel step-leaching approach for REE extraction from Acid mine drainage (AMD) in the Appalachian Coal Basin. AMD is an acidic and metal-rich water runoff from active and abandoned mines that is one of the primary water quality challenges in the Appalachian Coal Basin. AMD from coal mining in this region has been demonstrated to be enriched with REE relative to raw coal in multiple studies. Valorization of extraction from REE can encourage acid mine drainage remediation from abandoned mines or upwellings where mines are not directly responsible for remediation. REE is a critical material used to manufacture high-technology products and devices including smart phones, medical devices, airplanes, and automobiles. Global supply of REE is dominated by China, and 2010 threats by China to restrict the supply initiated widespread research efforts to develop a domestic REE supply.

In this paper, material balances and cost estimation are used to generate performance parameters for scale-up of REE extraction from AMD. Economic performance and sensitivity to key variables will be presented. As alternative sources of REE, such as AMD, progress it is important to consider the type of regulatory changes and incentives needed to develop a viable supply chain. The paper will close with discussion of the opportunities and challenges identified by this analysis in developing a domestic supply of REE from coal.

P5.2 An Updated CoalQual for Utilization of Abundant Domestic Coal

Priscilla Prem, Evan Granite, Murphy Keller, Ward Burgess, National Energy Technology Laboratory, USA

Coal is notoriously difficult to sample due to its inherent heterogeneity as it varies greatly by region, coal rank, and sample depth. Since the 1970's, the U.S. Geological Survey (USGS) has maintained a vital national coal quality database (USCHEM), of which COALQUAL is its primary, searchable subset. COALQUAL version 3.0 was published in 2015, with the purpose of addressing missing information stemming from software size limitations present in earlier versions of the database. By including qualifiers and estimates of crucial parameters, the authors of COALQUAL version 3.0 sought to provide a more complete understanding of U.S. coal reserves. This approach is arguably sufficient for Eastern and high-ranking coals for which there is an adequate amount of data available for making such estimates. However, many Western and low-ranking coals lack adequate sampling data since these regions were generally overlooked during the vast sampling efforts carried out in the 1970's and 80's. In the 30 years since the last sample was entered into the database, more evidence for the utility of these coals has gained traction and justifies the undertaking of new sampling efforts.

Lignite coals show promise for rare earth element (REE) extraction, but it was found that these coals are vastly under-sampled compared to their proportion of overall coal reserves, and contain the highest amount of "B" data, especially in critical REE measurements. Additionally, several under-sampled regions show promise for REE

extraction, including the subbituminous coals in the Green River Region in Wyoming and the lignite coals in the Texas Region of the Gulf Coast Province. To optimize new sampling efforts in these regions and others, updated analytical techniques should also be considered. Several of the analytical methods used at the time are now outdated and may be contributing to excessive "L" data. By switching to ICP-MS for most elemental analyses, many of these "L" data will no longer fall below detection limits. CoalQual is a treasure trove of critical information on abundant domestic coal. New sampling efforts and updated analytical techniques would enhance the CoalQual database to continue meeting the United States' needs for the 21st century.

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P5.3 Rare Earth Transformations During Coal Combustion – Implications for Potential Recovery

Jeremy Rivkin, Murphy Keller, Ward Burgess, Evan Granite, National Energy Technology Laboratory, USA

Rare earth elements are present within abundant domestic coals and coal byproducts such as fly ash and bottom ash. The United States typically produces around a billion tons of coal annually, with most of the coal being burned to generate electricity. The combustion chemistry within coal-fired power plants is complex and fascinating, presenting great opportunities for recovery of the rare earth and other critical elements. This project aimed to answer what happens to rare earth elements (REEs) during coal combustion and why their extractability varies between coal and ash. Answering these questions required two separate efforts: (1) conducting a literature search to find studies characterizing the association of REEs in coal and ash and (2) comparing data from extraction experiments using 2M acetic and sulfuric acids to extract REEs from a class C fly ash. It was necessary to understand how REE associations change during combustion and how factors like coal rank, major element composition, and solvent type affect REE extractability. For these examinations, the following analytical techniques were employed: x-ray diffraction, scanning electron microscopy, thermogravimetric analysis, and inductively coupled plasma mass spectrometry.

As coal is burned in a power plant, rare earth bearing organic and inorganic constituents will react with other components of coal and a homogeneous flue gas mixture. This occurs as aluminosilicate glass forms from the combustion of silicate clay minerals. The grains of rare earth mineral monazite can retain their material structure during coal combustion, resulting in entrapment within the aluminosilicate glass matrix. Trace amounts of rare earth elements can also be distributed throughout these glass particles. The primary implication of this reassociation is the necessity for aggressive separation techniques capable of breaking down the glass matrix to isolate REEs and rare earth minerals. Acetic acid was effective in extracting 72% of REEs from the fly ash while sulfuric acid extracted 53% of REEs. This could be attributed to the precipitation of gypsum during sulfuric acid leaching which inhibited extraction by locking these metals into its lattice structure. Both procedures will need improvement due to low REE extractability relative to other acidic extractions capable of capturing over 90% of REE content.

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