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ABSTRACTS BOOKLET

Clean Coal-based Energy/Fuels

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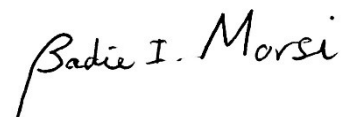University of
Pittsburgh

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This Abstracts Booklet is prepared solely as a convenient reference for the Conference participants. Abstracts are arranged in a numerical order of the oral sessions as published in the Final Conference Program. In order to facilitate the task for the reader to locate a specific abstract in a session, each paper is given two numbers: the first designates the session number and the second represents the paper number in that session. For example, Paper No. 12.1 is the first paper to be presented in the Oral Session #12.

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On behalf of the Thirty-Ninth Annual International Pittsburgh Coal Conference, I wish to express my sincere appreciation and gratitude to Ms. Nicole Drebsky for her meticulous guidance of the entire conference. My profound gratefulness goes to Mr. Rui Wang for his crucial assistance and dedication in preparing this Abstracts Booklet.

Thank you,

Badie I. Morsi

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

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1.1   (8:05-8:25) Performance Testing of a Moving-Bed Gasifier Using Coal, Biomass, and Waste Plastic Blends to Generate White Hydrogen

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The objective of this DOE-funded project by the Electric Power Research Institute, Inc. (EPRI), Hamilton Maurer International (HMI) and Sotacarbo S.p.A. (Sotacarbo), is to qualify coal, biomass, and plastic waste blends based on performance testing of selected pellet recipes in a pilot-scale updraft moving-bed gasifier. The testing will provide relevant data to advance the commercial-scale design of the moving-bed gasifier to be able to successfully use these feedstocks to produce hydrogen. In particular, the effects of the waste plastics on feedstock development (i.e., blending and pelletizing) and the resulting products (i.e., syngas compositions, organic condensate production, and ash characteristics) are a focus. The gasifier is Hamilton Mauer International, Inc. (HMI)'s moving-bed gasifier, which has been proven capable of gasifying nearly all coal ranks. It has also shown the ability in prior testing work to gasify wood chips. However, mixtures of these fuels with plastic wastes have not been prepared and gasified together. The feedstocks will be prepared by California Pellet Mill (CPM) under contract to HMI.

The technical tasks and current status for this two-year research project are:
•   Feed Procurement and Preparation: Nine different feedstocks were prepared from varying compositions of PRB coal, corn stover biomass, and car fluff waste plastics. Fuel pellets were produced by California Pellet Mill and shipped to Sotacarbo's test facility in Italy.
•   Test Plan Development: A test plan was created to define the test runs to be performed. The test plan detailed the different tests that were run, instrumentation used, extractive samples taken, and relevant figures of merit.
•   Gasifier Testing: Tests are currently being performed in the pilot-scale gasifier at Sotacarbo using nine different fuel feedstocks generated from varying mixtures of coal, biomass, and plastic wastes. The testing will provide information on gasification reaction efficiency/performance, yielding relevant data for models used to scale up the gasifier design. This task will also include work to reassemble the gasifier at Sotacarbo and perform a baseline 100% coal run.
•   Data Analysis and Reporting: Review of the data, determination of figures of merit, and interpretation of the results to be reported. The results will be used to specify the range of feedstock blends that can be successfully gasified as well as quantify gasifier outputs based on specific blends.
This paper will be summarizing the pelletizing procedure that ensures the viability of the tri-fuel pellets for the gasification runs that are being performed at Sotacarbo's 30 mm up draft moving bed gasifier. Initial gasification tests and all the lab scale tri-fuel pellet gasification runs will be completed by the fall of 2022. Performance data will enable modeling of a full-scale HMI industrial scale gasifier supporting both CHP and Hydrogen production.

1.2   (8:25-8:45) Study on the mineral transformation and catalytic mechanism of petroleum coke gasification based on ash addition

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Petroleum coke, a by-product of crude oil refining, can be utilized as a gasification feedstock. However, the extremely low gasification reactivity inhibits the large-scale utilization of petroleum coke. Previous studies have shown that AAEMs can effectively promote the gasification reactivity of petroleum coke. Power plant ash is rich in AAEMs, which can be used as catalysts to promote the gasification of petroleum coke. However, the existence of AAEMs in ash with different characteristics is inconsistent, so it is necessary to deeply study the mineral transformation behavior of ash in the process of catalytic gasification of petroleum coke and explore the catalytic mechanism, so as to provide theoretical support and technical guidance for the large-scale utilization of petroleum coke.

In this work, experiments were conducted on a Self-designed TG. Four kinds of power plant ash with different characteristics (two kinds of coal ash and two kinds of biomass ash) were selected and mixed with petroleum coke for catalytic gasification. Based on XRD, XPS and SEM-EDS and other test methods, the mineral transformation behavior during catalytic gasification was explored, and the relationship between gasification reactivity and mineral properties was tentatively constructed. This can not only provide a new way for the reuse of coal ash/biomass ash, but also provide a strong theoretical support for the subsequent large-scale utilization of petroleum coke.

1.3   (8:45-9:05) Rule of heat and mass transfer during the pyrolysis process of organic solid waste particles

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In order to study the rule of heat and mass transfer in the pyrolysis process of organic solid waste, and further clarify the mechanism of heat transfer on the pyrolysis reaction process of organic solid waste, this paper selected pine sawdust, furfural residue and corn straw as the research objects of organic solid waste, modeling the pyrolysis process of single particle of three raw materials. The model adopted multi-step dynamics, establishing the correlation between reaction kinetics and raw material types. And it improved the suitability of pyrolysis model for different raw materials. At the same time, the secondary carbonization and the secondary cracking reaction of tar, the heat and mass transfer process of volatile in particle pores, as well as the endothermic effect of pyrolysis and the convective heat transfer effect of volatile escape were considered. The changes of temperature, tar and light gas content at different radial positions during pyrolysis of pine sawdust, furfural residue and corn straw particles over time were studied. Additionally, the effects of particle size and final pyrolysis temperature on particle center temperature and conversion were also investigated. The results showed that the temperature distribution during the pyrolysis of pine sawdust, furfural residue and corn straw was consistent, there was an obvious temperature gradient between the particle surface and center, and the "platform" phenomenon appeared in the particle center. However, due to the differences in the thermal conductivity and thermal endothermic effect of the three raw materials, the "platform" appeared at different times. The uneven distribution of particles heat led to different initial time of weightlessness at different radial positions of the particles, resulting in a "lag" phenomenon. With the increase of temperature, the content of solid residue gradually decreased, and the gas products and liquid products increased. When the temperature was higher than 900 K, the output of gas and pyrolysis liquid showed an obvious inverse relationship. The uneven temperature distribution in particles led to uneven distribution of each component concentration.

1.4   (9:05-9:25) Effect of pyrolysis conditions on physiochemical properties of petroleum coke and its subsequent gasification reactivity

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Petroleum coke is widely used as a fuel due to its high carbon and high calorific value. However, extremely low gasification reactivity limits the large-scale utilization of petroleum coke, and it is urgent to find a way to improve the gasification reactivity of petroleum coke. Most of the existing gasification research is based on TG, and the processes of pyrolysis and gasification are artificially separated, which is quite different from the actual industrial application. It is necessary to fully understand the influence of pyrolysis conditions on the structure of petroleum coke, and to explore the influence of structural differences on the reactivity of subsequent gasification. This provides theoretical support for the optimization of subsequent gasification reactivity research.

In this work, firstly, the effects of pyrolysis temperature, heating rate and residence time

on the structure of petroleum coke were investigated based on a fixed bed reactor, and the relationship between structural parameters and pyrolysis conditions was established. Second, the effect of coke structure on the reactivity of subsequent gasification was investigated on commercial TG and self-designed TG, respectively. The above studies show that the influence of the pyrolysis process cannot be ignored in the study of the intrinsic gasification reactivity of petroleum coke.

1.5   (9:25-9:45) Effect of microwave dehydration and upgrading on lignite thermal conversion characteristics

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Lignite is an important energy and resource with huge reserves and good reactivity, but its utilization and development are greatly restricted due to its large moisture content. Microwave heating has the advantages of selective heating, safety, rapidity and high efficiency, and is a potential application technology for dehydration and upgrading of lignite. In the current literature, there are many studies on the microwave dehydration process and the properties of their products, however, relatively few studies on the influence of microwave upgrading process on their thermal conversion characteristics of products. This paper describes the effect of microwave dehydration and upgrading on the pyrolysis, volatile releasing and gasification characteristics of lignite. The pyrolysis behaviors and its gas products before and after microwave dewatering were determined using a thermogravimetric-Fourier transform infrared (TG-FTIR) spectroscopy instrument. Atmospheric pressure and pressurized gasification characteristics of pyrolysis coal char (come from the raw lignite and its microwave upgraded products) were studied on pressurized gasification thermogravimetric experimental device. The results show that the pyrolysis process moved towards the high-temperature and bituminous coal region. The characteristic parameters of pyrolysis indicated that the thermal stability of the coal structure was improved. The pyrolysis kinetic parameters were calculated, and the activation energies before and after modification were obtained at the same time. According to the TG-FTIR results, the amount of released gas products from stable and saturated components (such as p-xylene, phenol and CH_4) increased, whereas the amount of released gas products from unstable and unsaturated components (such as CO_2, CO and formic acid) decreased. The unstable structure and components in the lignite were decomposed and transformed, and a stable structure and phase were created. Moreover, pyrolysis activity declined, and thermal stability improved. The difference is that the gasification activity of upgraded coal has increased. Due to the increase in diffusion resistance and the shift of the chemical reaction to the left side of the equation, the rate of gasification reaction decreased with increasing pressure at relatively low temperature. In general, microwave treatment is a relatively mild dehydration and upgrading method. As the treatment temperature increased, the effects were more obvious. Meanwhile, the pyrolysis and gasification characteristics of the coal sample did not change much after upgrading, and the high thermal reactivity of the raw coal was still retained. This is of great benefit for the large-scale application of lignite after microwave upgrading.

SESSION 2 (8:00 – 9:45)
COAL SCIENCE – 1
Brian Shaffer and Leslie Ruppert

2.1   (8:05-8:25) ANALYSIS OF HIGH TEMPERATURE BEHAVIOR OF CRYSTAL COMPONENTS IN ASH OF VIETNAM COAL USING XRD AND TEM

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We have already reported the thermal behavior of four types of Argonne standard coal. From the results, it was found that needle-shaped crystals appeared after calcining with two types of Argonne standard coals. In the course of our study, we are interested in Vietnamese coal. Data for these coals may be short compared to those of Argonne premium coals. In this study, we investigated changes in the behavior of ash components in Quang Ninh (QN), Lang Son (LS) and Thai Nguyen (TN) Vietnam coals with high temperature treatment.
Three coal samples were used: Quang Ninh (QN) anthracite, Thai Nguyen (TN) subbituminous, and Lang Son (LS) lignite from Vietnam. In order to obtain 0.7 g of coal sample for XRD measurement, it was processed in a calcining furnace in an air atmosphere at a gas flow rate of 100 ml/min, 800°C, 1000°C and 1200°C and a heating rate of 10°C/min. X-ray diffraction measurements were performed to investigate the crystal structures of ash components in coal samples treated under air atmosphere. As

the X-ray diffractometer, Ultima IV (Rigaku) was used.
From the results of industrial analysis and elemental analysis of each coal, the ash content was in the order of TN> LS> QN. QN coal was a coal with very low ash content compared to the other two coals. The fixed carbon and C contents decrease in the order of QN> TN> LS, and the coal rank can be considered to decrease in the same order. From the results of ash component analysis, QN and LS contain a large amount of SiO_2 and Al_2O_3, but a low content of CaO. On the contrary, TN contained a large amount of CaO but a low content of SiO_2 and Al_2O_3.
In XRD of QN, only the peak of kaolinite ($Al_4Si_4O_{10}(OH)_8$) was confirmed in the sample before calcination. A broad peak was observed around 20-30° as before calcination. This is likely to be carbon amorphous. After calcination, kaolinite disappeared and peaks of illite [($KAl_2(Si_3Al)O_{10})(OH)_n$] and anhydrite ($CaSO_4$) appeared. As a result of ash analysis, anhydrite was observed at all temperatures after calcination despite the low CaO content, suggesting that anhydrite is a mineral which is easily crystallized. The illite peak which appeared at 800°C decreased at 1000°C and disappeared at 1200°C. On the other hand, mullite ($Al_6Si_2O_{13}$) appeared at 1000°C, and the peak intensity increased at 1200°C. From these facts, it is considered that the change from kaolinite to illite and then to mullite occurred. The quartz peak appeared at 1000°C and increased significantly at 1200°C. It is considered that the carbon content was reduced by calcination. In XRD of LS, kaolinite and pyrite were observed before calcination. Similar to QN, the kaolinite peak disappeared by calcination, the illite peak appeared, and mullite was observed at further increase in temperature. It is probable that the change from kaolinite to illite and mullite also occurred in LS. Quartz, unlike QN, was found at all temperatures after calcination, with a reduced peak at 1200°C. Hematite (Fe_2O_3) was observed at all temperatures after calcination because pyrite was oxidized and changed to hematite.
In TEM image of QN, no crystalline substance could be confirmed in the raw coal. In those calcined at 800°C and 1000°C, needle-like crystals and a collection of very small particles were also observed around the large particles, although the number was small. They disappeared when calcined at 1200°C, and a collection of black particles at about 50 nm was observed. In XRD, illite was the only mineral characterized by peaks appearing at 800°C and 1000°C and disappeared at 1200°C, indicating that the acicular crystals observed may be illite. Needle-shaped crystals could also be observed in LS and TN. As with QN, needle-shaped crystals could be observed in LS samples calcined at 800°C and 1000°C. On the other hand, observable crystals of TN were thicker and longer than the needle-like crystals seen in QN at 800°C. In addition, illite peaks appeared at 800°C and 1000°C in LS, but not in TN. From these results, it could be considered that the needle-shaped crystals observed in LS may be illite like QN, but the needle-shaped crystals observed in TN would be another mineral.

2.2   (8:25-8:45) Effect of microwave irradiation on spontaneous combustion and high temperature combustion characteristics of Shenmu bituminous coal

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Microwave irradiation is widely used in coal industry including drying, desulfurization, pyrolysis and so on. In recent years, many researchers have investigated the possibility of using microwave irradiation to change the pore structure of coal seam for exploiting coal bed methane. However, it is not clear whether this pretreatment will change the reactivity of coal, such as spontaneous combustion and high temperature combustion. In this work, Shenmu bituminous coal is subjected to microwave oven at 700 W for different time to get modified coal samples. The spontaneous combustion is studied by programmed temperature-rising experiments based on national standard of China, while the high temperature combustion is investigated by thermal gravity analysis (TGA). In the programmed temperature-rising experiments, gas production of CO, CO_2, C_2H_6, C_3H_8 were observed to compare the critical temperature of modified coal samples. When the microwave time increases, the tendency of spontaneous combustion increases first and then decreases. As for TGA, the initial and ending temperatures are 30°C and 1000°C, respectively, and the heating rate is 10 °C /min. The TG curve indicates that microwave treatment lower the ignition point and increase the oxidation reaction rate of coal. The activation energy E and pre-exponential factor A were obtained after processing the TG and DSC curves, shown in Fig. 1. E increases and then decreases with increasing microwave time, while A changes in the opposite direction. This indicates that the high temperature combustion reactivity of the modified coal increases and then decreases with the increase of microwave treatment time.
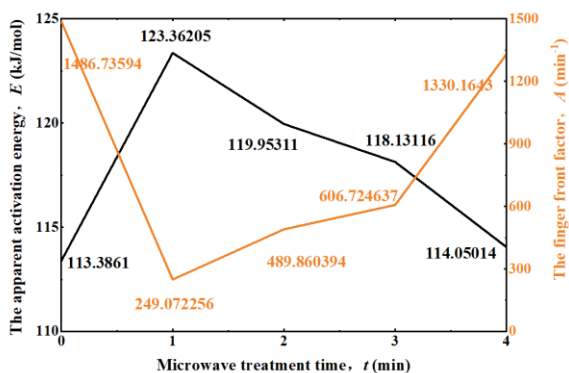
Fig. 1 effect of microwave time on kinetic parameters

2.3 (8:45-9:05) Research on the surface composition and interfacial structural model of macerals

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Jurassic low rank bituminous coal is rich in inertinite, which seriously restricts its efficient chemical conversion and utilization. If the coal and rock components are selectively crushed and separated effectively, it will be an effective way to solve this problem. However, the key to selective crushing is to figure out the interface characteristics of coal-rock components. In this paper, taking Shenmu Wangjiagou coal as the research object, using coal-rock microscope, infrared spectroscopy, X-ray photoelectron spectroscopy and other research methods, the embedded features of Shenfu coal and rock components and the surface structure of different coal and rock components were systematically studied, and finally established the coal-rock component interface interaction model. The results show that the ash of vitrain was lower than that of fusain, total sulfur content of fusain was as twice as vitrain's. Vitrinite had numbers of alkyl side chains, some Cationic groups -NH2, -NH-, while the inertonite contains more aromatic structure and oxygen-containing functional groups. Van der Waals forces and hydrogen bonding dominate. The inertinite is rich in medium and large pores, and the surface area is much larger than that of the vitrinite.

Key words: low rank bituminous coal, coal rock composition, structural model, embedded features, oxygen-containing functional groups, Van der Waals forces

2.4 (9:05-9:25) New Method to Estimate Kinetic Parameters in Distributed Activation Energy Model (DAEM) by Using Neural Network

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In this study, we proposed a new estimation method of kinetic parameters in Distributed Activation Energy Model (DAEM). In the proposed method, the formula of DAEM is regarded as a feedforward computation of a 3-layer neural network, and the kinetic parameters of DAEM are optimized by the supervised learning of the neural network. The proposed method does not require a priori assumption for kinetic parameters of DAEM. For validation, the kinetic parameters were estimated by applying the neural network with 64 hidden layer nodes or by applying the conventional methods to the reaction data generated by the numerical simulation. In addition, the obtained kinetic parameters were used to predict the conversion progress, and the prediction accuracy was compared between the neural network and the conventional methods. The kinetic parameters obtained by the neural network were very close to the true value. Also, the conversion progress predicted by the neural network was more accurate than those by

the conventional methods.

2.5 (9:25-9:45) Hydrodynamics modelling of the spray drying process within a laboratory-scale, semi-dry FGD scrubber

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Scrubber techniques are used widely for the desulfurization of flue gas from coal powered plants. Semi-dry flue gas scrubbing technology affords high desulphurization efficiencies and low water utilization, averting the need for downstream slurry handling and associated water treatment requirements. However, industrial spray-dry scrubbing systems are plagued with low desulphurization efficiencies which can be addressed by accurate modelling and optimization exploits. In the semi-dry process, an alkali slurry is atomized into hot flue gas where the SO2 is absorbed into the droplets, reacting with the alkali sorbent, whilst simultaneously removing water from the droplets to form dry particles. An accurate representation and fundamental understanding of the semi-dry FGD process requires the three main mechanistic processes (drying, absorption and reaction) to be deconstructed and evaluated in further detail before integrating the holistic model to describe the overall behavior of the semi-dry FGD scrubber. The absorption of SO2 occurs faster in the presence of water; the desulphurization efficiency of the flue gas is therefore limited by droplet drying dynamics. In order to accurately model the drying dynamics, the system hydrodynamics, including accurate capture of the atomization process and hence the convoluted multiphase interaction is paramount, necessitating the use of computational fluid dynamics (CFD) modelling in the formulation of the heat and mass transfer processes.

In the current work, the modelling of the spray drying dynamics of sorbent slurry droplets in a laboratory spray dryer is conducted. The numerical modelling is done systematically using CFD (employing StarCCM+ commercial platform) and verified with experimental data. The analysis started with rigorous modelling of the single–phase process capturing the complex hydrodynamics which included the effect of the downstream cyclone as a sub–model, convective and radiative heat flux, and heat loss to the environment. The model validation with experimental data showed a non-uniform chamber entrance velocity profile with the gas impinging preferentially on one side of the column. A bias in the temperature profile of the gas entering the spray chamber was also observed. The entrance dynamics results were then mapped onto a two–phase model that included slurry atomization by a two–fluid nozzle using the Euler–Lagrange framework. Three droplet drying models, the perfect shrinkage model, the classic d2 law and a mechanistic hindered-evaporation model were investigated and the results compared to experimental data. The work done has highlighted the importance of accurate modelling of both the hydrodynamics and drying kinetics in modelling spray dry-scrubbing systems, giving insights into the applicable processes as found in industrial scale scrubbers.

SESSION 3 (9:55-11:35)
GASIFICATION TECHNOLOGIES – 2
Francis Lau and Gary Stiegel

3.1 (9:55-10:15) Evaluation of the conditioning effect of an RO-plant saline solution on the resistivity of South African fly ash.

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Fly ash resistivity is an important characteristic which not only affects the electrical charge rate of fly ash particles but also the ultimate performance of Electrostatic Precipitators (ESP) used for fly ash separation and collection. South African fly ash has been found to be highly resistive, therefore limiting the collection efficiency of ESPs at several coal-fired power generation plants in South Africa. Several flue gas conditioning studies (e.g., duct injection of SO3) have shown to be effective in lowering fly ash resistivity to subsequently improve ESP performance. A previous industrial testing campaign involving the injection of a reject saline/brine solution (containing primarily sodium sulphates and chlorides) into the boiler of one of Eskom's coal-fired power station units showed a subsequent reduction in particulate emissions. The results observed therefore highlights the possibility of using a waste stream, in this case an industrial RO (reverse osmosis) plant saline reject solution, as a suitable and cost-effective alternative to other flue gas conditioning agents such as SO3.

An assay of the RO-plant saline solution also showed the presence of other ionic species (e.g., Ca, K, Fe, etc.), although in lower concentrations, could have also contributed to the observed reduction in particulate matter emissions. The observed improvement in particulate matter emissions on industrial scale therefore necessitated further investigation to elucidate the effect of saline conditioning on fly ash resistivity. Fly ash samples (PS-1 & PS-2) from two Eskom coal-fired power generation stations were sampled and conditioned (treated) with the RO-plant saline solution in different weight ratios (5, 8, 10, 20, 30 and 35 wt.% for PS-1 and 20, 30 and 35 wt.% for PS-2 respectively). Selection of these mixing ratios were based on typical flue gas volumetric flow rates (i.e., between 500 and 680 Nm3/s) under varying load factors as well as brine injection rates used during the industrial pilot testing campaign (i.e., 5 and 25 m3/hr). After being dried at ambient conditions, the samples were crushed to obtain a homogenous fine powder. Physiochemical characterization of the unconditioned and conditioned fly ash samples was done using several techniques (proximate analyses, thermogravimetric analysis (TGA), particle size distribution analyses, X-ray fluorescence (XRF) and QEMSCAN (Quantitative Evaluation of Materials by Scanning Electron Microscopy)), while an experimental resistivity rig was employed to measure ash resistivity. The latter was performed under dry and humid (7 wt.% moisture) conditions for both ascending and descending temperature increments (90 to 330 ℃) with the observed measurements found to be well within the acceptable error ratio as stipulated by the IEEE standard. Under dry conditions the resistivity measurements for the ascending and descending runs followed the same trend for both power station ash samples. The resistivity measurements for temperatures below 240 ℃ (range representative of surface resistivity) exceeded the optimum operating range for ESPs (1 x 1011 Ω .cm in the temperature range between 115 and 150 ℃). While the average resistivity of the dry ash samples, over the entire measurement range, decreased monotonously with increasing temperature; the average resistivity of the 7 wt.% ambient moisture ash samples (unconditioned and conditioned) showed an eccentric curve with a local maximum in the range between 130 and 180 ℃ for both the ascending and descending temperature measurements.

For temperatures below 210 ℃, initial ascending resistivity measurements for the conditioned ash samples (under dry conditions) were found to be substantially lower than the descending runs, while subsequent repeats of the ascending runs showed a similar trend to the results obtained for the descending runs. The observed disparity for the initial ascending runs could be attributed to volatile and soluble chemical species (e.g., carbonaceous impurities not detected with the saline solution assay) adsorbed onto the ash particles and removed when heating the ash samples. Furthermore, with moisture injection, it was concluded that the fly ash resistivity for both PS-1 and PS-2 decreased with an increase in saline solution loading (subsequent increase in sodium

sulphate/chloride species concentration). Ash samples conditioned with a higher ratio of saline solution (> 20 wt.%) provided resistivity results within the desired ash resistivity range for optimum ESP performance.

3.2 (10:15-10:35) Gasification: A Viable Choice for Production of Clean Hydrogen

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Hydrogen is considered a potential breakthrough source of clean energy in the anticipated decarbonized economy of the future. When consumed for electricity generation or as a fuel in industrial processes, no greenhouse gas emissions occur. In fact, hydrogen utilization is counted on to help meet the Administration's carbon and greenhouse gas reduction targets a 50 percent reduction in emissions by 2030, 100 percent clean electricity by 2035, and net-zero emissions by 2050. However, most of the hydrogen produced worldwide currently comes from reforming of natural gas or by gasification of coal and petcoke/petroleum residuals; such production methods have significant carbon footprints.

Clean hydrogen is currently defined as hydrogen produced with a carbon intensity equal to or less than 2 kilograms of carbon dioxide-equivalent produced at the site of production per kilogram of hydrogen produced. However, this standard may be revised in the future to become more stringent yet. Fossil fuel-based clean hydrogen production must therefore use intensive carbon capture to meet the clean hydrogen standard. Gasification has a unique combination of advantages for carbon capture cost and efficiency stemming from the inherent efficiency of integrating pre-combustion capture into syngas-based systems, and the potential use of inexpensive carbon-neutral feedstocks such as biomass. Gasification technology is a viable contender for clean hydrogen production in the near future.

The U.S. Department of Energy/National Energy Technology Laboratory is currently focusing on fostering development of technologies to support cost-competitive gasification-based clean hydrogen production. This presentation will provide a comprehensive overview of the portfolio that is spurring advances in modular and process-intensified gasifiers, novel and/or integrated oxygen production methods, in situ hydrogen separations, and more.

3.3 (10:35-10:55) OVERVIEW OF DOE/FECM R&D FOR CLEAN HYDROGEN PRODUCTION

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The Gasification Systems Program, conducted under the U.S. Department of Energy's Office of Fossil Energy and Carbon Management (FECM), is focusing on development of advanced technologies that reduce the cost of co-gasification of blended waste streams such as waste coal, waste plastics, municipal solid waste (MSW) and biomass enabling high efficiency and excellent environmental performance for net zero or net-negative carbon emissions with the integration of pre-combustion carbon capture (CCS) to produce clean hydrogen.

Due to high capital investments and operating cost required for large commercial gasification plants, the FECM Gasification Systems program is focusing on small-scale modular systems, process intensification and solutions for process issues arising when wider feedstock blends are deployed for clean hydrogen production with improvement of the efficiency and availability and offering flexibility in meeting location-specific needs.

This talk will highlight a broad overview and current progress that the DOE's FECM Gasification Systems program has made on small-scale, modular gasification systems and cost reduction of each component of the overall gasification system along with a detailed discussion of future co-gasification technology advances of blended waste streams as feedstocks for clean hydrogen production.

3.4 (10:55-11:15) A Novel Two Stage Gasification Reactor for Generating H2-Rich High Calorific Value Gas by Low Grade Coals

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High ash content in coal, by the virtue of potential ash fusion and agglomeration render conventional gasification approaches either impractical OR prohibitively expensive. Ash agglomeration and clinker formation, primarily due to high localized temperatures, are required to be addressed through appropriate technological interventions to enable gasification of high ash coal. In the current work, the challenge of high ash coal gasification has been addressed by separating the exothermic high temperature combustion zone and endothermic gasification zone in a two-stage gasification. The high temperature zone has the feed coal in highly mobile phase while the gasification zone has the char in the form of the packed bed collectively enabling handling of high ash coal without facing any ash fusion issues. The two separate, but connected stages enable independent control over the combustion and gasification. A pilot scale gasification system of 150 kW thermal gasification capacity has been designed and tested with coal of range of high ash Indian coal. In stage one, coal if fed into the mobile phase reactor with air as the carrying media where mostly devolatization and volatile combustion takes place. Appropriate mechanisms enable controlling the residence time of the coal in the mobile phase. The devolatized char generated is subsequently transferred to the second stationary bed reactor for Oxy-steam gasification. The process parameters are optimized for high carbon conversion and cold gas efficiency without clinker formation. The typical volume percentage of CO, CO2, CH4 and H2 are 30-40%, 15-20%, 0.5-2% and 40-50% respectively yielding a syngas of calorific value 11.2 MJ/kg. Carbon conversion greater than 80% has been achieved.

3.5 (11:15-11:35) Rheology and Phase Behavior of Coal-Plastic-Biomass Mixtures for Entrained Flow Gasification

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Entrained flow gasification (EFG) is a promising technology for the generation of hydrogen. While it provides an avenue to produce next generation fuels, the technology is still heavily reliant on the use of coal as a feedstock. One of the primary goals in the near term is to replace a portion if not all of the coal with cleaner opportunistic feedstocks. Two obvious choices are biomass and waste plastic. Biomass is favorable due to its high water content and the fact that it is renewable and carbon neutral. Waste plastic provides an opportunity to displace some of the waste materials that would otherwise enter landfills. The combination of coal, biomass, and waste plastic is encapsulated in a recent funding opportunity announcement from the Department of Energy. EFG is a leading candidate among the gasification technologies as it allows for high temperatures of around 1300°C and high pressures exceeding 300 psi. At these conditions, conversion to products is rapid and complete with residence times of less than 15 seconds. One of the biggest challenges in feeding coal, biomass, and plastic is the fact that the materials are physically and chemically very different. EFG commonly utilizes coal-water slurry as the delivery method of fuel with coal concentrations reaching up to 70wt% coal. Biomass and plastic interact very differently with water and would complicate the use of a water-based slurry. Not only is biomass very heterogenous, but the crushing of biomass and plastic down to a small enough particle size for feeding is energy intensive.

At the University of Utah, blended fuel mixtures are prepared using biomass and plastic as liquids, with coal being the only solid. Biomass pyrolysis liquid (bio-liquid) produced by Ensyn, and plastic oil produced by Renewlogy are combined as the solvent for fuel delivery. The bio-liquid is produced via a fast pyrolysis process that operates with very short residence times. The plastic oil is produced via a low energy catalytic liquefaction process that can generate up to one ton of oil daily. The bio-liquid contains roughly 21 wt% water meaning a significant amount of steam is generated to be used as a gasifying agent. The plastic oil is similar to a diesel fuel and can be thought of as a thinning agent in the blended fuel mixtures. The primary challenge in feeding bio-liquid/plastic oil-based slurries is the high viscosity compared to water, and the complex phase behavior of the coal and liquid phases.

Here, 12 baseline slurry mixtures are evaluated for their rheological properties and phase behavior. In all cases, the slurries exhibit shear thinning characteristics. Without the inclusion of additives (i.e. surfactants and dispersants) 40 wt% coal was the maximum possible coal concentration among the 12 baseline slurries. Furthermore, the inclusion of greater than 20 wt% plastic oil led to a rapid separation of the two liquid phases. Three candidate slurries were identified as being viable for use at the next scale. These slurries contained 15, 25, and 30 wt% coal and exhibited viscosities of less than 3000 cp at shear

rates of less than 1 inverse second. Temperature also had a significant effect on viscosity with slurries seeing a greater than 50% reduction in viscosity upon heating from 25 to 50°C. Viscosity as a function of temperature can be roughly modeled following an Arrhenius type expression. Separation tests indicated that the plastic oil and bio-liquid are immiscible as a binary pair but are partially miscible when coal is present indicating that coal acts as a sort of binder between liquids. The mixtures contain two primary phases being the (separated) plastic oil and the combined coal-bio-plastic phase. Mixtures containing 25 wt% coal were pumped against a backpressure of 300 psi using a progressive cavity pump at roughly 10 gal/hr proving the viability of coal-plastic-biomass mixtures for use in a 1-ton/day high pressure entrained flow gasifier.

SESSION 4 (9:55-11:35)
COAL SCIENCE – 2
Leslie Ruppert and Allan Kolker

4.1 (9:55-10:15) DEPOLYMERIZATION OF COAL UNDER MILD CONDITIONS VIA REDOX REACTION BY OXYGEN AND FORMIC ACID

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Coal has widely been applied as the raw material of value-added chemical products. Coke, carbon black, graphite electrode, carbon fiber, aromatic chemicals, etc. can be produced by appropriate processing of coals. In order to make the most effective use of the limited resource, depolymerization under mild conditions must be one of the key technologies to be developed. If coal's low-molecular-weight compounds (LMWC) can be increased, the thermoplasticity of coal would be enhanced, which is favorable for coke production, and the yield of tar would also increase, which means more value-added chemical products could be prepared from coal. In this study, the authors have proposed a novel coal treatment method that combines oxidation reactions by molecular oxygen and the following reduction reactions by coexisting gaseous formic acid to upgrade a bituminous coal at 90 ℃-150 ℃ under atmospheric pressure. The coal was expected to be depolymerized by the oxygen oxidation reaction and formic acid was expected to provide H radicals immediately to stabilize the radicals generated by the oxygen oxidation reaction. It was found that the softening and melting ability of the treated coals were increased when oxygen and formic acid existed in gas phase at the same time at 90–130 ℃. The LMWC amount of the coal treated at 90 ℃ in oxygen/formic acid significantly increased by 29.0 % on raw coal's LMWC basis which was measured by a coal fractionation method proposed previously by the authors. Surprisingly, the oxygen content of the coal decreased even in the presence of molecular oxygen when formic acid coexisted. FT-IR measurement showed that coal's hydroxy groups decreased through the treatment. Hydroxy groups can cause cross-linking reactions in thermal processes which were considered to inhibit depolymerization. It is therefore possible for the proposed method to achieve the depolymerization of coal not only by stabilization of the radicals generated by oxidative depolymerization but also by removing hydroxy groups under mild conditions. This method can be expected to contribute to more efficient utilization of coal for carbon materials and value-added chemical production.

4.2 (10:15-10:35) The role of hydrous pyrolysis pretreatment on the synthetic graphitization of lower-rank bituminous coal

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The synthetic graphitization of lower-rank bituminous coal is always difficult because of the abundant non-graphitized carbon, so the necessary pretreatment is important. The synthetic graphitization of anthracite will result in the appearance of a layered graphite structure, the higher order degree of aromatic fringes and the growth of aromatic fringe sizes. Thus, one possible approach is to convert low-rank coal into high-rank coal, then the artificial hydrolysis pretreatment is suitable. The well-restricted conditions of hydrous pyrolysis in a semi-closed simulation system include temperature, high pressure and water. In our study, a natural lower-rank bituminous coal, sub-pyrolyzed coals and corresponding residue after the synthetic graphitization are used to describe the structural evolutions of coals and corresponding residues, obtain the yields of graphitization and analyze the connections in the structure before/after the synthetic graphitization. There are significant increases in the mean random vitrinite reflectance (Rran) of pyrolyzed coal with enhanced experimental conditions. The yields of graphitization are positive with Rran of coal. The quality of heated residues is mostly about 60 % to 70 % of carbons presented in aromatic rings of pyrolyzed coals. The higher/larger crystallinity and crystal sizes of the pyrolyzed coals, the higher/larger degree of graphitization and crystal sizes of corresponding heated residues. The graphitization and order degree of aromatic rings of pyrolyzed coal after the synthetic graphitization will reach maximum at about 2.0 % Rran and then increase slightly. Also, the pyrolyzed coal with Rran more than about 2.0 % can be graphitized after 3000 °C treatment or the heated residue can be defined as graphite according to the graphite classification from the ICCP system based on the interlayer spacing (d002). Then, the role of hydrous pyrolysis pretreatment on the synthetic graphitization of lower-rank bituminous coal is clear. Therefore, the pretreatment of hydrous pyrolysis is beneficial to the synthetic graphitization of lower-rank bituminous coal. Appropriate pretreatment conditions can convert lower-rank bituminous coal into graphite after the synthetic graphitization. This work is expected to provide information for effective utilization of low-medium rank coal into graphite via the pretreatment of hydrous pyrolysis.

Keywords: Synthetic graphitization; Hydrous pyrolysis: Lower-rank bituminous coal; Pretreatment; Yield; Crystal structure

4.3 (10:35-10:55) Study on Influence of Sulfur in Coal on Graphitization of Coal

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Ten coal samples with different sulfur content were selected as the research objects to study the effect of sulfur content on the graphitization of coal based on the basis of proximate analysis, ultimate analysis, petrography analysis and coal facies analysis. Malan coal sample is special low sulfur coal, Baiyinhua3-10 coal sample is low sulfur coal, Donglutian11-1 and Donglutian11-4 coal samples are medium sulfur coals,

Baiyinhua3-2 and Baiyinhua3-17 coal samples are medium-high sulfur coals and Baiyinhua3-11, Donglutian11-10, Chonggu6-7 and Chonggu6-9 coal samples are high sulfur coals. Wherein, Baiyinhua3-2, Baiyinhua3-11, Donglutian11-1, and Donglutian11-10 coal samples are high organic sulfur coals and Chonggu6-7 and Chonggu6-9 coal samples are super-high-organic sulfur coals. The main macerals of Baiyinhua and Chonggu coal samples are collotelinite and collodetrinite, the main macerals of the Donglutian coal samples are telinite, collotelinite and vitrodetrinite, and the main macerals of the Malan coal sample are semifusinite and fusinite. The selected coal samples are mostly dull coals and semi-dull coals. The study shows that the yield of coal-based graphite increases with the increasing of reflectance of coal. The yield of coal-based graphite has a strong negative correlation with ash yield of coal and a strong positive correlation with volatile yield of coal. The yield of coal-based graphite has a strong negative correlation with the organic sulfur and total sulfur in coal. The organic sulfur in coal obviously hinders the yield of coal-based graphite. This may be caused by the inhibition of sulfide gas during graphitization, which will produce sulfur-containing mineral precipitates after graphitization. However, there is no correlation between the content of pyrite in coal and the yield of coal-based graphite. The yield of coal-based graphite is also not correlated with the macerals and minerals content of coal, and the correlation between coal-based graphite yield and parameters of coal facies is weak. These research results allow for us to better understand the influence of the degree of graphitization of coal and the yield of coal-based graphite, which puts forward the guiding significance of scientific theory for the efficient utilization of coal with different sulfur content in the field of coal-based carbon materials.

Key words: sulfur in coal, macerals, graphitization, coal-based graphite

4.4 (10:55-11:15) Preliminary Field Tests of Pyrolyzed Coal as a Soil Amendment

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Coal resources may have alternative use as a soil amendment in the agriculture sector. Pyrolyzed coal (coal char) which is a porous carbon material obtained from the pyrolysis of coal. High organic carbon, large surface area, and low bulk density of the coal char can have potential benefits for enhancement soil properties and plant growth. This study evaluates the soil health and sugar beet crop yield along with the plant growth parameters of soil treated with coal char. This field experiment was performed in a sandy loam (Haverson 41%, Ustic Torrifluvents and McCook 39%, Fluventic Haplustolls) soil at the Sustainable Agricultural Research and Extension Center (SAREC), Lingle of University of Wyoming, USA, in 2021. Corn was used as the test plant in the field. Coal char (CC) and Biochar (BC), chars alone and combined with manure, were used as a soil amendment to evaluate the difference in corn yield and soil health parameters. Two different rates of CC and BC: 10 and 20 tons acre-1 were applied in the field with four replicates for each treatment (Fig. 1). Manure was also added with CC and BC to see the combined effects on corn yield and soil health parameters. Soil samples were taken from each treatment during the middle of the growth period.
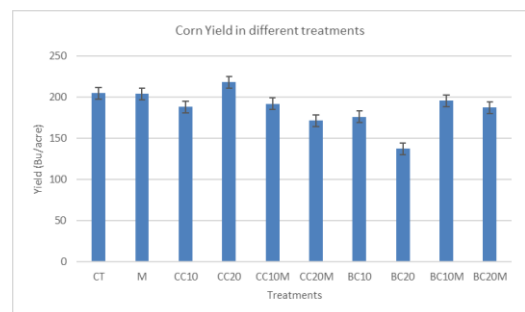

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Fig.1. Effect of coal char and biochar on corn yield. CT, control; M, manure; CC10, coal char 10 ton-acre; CC20, coal char 20 ton-acre ; CC10M, coal char 10 ton-acre with manure; CC20M, coal char 20 ton-acre with manure; BC10, biochar 10 ton-acre ; BC20, biochar 20 ton-acre ; BC10M, biochar 10 ton-acre with manure; BC20M, biochar 20 ton-acre with manure. Error bars indicates ±1 standard error.

None of the coal char treatments resulted in corn yields significantly different than the untreated control plots (Fig. 1). This is also true of the soils to which biochar was applied; corn yields from all biochar treatments, including the treatment with added manure and biochar, were not significantly different than the control. Additionally, no significant differences were found among the coal char treatments and biochar treatments. The only treatment performed better than CT is CC20, which was the greatest (218.41 Bu acre-1) corn yield among all treatments and that is 7% higher yield than non-treated plot corn yield (205 Bu acre-1) in this field study.

Soil laboratory tests were performed on samples collected from the field during the middle of the plant growth season. Preliminary soil test results (Fig.2) showed Soil pH was not affected by the CC and BC treatments regardless of altered application rates and combination with manure. This indicates the pH buffering capacity of soil is very high or application rates were not great enough to alter soil pH. Organic matter (OM) appeared to be varied according to the treatments. CC10 and 20; BC10M and BC20M treatments have significant higher OM content followed by CC 10 and 20 (Fig.2). Average Nitrate nitrogen (NO_3-N) content in all treatments displayed great increase compared to control plot, however, abundant variation among the char treatments. Further investigation is needed to find the cause of variation. The highest Cation Exchange Capacity (CEC) was noticed on CC 20 treatment (21.1 meq/100 g) followed by BC 10 (21 meq/100g), and was not significant difference among any treatments.
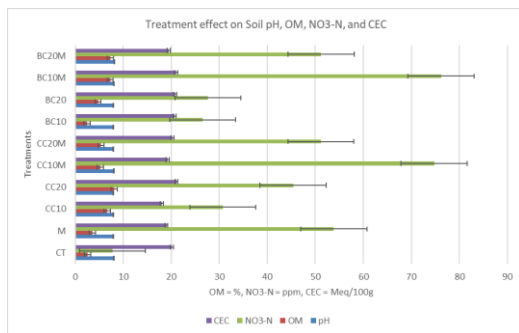

Fig. 2. Coal char, biochar and manure treatment effects on soil pH, OM, NO_3-N, and CEC levels. Error bars indicates ±1 standard error.

Coal char and biochar increased the OM content in the soil compared to non-amended soil which is due to the organic carbon content of the char materials. Nitrate nitrogen in the treated soils exhibited higher value than control soil that may be because of nutrient absorbed or retained by the char materials that remain in the soil. The sandy loam soil of the experimental site may not have retained the applied fertilizer in the plots where biochar and coal char were not added. Increased OM on treated soils did not justified to the CEC of the treatments and that may be due to the activated carbon in the char materials which may remain inert in the soil.

4.5 (11:15-11:35) Performance and Economic Analysis of Lignite Coal Dewatering with Supercritical Carbon Dioxide

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Residual moisture in power plant feedstock materials like coal inhibits power plant performance and results in higher CO2 emissions per unit amount of energy produced. Therefore, feedstock materials must be pre-dried to improve utilization and reduce the CO2 emissions. Conventional thermal drying is energy intensive due to high latent heat of water, so alternative methods of drying/ dewatering are of interest. In this research,

dewatering of lignite coal (North Dakota coal – 33% initial moisture) was performed with supercritical carbon dioxide. Moisture is removed from the coal pores by dissolution into and mechanical displacement by supercritical carbon dioxide. Coal dewatering experiments were performed in a 1-liter supercritical fluid extraction system under various operating conditions such as operating pressure, temperature, equilibrium time, and coal loading rate. Best operating conditions for coal dewatering was identified as: 10 minutes cycle time, 100 bar pressure, 100 g/L coal loading rate, and 100 °C vessel temperature. About 15% reduction in moisture content was obtained under these conditions. Contrary to published literature, surfactant had little effect on the dewatering rate, possibly, because initial moisture content was only 33% as opposed to more than 50% found in the literature. Also, coal is microporous, so water removal rate from micro-pores is more difficult than from macropores. Techno-economic analysis of coal dewatering process with supercritical carbon dioxide was performed for a reference 650 MW net power plant assuming same performance in the scaled-up system. Up to 0.45% increase in power plant efficiency is expected from 36.2% for conventional power plant with no pred-dying to 36.65% for power plant with supercritical CO_2 dewatering technology. As a result, the levelized cost of electricity (LCOE) reduces from $ 101.5/MWh for conventional power plant to $ 101.1/MWh. Additionally, up to 52 kilo tons in annual fuel savings can be realized. However, supercritical CO2 drying might not be more advantageous over thermal drying, where the LCOE was about $ 101.08/MWh. Supercritical CO2 drying performance is more pronounced in macroporous materials with higher moisture content, where a definite advantage over thermal drying can be obtained. This research work was performed as a part of Small Business innovation Research (SBIR) Phase I grant, supported by the Department of Energy, under Award no. DE-SC0021486.

SESSION 5 (12:35 – 14:15)
GASIFICATION TECHNOLOGIES – 3
Francis Lau and Alberto pettinau

5.1 (12:35-12:55) Modeling Ash Partitioning in Slagging Energy Conversion Systems

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Optimizing the performance and reliability of slagging systems such as entrained flow gasifiers and cyclone-fired boilers requires the ability to predict the partitioning of fuel impurities between the slag and entrained ash species. For example, in entrained flow gasification systems, the ash partitioning not only impacts the slag flow behavior but also has a significant influence on fouling of syngas cooling equipment. In addition, minimizing NOx emissions in a cost-effective manner in cyclone-fired utility boilers without causing freezing of the flowing slag layer and partitioning that causes fouling poses a significant operational challenge. Microbeam Technologies Inc. (MTI) and University of North Dakota (UND) are developing an integrated approach to predict ash partitioning at varying plant operational conditions. This approach combines the understanding of behavior of fuel impurities based on the data collected at a power plant during a field test with Computation Fluid Dynamic (CFD) methodologies. Understanding the partitioning of ash within a cyclone combustion barrel or the first stage of an entrained flow gasifier along with the composition and viscosity of the molten slag are keys towards ensuring a steady slag flow when sub-stoichiometric conditions are used to reduce NOx emissions and to produce a high hydrogen syngas. The existing CFD methodologies commonly use particle Weber number to assess the slagging and fouling propensities. However, a lack of consistency in reporting the values of critical sticking viscosity, in conjunction with an inability to track changes to the ash composition are major shortcomings inherent in current CFD methodologies. This is because the ash partitioning is related to the form of occurrence of inorganic components within the parent coal. These limitations are alleviated in the unique framework presented in this paper where CFD simulations in conjunction with fuel characterization data are used to predict ash partitioning within a cyclone-fired utility boiler firing lignite coal and are currently being extended to slagging gasification systems. First, standard fuel analyses are performed that include proximate, ultimate, and ash composition analysis along with computer-controlled scanning electron microscopy and chemical fractionation methods are employed to determine the size, composition, abundance, and modes of occurrence of the inorganic constituents. This information is then incorporated into MTI's Ash Generator program to generate the distribution of ash species in the form

of gases, liquid, and solid components during the energy conversion process. By utilizing the ash generator output, the CFD simulations predict the ash partitioning as well as the chemical compositions and viscosities of the silica rich slag reasonably well. The work improves the ability of CFD to simulate the impact of sub-stoichiometric operations on ash behavior in slagging energy conversion systems. Examples of the predicted partitioning behavior will be presented as part of this paper.

5.2 (12:55-13:15) Making Coal Relevant for Small Scale Applications: Modular Gasification for Syngas/Engine CHP Applications in Challenging Environments

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This project will demonstrate the practicality of small-scale, modular, coal gasification units to provide low-cost fuel for firing reciprocating engine generators with syngas and pyrolysis tars/oils. This project would repurpose the site of a former refinery, which has since been demolished, within the City of North Pole, where the heat and power can be used to power a proposed 20- acre greenhouse. The current site occupant, Marathon Oil, operates a fuel terminal. A district heat system will be installed to provide economically priced heat for Marathon, for an anticipated commercial district with 200,000 square feet, for the city utilities, and for 240 homes that are planned for construction in a new, nearby subdivision.

The project would construct a CHP plant and 20-acre greenhouse operation, sited on 20 or more acres of land inside the boundary of the Marathon Fuel Depot Terminal. Coal would be delivered to the facility via truck and stored in a silo onsite. Two gasifiers would convert the coal into syngas, which would be fed through a gas cleanup train and then combusted in six reciprocating engines driving electric generators. Heat recovery on the engine cooling loops and exhaust trains would provide heat to a glycol/water circulation system for use in the greenhouse and in the Marathon facilities. Natural gas would fuel two additional engine generators and would also be available to supplement the syngas-fired engines as required. The Project would provide electricity to industrial customers or Golden Valley Electric Association and has the potential to provide district heat to the City of North Pole and other end-user.

5.3 (13:15-13:35) COMMERCIAL-SCALE TRIAL FEEDING WASTE ACTIVATED SLUDGE TO A SASOL FIXED BED DRY BOTTOM GASIFIER

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Global trends and Sasol environmental strategies support the need to move waste streams away from incineration and to proceed up the waste hierarchy, recovering energy or valuable components from these streams rather than just thermally destroying them. This is what motivated the Sasol research team to develop a process setup, to test on commercial scale, whether one can co-feed high moisture content waste activated sludge (WAS) to the existing SASOL FBDB (fixed bed dry bottom) gasifiers in Secunda. This would effectively utilize existing assets to manage the WAS in a more efficient way, deriving synthesis gas from the carbon still contained in the sludge. Since the SASOL FBDB gasifiers are typically known for dry, coarse coal type feed, there was quite some uncertainty as to how these gasifiers would operate with injection of a high moisture content sludge feed that contains micron sized biological cells, albeit at a low ratio of sludge to coal fed into the gasifier. The thickened WAS is known to behave as a non-Newtonian, shear thinning liquid, which made pump designs for gasifier injection very challenging. To overcome this, the team incorporated thermal hydrolysis pre-treatment of the WAS to reduce its viscosity and kill the pathogens associated with the sludge as a process step in the trial run setup. Several combinations of thermal hydrolysis

reactor temperature and residence time were evaluated to find the combination that yields the lowest sludge viscosity. The reactor temperature, as determined by the pressure in the vessel was found to be the governing factor, and optimization of this variable resulted in the lowest sludge viscosity. After thermal hydrolysis, the sludge was transferred to the gasifier in road tankers. At the gasifier injection site, the thermally treated sludge was injected at a controlled flow rate into one gasifier, which was still operated under normal conditions with coal, steam and oxygen fed to this unit. In total seven gasifier test conditions were evaluated, that being combinations of gasifier load and steam to oxygen ratios. These results were compared to baseline tests at the same test conditions to quantify the impact of the sludge injection on the gasifier operation and main output streams that were sampled during the tests (raw synthesis gas, ash, primary tar and condensed steam (gas liquor)). It was concluded that the sludge injection did not negatively impact the gasifier operating stability, as most of the operating variables remained in expected ranges. The sludge injection, at a low ratio relative to the coal feed rate, also did not have adverse consequences on the main gasifier product streams. This trial run has proven that it is technically feasible to route WAS to the SASOL FBDB gasifiers, which in the Sasol application enables the development of a more efficient process scheme for internal re-processing of the material.

5.4 (13:35-13:55) Pyrometamorphism from Underground Coal Gasification

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Underground coal gasification uses high temperature conversion reactions to alter deep coal seams into a synthetic gas that can be utilized for electricity production. The in situ gasification of coal at temperatures in excess of 1000 °C, results in thermal alterations to the sedimentary strata around the coal seam. Pyrometamorphism or combustion metamorphism is generally used when coal burns with enough energy to bake or fuse the surrounding rocks. The growth of the UCG cavity can be a complex process but invariably involves spalling and intermediate-scale fracturing coupled with collapse activities. All of these actions results in a chaotic rubble-filled cavity characterized by pyrometamorphosed mineral assemblages. Changes in mineral assemblages observed in metamorphosed rocks can be used to provide a qualitative estimate of the conditions of metamorphism based on deduced changes in temperature and the reconstruction of the temperature profile in the gasifier.
Two cores drills were drilled in a spend UCG pilot plant to intercept the gasification zone with the aim of retrieving samples to compare to an off cavity drill core. The visual analysis of the verification boreholes showed macroscopic signs of extreme heat interaction. These features were more prominent in the overburden which contained an ash layer, buchite and paralava sections with vast amount of visible vesicles. The majority of the visible pyrometamorphic features were limited to within 2 m of the overburden-char contact.
The following mineral alterations or crystallization of secondary minerals was confirmed: Pyrite transformed to pyrrhotite. This alteration was seen by an inverse relationship in the profiles of pyrite and pyrrhotite. As pyrite level reduced the pyrrhotite levels increased beyond background levels. Significantly high temperature mineralization of cordierite was detected in the overburden which was higher than the background values recorded. Appreciable quantity of high temperature silica polymorphs, tridymite and cristobalite, were detected in the overburden.
In general, the extent of overburden alteration was not the same within the gasification zone. This shows the heterogeneous nature of gasification in a UCG chamber where different sections experience changing temperatures resulting in a varied temperature profile across the geo-reactor.

5.5 (13:55-14:15) A Study on Gasification Behavior of Soma Coal in a Bubbling Fluidized Bed Gasifier

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The objective of this study is to determine the gasification characteristics of Turkish coal in a fluidized bed. Soma coal was used for the experimental studies. Air was used as the gasification agent. The experimental studies were carried out under atmospheric conditions using a bubbling fluidized bed gasifier with a capacity of 20 kg/hour and changes in the operating conditions, such as the equivalence ratio (ER) and gas components were analyzed. By decreasing equivalence ratio, it was observed that CO, H_2, CH_4 concentrations and the heating value increased; while CO_2 concentration, carbon conversion ratio and cold gas efficiency decreased. In the experimental studies where the equivalence ratio was decreased from 0.41 to 0.24, the heating value of syngas changed from 2.5 to 3.4 MJ/Nm^3.

6a.1 (12:35-12:55) Prototype Fabrication, Mechanical Testing, and Material Characterization of Coal-Based Bricks & Blocks (CBBs)

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Advancing new markets for coal can enhance U.S. national defense security, bolster the nation's energy and mineral security, enhance its environmental objectives and contribute to the United States' economic prosperity. Given that the market price of coal species currently averages around ~$0.04/kg, there is a clear economic incentive to use available U.S. coal resources as a basis for high-value products. A preliminary cost model for coal-based bricks and blocks (CBBs) projects competitive prices compared to clay and cementitious products (~ $1 - $2 per unit) while offering technical superiority. Coal or coal by-products can be incorporated into novel materials to improve performance, decrease costs, or both. Coal-derived composites possess mechanical, thermal, and electrical properties that can be used to produce new types of building materials or superior versions of existing building materials. CBBs weigh about 50% less than clay bricks and can be manufactured with an interlocking design to promote ease of use for the novice builder.

Market appeal will be assessed based on market size, market growth rate, required attributes and competitive strengths of the coal-based bricks and blocks. A useful attribute of thermoplastics as binders is that they can be heated to their melting point, cooled, and reheated again without significant degradation. Advantages include low cost, availability, binding ability and processability. Both virgin and, where available, post-consumer recycled versions are tested for each thermoplastic species. Ideally, the incorporation of post-consumer recycled thermoplastic will decrease material acquisition costs and increase product sustainability. The primary goal is a relatively light-weight composite product with superior compressive strength. Optimizations in fabrication and thermoplastic loading, etc., are therefore generally based on compressive strength tests. Strength comparisons between composites made with surrogate aggregates and those made with coal demonstrate good compatibility between the thermoplastic matrix and anthracite without the need for surface modification of the anthracite. Initial methods of fabrication using hot-press molding and extrusion have been extended to include injection molding. Preliminary findings suggest extrusion is better than hot-press molding at homogeneously mixing the two components.

CBB formulation is evaluated according to a design-of-experiments (DoE) approach. DoE variables are a) relative weight fractions of binder, b) relative proportions of large versus small (milled) anthracite size fractions, and c) additive percentage. CBBs are tested for compressive strength, modulus of rupture (by flexure test) and water absorption per ASTM C67, with density determined by the Archimedes drainage method. Fractured interfaces are examined by SEM (Scanning Electron Microscopy) to resolve fracture dynamics and interior microstructure uniformity. Differential scanning calorimetry (DSC) is used to compare plastic transition temperatures i.e., glass and melting temperatures to contrast virgin with post-consumer recycled thermoplastics and optimize their usage. These results are used in the DoE analysis to identify the binder and relative weight percentages for optimum strength, density and porosity. For example, a higher loading of small anthracite particles (149 to 250 microns) acts to fill void spaces in the material matrix, resulting in stronger CBBs. Optimal thermoplastic loading for hot-press molded bricks, as determined by compressive strength testing, is 38% of total composite weight, while the optimal loading for extrusion is still under investigation but estimated using currently available data to be ~10% higher. Overall, CBBs possess strength comparable to clay-based bricks but are non-permeable and hydrophobic, and hence resistant to degradation by freeze-fracturing, corrosion, and efflorescence. The strongest composites have been made with the following thermoplastic binders (in order of strength): high-density polyethylene crosslink resin, high-density polyethylene, nylon 6/6, and polypropylene. An investigation of their onset and degree of deformation is ongoing and will dictate their applications.
TEA (Techno-Economic Analysis) examines both technical and economic details for the coal-based manufacture of bricks. Economic analysis includes capital and operating cost estimates over the equipment service life. Notably, CBBs do not require the high temperature calcination needed to produce cement, nor do they require firing in the 1600-2400 °F range for three days using natural gas, as do clay brick equivalents. Instead, CBBs are heated to a modest <600 °F according to the melt flow index of the

thermoplastic binder. Existing anthracite mines can be expanded to produce CBBs (see "Process Schematic & Material Flow" image) to reduce aggregate transportation costs and emissions that exist for clay bricks. Hence, their projected energy cost and CO2 footprint are much lower. TEA reflects this reduced energy cost while a comparative CO2 emission analysis quantifies the reduced environmental footprint, allowing for a prediction of the expected economic advantages of CBBs considering a future carbon tax.
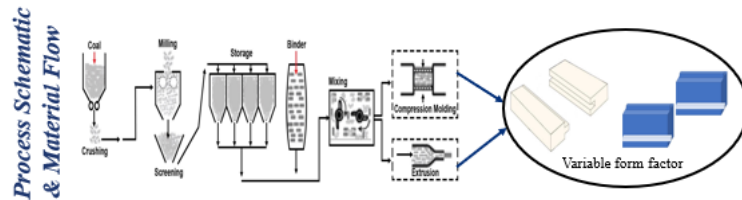
6a.2 (12:55-13:15) Evaluation of the product quality and market suitability of synthetic gypsum produced from Eskom's wet flue gas desulphurization (FGD) process.

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To drastically improve air quality, both existing and new coal-fired power generation facilities are required to comply with more stringent emission limits as stipulated by the relevant South African Environmental legislation. More recently, a significant reduction in SOx (sulphur dioxide- and trioxide) emissions from Eskom's coal-fired power station fleet has also been prioritized. To achieve this goal, six commercial wet-FGD (flue gas desulphurization) units were installed as part of the construction and commissioning of one of Eskom's new power stations. Apart from its high SO2 removal efficiencies, wet-FGD processes have the added advantage of producing synthetic gypsum. The production of FGD gypsum presents an ideal opportunity to explore potential international and local markets (e.g., cement manufacturing, agricultural, wallboard industry, etc.) for using this coal combustion by-product (CCP), as a means of stimulating further revenue. Unfortunately, in South Africa, the commercial uptake of large amounts of FGD gypsum remains relatively poor at this stage and results in significant environmental and economic impacts for Eskom (e.g., safe and responsible disposal leads to high landfill disposal costs). It is, however, envisaged that the demand for FGD gypsum will increase in the, not too distant, future especially as natural occurring gypsum resources are depleted. The various commercial uses are, however, dependent on the different grades and qualities of gypsum. The purpose of this study was therefore to assess the key quality parameters of the produced FGD gypsum and evaluate its comparability to other commercially available gypsum products using both international analytical standard methods and alternative techniques.
Representative samples of FGD gypsum were acquired from the gypsum drying belt of one of the FGD units, while three different grades (agricultural, cement and wallboard grade) of commercially available gypsum were obtained from a reputable, local natural gypsum supplier. The key quality parameters considered during this investigation included gypsum purity (i.e., based on the wt.% of $CaSO_4.2H_2O$), moisture content, excess limestone / $CaCO_3$ content, chloride content as well as sulphite (SO_3^{2-}) content. Evaluation of these parameters involved the application of gravimetric and titration techniques, as prescribed by international best practice (e.g., VGB-M 701e), on both the FGD (i.e., FGD#1, FGD#2, FGD#3) and commercially supplied gypsum samples (i.e., AGRI#1, CMNT#1 and WLBD#1). Additional, non-standard, analytical techniques

such as X-ray fluorescence (XRF), X-ray diffraction (XRD) and QEMSCAN (Quantitative Evaluation of Materials by Scanning Electron Microscopy) were also employed to evaluate their analytical comparability with standard methods as a means for consideration as suitable alternatives for assessing some of the main quality parameters.

From the results (based on standard methods), it was evident that the three commercial grade samples exhibited quality characteristics similar to those specified in open literature. For the FGD samples the following quality parameters (averaged basis) were determined: a moisture content of 0.05 wt.%, a gypsum purity of 92.7 wt.%, an excess limestone concentration of 3.3 wt.%, a chloride content of 0.02 wt.% and a sulphite concentration of around 0.71 wt.%. A comparison between the results and the required industry specific specifications indicated that the FGD gypsum may be considered a suitable alternative for the cement and agricultural gypsum industries, by replacing the natural gypsum used in these industries. Further improvement in the gypsum quality parameters is expected once all units of the power station reach beneficial operation and further plant optimization efforts are implemented. Good comparability was achieved between the gypsum purity and excess limestone (or $CaCO_3$ content) results obtained from thermogravimetric analysis (TGA, standard method prescribed by VGB-M 701e) and those derived from QEMSCAN, XRF and XRD therefore suggesting that these techniques could, within a reasonable margin of error, provide acceptable estimates for the aforementioned quality parameters.

6a.3 (13:15-13:35) Making large-scale construction of complex structures more accessible with PyMOL

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The complexity of coal, other kerogens, and their products has limited out ability to portray realistic structural representations that effectively capture these structural features. While some advances have been made they often rely on expensive molecular modeling software and a variety of difficult to obtain in-house scripting. Here the use of PyMOL is demonstrated with the intent of making more meaningful larger-scale (>50,000 atoms) construction strategies available. Specifically, with limited scripting and Excel to populate the sequence of command line entries to build structures from the bottom-up: 1) generate a desired distribution of PAH molecules (rank appropriate), including internal 5-membered rings with Si atoms in the "peaks", 2) displace those molecules into a grid structure (to aid viewing the structural transformations), 3) replace random hydrogen atoms with appropriate aliphatic and heteroatom function groups, 4) replace 5-membered "peak" Si atoms with O, N, S, and C, to generate dibenzofuran etc. type structure within the PAH molecules, 5) replace non-hydrogen bonded sp2 carbon with quaternary nitrogen, 6) displace the molecules into random "slices" in the z-direction to permit desired cross-linking frequency and creation of molecular weight distributions (also to reduce H content). Using this approach, we can better address "hidden" assumptions (ratio of phenanthrene to anthracene, 5-member ring placement etc.) and better visualize the structural transitions and structural features prior to assembly of the molecules in 3D space. The approach is rapid (minutes) as it is non-iterative (you build to suit rather than build and check), adds a visual 2D capability often lacking in construction strategies, negates any high-level modeling approaches, while using only personal computing resources.

6a.4 (13:35-13:55) Phase Mapping using Images from Backscattered Electron Imaging and Energy Dispersive Spectroscopy of Ash

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A method is shown for mapping backscattered electron (BSE) images and images derived from energy-dispersive spectroscopy (EDS) in a scanning electron microscope (SEM) to generate improved images of samples such as ash deposits on heat transfer surfaces.

SEM imaging using BSE and EDS is used on polished cross-sections of deposits taken from a coal-fired boiler. The BSE image shows some basic information about chemistry (average atomic number), but also shows textural information such as porosity and fine details of the image. The elemental maps show the relative concentration of inorganic elements in the sample.

Images and chemistry information from the SEM are mapped onto a perceptually uniform colorspace. The perceptually uniform colorspace CIECAM02-UCS is used to show differences in color. In this application it is used to classify and differentiate different types of phases in ash related materials. The lightness correlate J is assigned to the BSE image. The red-green correlate ac is assigned to the concentration of acids (Si+Al+Ti) in the material. The blue-yellow correlate bc is assigned based on the concentration of bases (Na+Mg+K+Ca+Fe) in the material.

Examples are shown and discussed. The phasemapping technique outlines features of the sample that are difficult to see via separate BSE/EDS images and maps. The use of phasemapping utilizing CIECAM02-UCS easily shows the difference between quartz, iron-rich, and aluminosilicate particles. The phasemap also discriminates between Na-rich and Ca-rich aluminosilicates as well as pure aluminosilicates (those with low levels of network modifiers such as Na and Ca). Consistent features of ash materials observed during analysis of the phase map data were summarized.

The phasemapping technique shows both physical and chemical features of the sample that provide highly useful data for understanding the interaction of different phases in complex mixed inorganic materials such as fly ash and ash deposits. The ability to classify phases present in ash materials is important in ash utilization and processing as well as managing the impacts of ash on plant performance.

SESSION 6b (13:55 – 14:15)
CLEAN COAL DEMONSTRATION AND COMMERCIAL PROJECTS - 1
Tom Sarkus and Dan Connell

6b.1 (13:55-14:15) Engineering and Design of the 1.5 Million Tonnes per Annum Post-combustion CO2 Capture Facility at the China Huaneng Longdong Energy Base

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This paper will present the Front-End Engineering Design (FEED) of the large-scale post-combustion CO2 capture project using China Huaneng's next-generation HNC series amine technology (1–3). CO2 will be captured from the slipstream of Unit 1 of the 2x1,000 MW ultra-supercritical coal-fired power plant at the newly build China Huaneng Longdong Energy Base in Northwest China. The FEED study targets to capture over 90% of CO2 from the 1,230 tonnes/hour, 951,000 Nm3/hour flue gas. It will reduce 1.5 million tonnes per annum (Mtpa) CO2 emission, which equals over 29% of total CO2 emission when Unit 1 operates at 100% Boiler Rate Load (BRL). The project integrates innovative process designs including absorber inter-cooling, rich solvent split, advanced lean-rich heat exchanger design in series, lean vapor recompression, etc, with the specific reboiler duty reaching below 2.3 GJ/tonne CO2, while still maintaining the system operation reliability and economic feasibility. The solvent performance, engineering design, major equipment layout, energy and material balance will also be presented. The captured CO2 will be transported via pipeline in the supercritical phase at pressures over 12 Mtpa and stored via dedicated geological storage and enhanced oil recovery.

The detailed FEED study is currently underway, with the final investment decision (FID) approved in February 2022. The plant construction is targeted to commence in the 4th quarter of 2022. Once built by the end of 2023, this project will become the first million-tonne carbon capture and storage (CCS) facility in China in the power generation sector, and the largest post-combustion capture plant in the world.

The project will present a revolutionary low-cost decarbonization option for coal-fired power generation. The preliminary cost of the CO_2 capture plant is estimated at a total investment of just over 800 million CNY (>USD\$ 122 million, at CNY/USD exchange rate of 1/6.56), and the levelized cost of CO_2 captured is 220 CNY per tonne (USD\$33.5 per tonne CO_2, excluding tax) with an 8% discount rate and 15 years discount period, based on the coal price of 600 CNY per tonne (USD\$91.5 per tonne coal).

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SESSION 7a (14:25-14:45)
GASIFICATION TECHNOLOGIES – 4
Francis Lau and Alberto Pettinau

7a.1 (14:25-14:45) Strategic Importance of Coal Gasification For Türkiye

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The predominant production and consumption of coal around the world has shifted from west to east countries. No matter how shifting west to east coal's production is, coal continues to be at the forefront of the world's primary energy consumption. Türkiye's energy costs constitute more than half of the deficit because of dependency on primary energy sources.

It is an important national security issue to be able to process domestic coal resources with high technology and use them for gasification / liquefaction in order to reduce foreign dependency on energy. One of the major risk factors for Türkiye is a regional or global crisis that may arise in petroleum and natural gas. The most important way to become a self-sufficient country in energy is to increase the diversity of resources, as well as to transform domestic coal resources into high value-added products with local technologies.

In this study, the current status of coal, future of coal with predictions, and coal gasification information and future prospects are given globally and specifically so as to include Türkiye. Furthermore, emphasizing the strategic importance of coal gasification products for Türkiye, some suggestions made by analyzing the Turkish market.

Keywords: Coal, Coal Gasification, Gasification Products, Türkiye's Coal Strategy.

SESSION 7b (14:45-16:05)
COAL BED METHANE AND SHALE GAS
Dick Winschel and Dan Connell

7b.1 (14:45-15:05) A NOVEL COAL STRUCTURE INDEX AND ITS IMPLICATIONS FOR HYDRAULIC FRACTURING

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Investigation of structurally deformed coal (SDC) dual advantages of not only improving on the coalbed methane (CBM) production and avoiding gas outbursts during coal mining due to the mechanical strengths and physical properties difference. In this work, a novel coal structure index (CSI) was proposed based on extensive coal samples measure and analysis, which could improve accuracy for evaluating the mechanical properties of coal. The mathematical relationships between coal deformation and petrophysical properties was further set up based on CSI model. The results show that study area is dominate by undeformed and brittle deformed coal, and there is negative relationship between permeability and the value of in situ stress in the slightly brittle deformed coal zones. The compressive strength exponentially decreases with increasing CSI (avg.), of which the correlation coefficient of coal in a water-saturated state is higher than that of coal in a dry state. CSI also could help to evaluate the fracturing performance, there is a reversed U-shaped relation between CSI (avg.); for fracture

height, an inverse relationship would take hold. The sensitivity on fracturing follows the order Brittle coal >Undeformed coal >Ductile coal. The slightly brittle deformed coal is favorable target SDC type for hydraulic fracturing, which is mainly located in the central Fanzhang and southwestern Zhengzhuang coal zones. Thus, this study could provide a basis for the optimization of favorable areas in CBM reservoirs.

7b.2 (15:05-15:25) Study on Coal Methane Adsorption Behavior Under Variation Temperature and Pressure-Taking Shanxi Maozequ Mine Coal in China for Example

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Based on the Langmuir volume and Langmuir pressure of series isothermal adsorptions of lean coal of Shanxi Maozequ Mine in China, the four parameters of a temperature-pressure-absorbing equation (TPAE) have been regressed with 8% relative error. In the measured temperature (30~100℃) and pressure （0~30 Mpa) range, TPAE can not only simplify Langmuir parameters, but also picture the quantitative relationship around the temperature-pressure-adsorption. The TPAE has been used to calculate the temperature's effects under isobaric condition or the pressure's effects under isothermal condition. The partial differential of temperature proves that the temperature affects the adsorption amount negatively. The partial differential of pressure proves that the pressure affects the adsorption amount positively.

7b.3 (15:25-15:45) Experiment of low frequency vibration to increase the production of coalbed methane well

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China's coal seams are thin in thickness, high in metamorphism, low in porosity, low in permeability, complex in structure and low in output. However, the coal seams have high gas content and great resource potential. In order to improve the production of coalbed methane wells, we carried out physical simulation experiments of coal rock permeability and drainage under different vibration modes. (1) Experiment on the influence of low-frequency vibration on coal rock permeability: a total of 9 samples were tested, and vibration permeability experiments of no vibration, 10 Hz, 20 Hz, 30 Hz, 40 Hz, 60 Hz and 70 Hz were carried out respectively. Compared with no vibration, the permeability after vibration increases by 7.2% ~ 24.5%. The permeability increases with the increase of vibration frequency. (2) Experiment on the influence of low-frequency vibration on the output of gas discharge and production: fill nitrogen into the adsorption desorption tank (replace methane with nitrogen). The injection pressure is 2.5 MPa ±. After injection, wait for adsorption. When the pressure drops below 0.5 MPa, inject nitrogen again. Six operations are repeated, lasting for 98 days. The total gas injection is 109.9 ml, which ensures that the coal and rock can fully absorb gas. Then, in the natural gas production state, the production is discharged intermittently. The interval time is 3 days each time, and the output is gradually reduced. At the fourth time, the output of discharged production is reduced to 0, and the
accumulated gas production is 7.3ml. After that, it was transferred to vibration, with the vibration frequency of 45 Hz and the total vibration duration of 90h. It was drained again, and the gas production was 0.3 ml, which proved that vibration could increase the output of coalbed methane. (3) On the basis of experiments, the relationship between energy

and radius of vibration with different frequencies in coal seam is established. It is found that the higher the frequency, the more concentrated the energy of the vibration wave, but the shorter the radius of propagation in the coal seam; On the contrary, as the frequency of vibration wave decreases, the radius of propagation in the coal seam increases, but the energy density decreases. Through optimization, it is considered that the vibration frequency is optimal in the range of 90 ~ 120 Hz, which is suitable for coal-bed methane mining under the current well pattern in China.

Key words: Coalbed methane; Low frequency vibration; Desorption; Diffusion; permeability

7b.4 (15:45-16:05) Hydrocarbon generation potential of the Permian shales, India: Insinuation from source rock evaluation and kerogen-kinetics

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Unconventional petroleum system boom from the shale reservoirs provided the impetus for petroleum industries to address the energy demand-supply chain globally. In context to that, the Permian shales from the two contrasting basins viz; North Karanpura (NK) and Raniganj (RN) of the Damodar Valley, India have been studied in order to illustrate the petroleum storage and generation potential. The most widely geochemical screening technique Rock-Eval (RE) pyrolysis and light reflected microscope are used for the estimation of source rock and reaction kinetics study. Using Rock-Eval, heating-rates programmed as 5 °C/min, 15 °C/min, and 25 °C/min to resolve the kinetics potential of the studied shales. The results from the Rock-Eval and Petrography indicate that the NK shales fall in the zone of liquid hydrocarbon yielding potential, attributing their distinctive petrographic composition i.e., rich in type I-II kerogens. In comparison, the RN basin shales display contrasting potential indicating the presence of type III-IV kerogens and higher thermal maturity. Further, the kinetics data reveals the clustering of the samples in groups on the activation energy versus pre-exponential factor plot (E vs LnA). Highest reactivity was displayed by the samples rich in type I-II kerogens, whereas the samples rich in type III-IV kerogens, and those displayed elevated thermal maturity, were observed to fall under lower reactivity zone on the reaction kinetics model. One heat affected (igneous intrusion) sample from the RN basin showed the least reactivity which further revealed the highest RE S2 pyrolysis and oxidation stage Tmax and S4Tpeak, respectively, with considerable drop in hydrogen index (HI) effluent. This essentially signifies the role of the thermal aureoles (igneous emplacement) on the adjacent shales, causing the expelling the hydrocarbons and lowering their potential reactivity. The results reported in this work emphasis the role of petrographic composition i.e. macerals, a key controlling factor for the source-rock hydrocarbon generation potential and reaction kinetics of the studied shales. Significant presence of the framboidal pyrite together with type I-II kerogens in the NK shale samples further suggests some marine incursion during the depositional phase of the basin.
Keywords: Rock-Eval, TOC, Kerogen-kinetics, Kerogen types, Petrography

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SESSION 8 (14:25-16:05)
CLEAN COAL DEMONSTRATION AND COMMERCIAL PRODUCTS – 2
Tom Sarkus and Dan Connell

8.1 (14:25-14:45) Permitting the First Carbon Storage Hub in the United States

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Carbon capture and storage is a technically feasible and, with the development of storage tax credits, a potentially economic process for decarbonizing electrical generation from fossil fuel combustion. Advanced Resources International, Inc. (ARI) is developing Class VI UIC injection permits for the Kemper County Storage Complex, located near Mississippi Power Company's Plant Ratcliffe electrical generating station. Two Class VI permits will be submitted that will together be capable of geologically storing more than 50 Mt of CO2 over 30 years of injection. The documentation needed to fulfill the requirements for Class VI permits includes geologic site characterization, determination of the Area of Review (AoR), well construction, financial responsibility, testing and monitoring, well plugging and site closure, and emergency and remedial response. The characterization phase of the project lasted from 2017 to 2021 with the drilling of six characterization wells near Plant Ratcliffe, from which open-hole well logs and whole core were taken to assess potential storage reservoirs and confining units. The Lower-Cretaceous sands of the Paluxy Formation were selected as the target injection interval due to their high porosity and permeability, while the Tuscaloosa Marine shale will serve as the primary confining zone due to its excellent confining characteristics and structural simplicity. The Marine shale is situated below the deepest underground source of drinking water (USDW) in Kemper County. The geologic data was assembled into a 3D model from which the storage capacity and the AoR were determined. The lateral and vertical migration extent of the CO_2 plume, formation fluids, and the pressure front was determined by geologic site characterization and computational modeling. The projected CO2 plume was modelled for 30 years of injection and showed effective stabilization 20 years after the end of injection. This 20-year post-injection plume extent is used as the AoR for the Project. To assess the progress of the plume and pressure front, a series of monitoring wells will be drilled around the injectors, including five In-zone monitoring wells in the Paluxy Formation, two Above-Zone monitoring wells in the Upper Tuscaloosa Group (Formation above the confining zone), seven deep groundwater wells in the Eutaw Formation (lowest USDW), and seven shallow groundwater wells in the Wilcox Group (shallowest USDW). Monitoring at each of the wells will continue annually through the end of the post-injection site care period. A shutdown plan will be initiated for the injection well and the UIC Program Director will be notified in the event the CO2 stream may cause any endangerment to a USDW. This project is part of the CarbonSAFE Program and is financially supported by the USDOE-NETL and Mississippi Power Company. The project is managed by the Southern States Energy Board. Technical Support is provided by Southern Company Research and Development.

8.2 (14:45-15:05) The 21st Century Hybrid Gas / Coal Concept Power Plant: FEED Study for Planned Hybrid Gas Turbine and USC Coal Boiler Concept (HGCC) Plant with Post Combustion Carbon Capture and Energy Storage System at City, Water, Light and Power

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The City Water, Light, and Power (CWLP) power plant supplies both electricity and water to the city of Springfield – capitol of the state of Illinois. CWLP currently relies heavily upon Illinois coal and needs to reduce greenhouse gas emissions. Like many other power plants throughout the United States and the world, CWLP must make major, but cost-effective, modifications in its hardware and technology to meet current and future demands for clean, renewable, reliable, and affordable energy.

Under the 21st Century Power Plant initiative, a two-phase Front End Engineering Design (FEED) study is funded by the U.S. Department of Energy (DOE) to evaluate the feasibility of installing a 350 MW net power plant at CWLP that would meet the agency's FIRST requisites for future power plants (Flexible, Innovative, Resilient, Small, Transformative). The resulting design will maximize the following features:

• Small (up to 350MWnet) and modular units
• Capable of zero, or near-zero levels of regulated emissions
• Include a strategy for the final disposition of captured Carbon Dioxide (CO2)
• Have the capability for high ramp rates and minimum loads commensurate with estimates of renewable market penetration by 2050
• Have feedstock flexibility that improves the emissions, reliability, operability and/or economics of the plant, and/or mitigates an environmental liability
• Have capital and operating costs that could enable commercial success in a future business case
• Applicable to markets that will enable wide-scale replication without those markets being saturated by the output of just a few plants

Phase I of the project, which is 70% complete, is a pre-FEED feasibility study consisting of preliminary engineering designs, construction feasibility studies, environmental compliance evaluation, technoeconomic analysis, and workplace study. The plant under development is a hybrid gas turbine and ultra-supercritical (USC) coal boiler concept (HGCC) plant with post combustion carbon capture and energy storage system. This futuristic design (1) combines existing technologies in a novel way, making each of the components modular for easy replacement when repairs are needed and as future technologies are developed; (2) improves efficiency and reduces carbon emissions; (3) provides fast start-up and high ramp rates; (4) incorporates carbon capture to bring regulated emissions down to near-zero; (5) allows for flexible feedstock to reduce regulated emissions below zero; (6) includes an energy storage system and robust controls to provide rapid response to both changing grid demands and variable renewable inputs; and (7) uses algae cultivation to provide carbon utilization with wastewater treatment benefits.

The HGCC plant, under design by Doosan Heavy Industries, reburns the hot discharge from a gas turbine generator (GTG) in the boiler to enhance efficiency. The GTG is being designed so that the burners could be replaced with hydrogen burners in the future. The boiler is also capable of burning coal or a mixture of coal and biomass, providing net negative emissions. The plant also utilizes a battery energy storage system with associated controls for load compensation and high ramp rates, a carbon capture system, and an algae pond for carbon utilization.

The carbon capture system, designed by Linde, is an amine system that is being scaled up from 10MW to 350MW at 90 - 95% capture rate. The algae cultivation system, designed by Global Algae Innovations, will also be based on scaling up from a successful 8-wet acre algae farm in Kauai, HI.

The Phase II FEED study looks at the arrangement and assembly of modular components in a way that will best meet facility operation and repair/replacement needs. One important consideration will be the design of the plant for resiliency through its ability to burn a variety of fuels. For example, the natural gas burner is also being designed to be able to burn Hydrogen as well. This will give the plant manager flexibility to modify the feedstock as necessary. The study will also consider the plant's interaction with both changing demand and addition of renewables on the grid.

This HGCC 21st century power plant is truly the power plant of the future. Being flexible, innovative, resilient, small, and transformative, it will be able to meet the fluctuating needs of the customers, additions of renewables on the grid, future advances in technology, and changes in environmental requirements.

8.3 (15:05-15:25) Lessons Learned from Major DOE Projects

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Since 1986, the US. Department of Energy's (DOE's) Office of Fossil Energy & Carbon Management (FECM) has issued 10 competitive solicitations for major demonstration projects. These competitions have yielded more than 80 major projects, including successful Carbon Capture and Storage (CCS) demonstrations led by NRG Energy/Petra Nova in Thompsons, TX; Archer Daniels Midland (ADM) in Decatur, IL; and Air Products in Port Arthur. DOE project funding has been administered by DOE's National Energy Technology Laboratory (NETL) which has compiled a presentation on recent and historical lessons learned from both successful and unsuccessful demonstration projects. These lessons may be prescient given upcoming commercial-scale federal infrastructure programs on a variety of topics including integrated CCS demonstrations, carbon storage infrastructure, hydrogen hubs, long-duration energy storage, and rare earth elements & critical minerals.

8.4 (15:25-15:45) An Update on Design Optimization to Develop an Innovative Clean Energy Solution Using Waste Coal and Biomass with Carbon Dioxide Capture and Storage

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CONSOL Energy will present an update on its FEED (front end engineering and design) study, titled Design Development and System Integration Design Study for an Advanced Pressurized Fluidized Bed Power Plant with Carbon Dioxide Capture and Storage. The presentation will focus on the current design optimization efforts to engineer a carbon-negative power plant using pressurized fluidized bed combustion (PFBC), an amine-based carbon dioxide capture system, and geological CO2 storage. CONSOL will address key considerations affecting the design, siting, and commercial viability of the plant, including fuel and reagent supply logistics, boiler design, capital and operating costs, equipment availability, and CO2 disposition options.

The project is one of four studies to develop technically innovative clean energy solutions funded by the U.S. Department of Energy, National Energy Technology Laboratory (DOE NETL) as part of its 21st Century Power Plant Program. The project builds on a series of two previous studies, a conceptual design and a pre-FEED study, which CONSOL presented results from at the 2020 and 2021 Pittsburgh Coal Conferences. The current phase of the project is comprised of two parts: a design optimization effort, followed by a conventional FEED study. The overall period of performance is 34 months with completion targeted for March 2024.

The project's design seeks to capture and permanently sequester 97% of the generated CO2 emissions from the power plant at a storage volume of approximately three million tons annually, while delivering overall net negative CO2 emissions using a BECCS (bioenergy with carbon capture and storage) strategy by co-firing up to 10% (by heat content) forestry waste biomass. The project minimizes environmental impacts by incorporating controls to deliver near near-zero emissions of regulated pollutants, zero liquid discharge, and beneficial reuse of plant byproducts.

The location for the plant is expected to be at or near CONSOL's Pennsylvania Mining Complex (PAMC), where the potential for integration into existing mine site infrastructure promotes the sustainability of the coal supply chain. In addition, the project will incorporate environmental justice, workforce development, and local community growth initiatives as key goals.

The project strives to complement renewable power systems by providing sustainable, low-carbon baseload electric power supply, which is expected to be a critical component to meet the future needs of an evolving electric grid. Provided that the project produces favorable economics, and an efficient design, construction and commissioning of the plant could be completed before 2030.

8.5 (15:45-16:05) Dynamic Decarbonization Through the Melding of Prescriptive Maintenance and Minimally Invasive Condenser Treatments

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Decarbonization of the power industry is an immediate concern which has placed a substantial economic and technical challenge on operators. One potentially attractive option to simultaneously reduce the carbon footprint of existing power plants without the need for extensive capital investment is prescriptive maintenance, which can actively monitor the health and output of equipment and make suggestions as to how to implement small operating adjustments over time. One challenge with implementing such systems, however, is that they do not inherently increase the efficiency of underperforming or overburdened units, and to have the most impact, any underlying machine learning model must have a large volume of historical data as well as access to a broad swath of real time performance outputs.

This creates an unusual situation, in that prescriptive maintenance solutions typically do not mesh well with the implementation of new technologies that change the underlying fundamentals of a system and upend the historical baseline performance. Combine this with the paradox that only the most proven and de-risked technologies are allowed to be utilized in key systems such as a main condenser and creating the substantial leaps forward in decarbonization may be limited.

This work presents the benefits of designing and implementing an efficiency-improving internal condenser tube surface treatment with a lightweight prescriptive maintenance monitoring platform. While the surface treatment, commercially known as HeatX™, has already been successfully deployed in multiple case studies, pairing it with a standalone performance monitoring device capable of reporting out efficiency data proved to be a way of unlocking further decarbonization gains beyond the mere avoidance of unnecessary maintenance shutdowns. This standalone platform, known as ThermAI™, is based on an ensemble learning method specifically designed to impute and compensate for limited data inputs, and was trained on a hybrid digital twin model to detect the early onset of fouling buildup on treated surfaces where no past historical data was available. Implementation of this combined physical and digital efficiency solution can be scaled from systems as small as a single plate-and-frame exchanger to a heavily used condenser unit and have offered heat rate performance gains of as large as 7.5% based on overall reduced fuel requirements for heating, and lowered condenser backpressure.

SESSION 9 (8:05 – 9:45)
CARBON MANAGEMENT – 1
Nick Siefert and Alberto Pettinau

9.1   (8:05-8:25) 3D micro-structural changes of an artificial flow channel in wellbore cement under geologic CO2 storage conditions: combined effect of effective stress and flow

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Understanding CO2-induced micro-structural changes at the imperfections in wellbore cement is vital for assessing the risk of CO2 leakage through wellbore cement under geologic CO2 storage (GCS) conditions. To investigate the evolution of a flow channel width in cement under GCS conditions and the influence of effective stress and flow on the micro-structural changes of the flow channel in cement, we carried out a set of experiments in which the flow condition (flow-through vs. static) and the effective stress (3 MPa effective stress vs. no effective stress) were varied. Micro-structural changes of an artificial flow channel were investigated by X-ray micro-computed tomography (CT). CT images revealed a clear micro-structural change of the flow channel and distributions of Ca(OH)2/C-S-H dissolution and calcite precipitation zones near the channel after reacting with CO2-saturated brine. CT results showed that a flow rate of 0.01 mL/min through the channel turned channel self-sealing (as observed in the static scenario) into channel opening. Effective stress accelerated the dominant chemical reaction, i.e., enhancement of Ca(OH)2/C-S-H dissolution around the channel in a flow-through scenario and enhancement of calcite precipitation around the channel in a static scenario. It seems that effective stress and flow have a combined contribution to micro-structural change of the flow channel in hydrated Portland cement, which may increase the risk of CO2 leakage through wellbore cement when exposed to high concentration CO2.

9.2   (8:25-8:45) Study on the conversion mechanism of thermal plasma non-catalytic CH4-CO2 reforming system to syngas

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CH4-CO2 reforming to syngas is an efficient and clean technology path for large-scale comprehensive utilization of carbon and hydrogen sources and conversion of greenhouse gases. In this paper, thermal plasma is used as molecular activation method to analyze the composition of thermal plasma non-catalytic CH4-CO2 reforming system reaction products and the selectivity changes of CO and H2 through experiments under different feed ratios. Combined with HSC Chemistry thermodynamic calculation and Chemkin kinetic model, the reaction characteristics and reaction mechanism of CH4-CO2 reforming system were studied. The experimental results show that when the CO2/CH4 ratio is 6/4, the conversion rates of CH4 and CO2 can reach 92.1% and 81.9%, and the selectivity of CO and H2 are 87.0% and 75.2%, respectively. With the increase of CO2/CH4 molar ratio, the CO2 conversion and H2 selectivity showed a downward trend, while the CH4 conversion and CO selectivity showed an upward trend. The HSC performs thermodynamic calculations on the possible reaction types of the reforming system under simulated plasma experimental conditions. The results show that an appropriate excess of CO2 can promote the conversion of CH4, the conversion rate of CH4 and CO2 can be higher than 90%, and the average selectivity of CO is above 70%, indicating that thermal plasma can promote the cracking of CO2 and improve the selectivity of CO. The results of PSR kinetic analysis show that CH4 and CO2 will be cracked to form free radicals at the moment of contact with the plasma flame, and the types of free radicals cracked by CH4 are more than that of CO2. The stability of the four free radicals of CH4 cracking is CH2> CH3>CH>H. In addition, the temperature-sensitive ROP analysis of the concentration of the main gas components shows that the formation of CO and H2 is mainly caused by the collision of O-containing radicals and H radicals in the system after thermal plasma activation. Finally, the formation paths of CO and H2 in the thermal plasma non-catalytic CH4-CO2 reforming system are analyzed, which provides a new theoretical basis for the CH4-CO2 reforming system reaction.

9.3   (8:45-9:05) Effect of support on the catalytic performance of Ni-MgO/X catalysts for carbon dioxide reforming of methane

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The supports type has an important influence on the catalytic activity and stability of nickel-based catalysts since it would affect the active metal particle size and the interaction between active metal and support. In this work, a series of Ni-MgO/X (X = La2O3, ZrO2, SiO2, γ-Al2O3) catalysts were fabricated via impregnation method. It is found that support greatly influence the structure and catalytic performance of Ni-MgO/X catalysts. Catalytic activity evaluation presented that when La2O3 was used as support, its conversions of CH4 and CO2 was kept 70.3% and 55% at 750°C in 8 h. When ZrO2 was used as support, the conversions of CH4 and CO2 were decreased from 73.3% to 64.0% and 81.3% to 72% at 750°C after 8 h runs. On the contrary, the Ni-MgO/SiO2 and Ni-MgO/γ-Al2O3 catalyst possessed superior catalytic activity. Their conversions of CH4 and CO2 maintained at 83.4% and 89.4% in 8 h, and the H2/CO molar ratio was 0.92, which were close to the thermodynamic equilibrium values at 750°C (CH4 conversion, CO2 conversion and H2/CO molar ratio were 84%, 91% and 0.92, respectively). Furthermore, 100 h catalytic activity evaluation of the Ni-MgO/SiO2 and Ni-MgO/γ-Al2O3 catalyst was carried out to investigate their stability in detail. After 100 h runs, CH4 and CO2 conversion over Ni-MgO/SiO2 catalyst were decreased from 83.4% to 78.8% and 89.4% to 84.3%, and the H2/CO molar ratio was decreased from 0.92 to 0.86, while Ni-MgO/γ-Al2O3 catalyst still maintained high CH4 and CO2 conversion. By analyzing their structure and carbon deposition, it found that though Ni-MgO/γ-Al2O3 catalyst obtained higher carbon deposition (0.89 wt.%) than that of Ni-MgO/SiO2 catalyst (0.16 wt.%), the strong metal support interaction in Ni-MgO/γ-Al2O3 could inhibit the Ni agglomeration, which endowed Ni-MgO/γ-Al2O3 superior stability.

9.4   (9:05-9:25) CO2 Capture from Flue Gas over DEA-functionalized Activated Semi-coke

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CO_2 emission has resulted in a series of global problems such as global warming, tropical storm etc. The main source of CO2 emission is from coal-fired power plants. Therefore, it is very important to explore an effective approach for capturing and separating the CO2 in the flue gas so as to reduce the greenhouse effect and build a sustainable ecological environment. Solid amine sorbent has been proved to be a promising sorbent for CO2 capture from flue gas. However, the sorbents still suffer from low CO2 sorption capacity and the expensive carrier cost. In this work, a novel solid amine sorbent was synthesized by employing cheaply activated semi-coke as the carrier and diethanol amine (DEA) was impregnated in the activated semi-coke to investigate its characterization and adsorption/desorption properties of CO2 from flue gas. Results showed that the DEA dosage plays an overwhelming role in the CO2 sorption capacity of the amine-functionalized activated semi-coke. When the DEA dosage was 50 wt%, superior CO2 capacity (2.16 mmol/g at 60 ºC) was achieved, which was 95% higher than that of the activated semi-coke without DEA impregnation, and competitive to the sorbents with other carrier such as SBA-15, activated carbon etc. The CO2 sorption capacity still remains 90% after 10 cyclic regenerations, showing excellent cyclic sorption stability for CO2 capture and its separation from flue gas. The enhanced CO2 sorption performance was ascribed to the proper pore volume and the amount of effectively available amine.

9.5   (9:25-9:45) Reservoir Rocks Interacting with CO2/Brine under Subsurface CO2 Sequestration Conditions

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Carbon capture and storage (CCS) is identified as the key strategy for reducing the atmospheric concentration of CO2 - the main contributor to global climate change. The potential options for CO2 storage include underground geological formations such as saline aquifers, depleted oil and gas reservoirs, unmineable coal seams, and CO2 within enhanced geothermal systems. CO2 storage in saline aquifers is recognized as one of the highest estimated storage capacities within underground geological formations. Obtaining the knowledge of possible geochemically induced changes to the permeability and porosity of host CO2 storage sandstone will enable us to gain a deeper insight of the long-term reservoir behavior under the CO2 storage conditions.
An experimental study of the interaction of CO2/brine/rock on saline formations was conducted in a static system under CO2 storage conditions. Core samples from the Mount Simon formation in Illinois and the Cedar Keys-Lawson formation in Florida were exposed to the simulated in-situ reaction conditions for six months, while selected exposure experiments were conducted up to six months. In a typical experiment, core with a corresponding model brine were placed in a static reactor at 85 °C (or 55 °C for samples from the Cedar Keys-Lawson formation) and CO2 pressure of 23.8 MPa (3,500 psig) was applied to the reactors. CT, XRD, SEM, brine chemistry, porosity, and permeability analyses were conducted prior to and after the experiments.
Preliminary permeability measurements obtained from the sandstone sample showed a change after it was exposed to CO2-saturated brine for six months. The changes depend on where the samples were obtained as well as the major mineral contents in the core. This observation suggests that mineral dissolution and mineral precipitation could occur in the host deposit altering its characteristics for CO2 storage over time.

SESSION 10 (8:05 – 9:45)
VALUE-ADDED PRODUCTSFROM COAL - 1
Dick Winschel and Atsushi Ishihara

10.1 (8:05-8:25) Study on affecting factors of dehydration during one-step preparation of 9-fluorenylmethanol

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High temperature coal tar is rich in high value-added aromatics, and fluorene accounts for 1~2% or so. 9-fluorenylmethanol is one of the important downstream products of fluorene, which often used as the precursor of amino protectant or carboxyl protectant in polypeptide synthesis, and the synthesis of photoelectric materials. 9-fluorenylmethanol can be synthesize from fluorene by one-step or two-step method. In our previous research, the selectivity and yield of 9-fluorenylmethanol can reach 100% by using a two-step method. But there are still some drawbacks of the two-step method, such as costly, safety risks and long process. One-step method using paraformaldehyde as hydroxymethylation reagent is simple and economical. However, the process is difficult to control since 9-fluorenylmethanol is prone to alkali-catalyzed β-elimination reaction to produce the dehydrated product, 9-methylenefluorene, or reacts with another formaldehyde molecule to produce 9,9-bis(hydroxymethyl)fluorene further. This results in low purity and low yield of 9-fluorenylmethanol. Therefore, the dehydration of 9-fluorenylmethanol was investigated by considering the major factors, such as reaction temperature, substrate concentration and the amount of paraformaldehyde in N, N-dimethylformamide with potassium carbonate as catalyst. In addition, the influence of

alkali intensity was determined with potassium hydroxide as the contrast. Finally, it was applied to the one-step preparation of 9-fluorenylmethanol.

Key words: coal tar; alkali catalysis; 9-fluorenylmethanol; alcohol dehydration

10.2 (8:25-8:45) Effect of Alkali on Density, Compressive Strength and Thermal Conductivity of Char-Based Concrete Bricks

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Alkaline accelerators (e.g., sodium carbonate (Na_2CO_3) and sodium bicarbonate ($NaHCO_3$)) are often used to improve the rapid hardening ability and early strength in concrete. The Na_2CO_3 could increase the compressive strength up to 40% for the cement paste. The bicarbonate ions could reduce the expansion of mortar and improve the sulfate resistance of mortar when subjected to sulfate attack. The addition of $NaHCO_3$ could accelerate the hydration of cement paste and improve the compressive strength up to 8% in cement paste. In this study, the effect of addition of alkaline materials (Na_2CO_3 and $NaHCO_3$) on the mechanical and thermal properties of char-based concrete bricks (CCB) was investigated. The CCB samples were prepared with pyrolyzed char (60-70 w/w%), ordinary Portland cement (30-35 w/w%), and alkali (3-7 w/w%). The densities, compressive strengths, and thermal conductivities of CCB samples are in the ranges of 0.78-0.95 g/cm3, 2.6-9.1 MPa, and 0.18 to 0.35 W/m.K, respectively. Regardless of different pyrolyzed char contents, after curing 14 days, the thermal conductivities of CCB samples with alkali are similar to the baseline CCB samples (i.e., alkaline content = 0). However, comparing with the baseline CCB samples, the alkaline addition reduces the compressive strength of CCB samples 5 to 50%. At a fixed curing time, the effect of alkaline addition on the change in density is less than 5%. Hence, the density is not correlated with the compressive strength of the CCB samples in this study. Although the addition of $NaHCO_3$ and Na_2CO_3 is helpful for accelerating the ettringite formation, high content of Na^+ ions can partly replace the Ca^{2+} in the C-S-H gel, which leads to the discontinuity of C-S-H gel and the reduction in compressive strength due to alkaline addition.

10.3 (8:45-9:05) Effect of Carbonization Temperature on the Properties of Carbon-based Structural Unit

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A promising application for pyrolysis chars (PC's) is to utilize them for manufacturing carbon-based structural unit (CSU) as a potential building material. The CSU can be fabricated from PC as a solid filler material and coal-derived mesophase pitch (MP) as a binder material. The mixture of PC and coal-derived MP is expected to produce a stronger carbon-based construction material, which possesses similar or even better properties in terms of density and compressive strength than concrete and wood. In this study, CSU was prepared by mixing MP (coal) with PC in a mass ratio of 1:2, followed with mixture ball milled, dried, and pressed into cylindrical samples at 100 MPa. For thermal treatment of the compressed samples, they were firstly oxidized at 245oC and then carbonized at temperature from 700oC to 1600oC. With increasing the carbonization temperature, compressive strength firstly increased due to the higher degree of carbonization up to 900 ºC and then decreased with increasing temperature as more graphite appears and the mesophase pitch binding gets weaker. The compressive strength was 42.7 MPa at 700 oC, increased up to 88.1 MPa at 900 oC, and then reduced to 47.1 MPa at 1600 oC. The thermal conductivity increased from

0.175 W/m.k (at 700 oC) to 0.521 W/m.k (at 1600 oC) and the density increased slightly from 0.97 g/cm3 to 1.08 g/cm3 with increasing carbonization temperature. It can be concluded that the optimized carbonization temperature for CSU samples is 900oC. The application of these coal-derived CSUs as alternatives to concrete building products, from a performance perspective has shown to technically appealing. Furthermore, the techno-economics and practical feasibility of the substitution for concrete products are discussed.

10.4 (9:05-9:25) Field Trial of Anthracite Coal-Based Activated Carbon for Mercury Emissions Reduction in Flue Gas from Power Generation Unit

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A commonly used approach for removing mercury (Hg) from municipal solid waste incinerators and utility boiler flue gas consists of direct injection of a dry Hg sorbent. The method has been effective at removing Hg in the flue gas to levels mandated by environmental regulations. A low-cost, anthracite coal-based activated carbon (ACAC) candidate was used to perform bench-scale packed bed experiments, aimed at understanding the mechanism of Hg adsorption on the ACAC. The lab-made ACAC was activated from anthracite using a chemical activation method with potassium hydroxide in a horizontal tube furnace system. This ACAC achieved good results in terms of Hg adsorption at elevated temperatures in simulated flue gas, comparable to commercial activated carbon (CAC, Darco-HG). Following lab testing, a field test campaign was carried out to evaluate the Hg adsorption performance of the ACAC in a slipstream apparatus. The slipstream apparatus was designed to assess Hg adsorption ability using the lab-produced ACAC under real flue gas conditions and to compare the performance of the ACAC with four different CACs. Field test experimental parameters were as follows: the inlet flue gas temperature of the slipstream setup was kept at 212℃ (413.6 ℉); the injection rate of ACAC and CACs was kept at a constant value of 0.3 gram/min. The flue gas flow rate was around 500 lb/hr. The obtained adsorption results were very encouraging. The ACAC Hg removal efficiency reached up to 80%, which was comparable to the removal efficiency of the CACs. The high ACAC Hg adsorption performance demonstrated from this field trial would lead to additional work on ACAC to improve its performance and estimate the techno-economics of a potential ACAC product, which would be of interest to commercial companies and end-users looking for a low-cost Hg control sorbent. This also opens additional opportunities for the potential of applying the ACAC to other industrial applications, such as cement and steel industries, for Hg emissions reductions.

10.5 (9:25-9:45) Unexpected high Extraction of Oxygen Rich Subbituminous PRB Coal with Renewable Carbon Solvents to Produce Materials for Asphalt Markets

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Currently, about 25 million tons of asphalt binder are used each year in North America for paving and roofing applications, and more than 100 million tons are used each year globally. There is an ever growing push to reduce the carbon footprint for asphalt materials, and this has led to a paradigm shift for the asphalt industry as it triggers a critical search for new alternative sustainable binders. Of particular interest are binders produced from non-recyclable waste materials from other industries (such as tires and plastics) and especially those from biomass.

Coal reacted with bio-derived triglyceride feedstocks (vegetable or animal based) could provide a new high volume, highly consistent and tailored feedstock for alternative asphalt materials, such as binders and asphalt additives. Of particular interest for asphalt additives are recycling agents, or rejuvenators, which are used to increase the recycling of old pavement. To this end, a new solvent extraction (SE) method has been developed that converts up to 85% Powder River Basin (PRB) coal with renewable carbon triglyceride-based solvents into an asphalt product feedstock. The solvents work to breakdown the coal macrostructure to provide smaller molecules while also reacting with the oxygen groups in the coal to produce much softer, meltable and soluble products than what is traditionally produced by direct coal liquefaction using tetralin or aromatic oils. This new class of SE materials has properties that are compatible with petroleum asphalts. Additionally, follow-on chemistry can be applied using other renewable carbon triglyceride chemistry to further tune the properties and performance for various asphalt applications.

Experimental results surrounding the novel SE approach will be discussed, as well as, chemical and compositional characterization of these new materials in the context of paving and roofing applications.

SESSION 11 (9:55-11:35)
CARBON MANANGEMENT – 2
Nick Siefert and Alberto Pettinau

11.1 (9:55-10:15) Design the 1st ISO Verified Carbon Capture Unit in the World for Carbon XPRIZE Competition

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Delta CleanTech has developed its Low-Cost Design® (LCDesign®) Post-Combustion Carbon Capture technology to reduce the technology capital and operation costs as well as minimizing the emissions to atmosphere, effluent streams, and waste generation. Delta CO2 capture technology is based on the bulk removal of CO2 from high volume flue gas by the use of chemical absorbents. The design is made based on the flue gas composition, operating conditions, the clean-up target and the CO2 production capacity. In 2019, Delta LCDesign® technology was selected by InnoTech Alberta, a wholly owned subsidiary of Alberta Innovates, for the NRG COSIA Carbon XPRIZE Competition in Calgary, Alberta, Canada. The competition involves five finalists who have been competing on converting the captured CO2 into new different innovate and sustainable products. Some of these products will store CO2 permanently, like concrete and nanotubes, while some others will not, such as alcohols and fuels.
The plant was designed in modular concept allowing easy fabrication, transportation, installation, commissioning, operation & maintenance with a small footprint. The whole plant consists of three modules: Process Building with Towers, Heating System and Cooling System. It captures the CO2 from a natural gas-fueled turbine flue gas within Sheppard Energy Centre. The flue gas has very low CO2 content (3 to 5 volume %). At the test site, only electricity and water are provided to the plant operation and all other utility requirements, such as heating, cooling and instrument air, are provided as standalone utility units. Capture unit was designed for flexibility to enable future research and development to enhance carbon capture processes and effectively compare amine-based systems with other novel capture technologies. Enriching or reducing the CO2 content (consequently changing the O2 and N2 contents) in the flue gas can be

done to study different types of solvent and flue gas compositions and conditions. The plant is also equipped with Delta Reclaimer® unit that can reclaim most of amine solvents, which can be used in the Post-Combustion Carbon capture applications.
NRG COSIA Carbon XPRIZE hired a third party (350 Solutions from Raleigh, NC, USA) to validate all five finalists, including the CO2 Capture plant. The plant has confirmed to produce the CO2 product at purity of 99.9 Volume % dry for utilization by others. This is the first Post-Combustion CO_2 Capture plant in the world to be verified according to ISO-14034:2016 "Environmental Verification Technology" by a third party. 350 Solutions has issued a summary verification report. The ISO verification confirms the operational size/capacity, CO2 Capture efficiency, CO2 production rate, energy usage and water usage. The plant has confirmed to produce the CO2 product at a rate from 4.79-6.13 tonne CO_2 per day and at purity of 99.9 Volume % dry for utilization by others.
To complete this work, in addition to the Delta CleanTech design tools, a commercial rate-based process simulator was utilized during the design phase and the output from this tool is presented in this work. It has been found that the rate-based model provides a more realistic approach for the process design of the Post-Combustion Carbon Capture plant.

11.2 (10:15-10:35) Test Campaigns at ERTF Carbon Capture Pilot Plant

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The Emissions Reduction Test Facility (ERTF) Pilot Plant was built in 2010 to capture carbon dioxide (CO2) from any type of flue gases. The pilot plant is based on Delta CleanTech first generation technology which was known as Thermal Kinetics Optimization® Configuration or TKO®. The ERTF pilot plant was designed to accept any type of solvents although it was specifically designed based on a formulated solvent, RS-2® solvent. RS-2® was claimed to require low energy consumption which is within the range from 1.20-1.25 kg Low-Pressure saturated steam per kg captured CO2. Furthermore, the test pilot plant was design to capture 0.5 to 1 metric tonne per day of CO2 depending on the selected flue gas (composition & conditions), the solvent (type & concentration), the operating conditions, and the process configuration.
The ERTF is a good size pilot plant for solvent screening and configuration evaluation test campaigns. In addition to the coal flue gas source, it is recommended to add simulated flue gas source in order to conduct tests more frequently and at less cost than the actual coal flue gas. The simulated flue gas source can be a mixture of CO2 with Air or N2. To minimize the CO_2 consumption during the test campaign, the captured CO2 product can be recycled into the absorber feed. The three test campaigns presented in this work have been successfully completed by a common engineering team from Delta CleanTech and Doosan Babcock.
The first test run (Run #1) was conducted successfully to capture 1 TPD using RS‐2® solvent at CO2 recovery rate of 91.2%. The steam consumption of this test run was 1.33 kg steam per kg CO2. In this full load case (flue gas rate of 230 kg/h and solvent rate of 780 kg/h), it is not possible to achieve CO_2 rich loading more than 0.38 mol/mol because the absorption column is slightly under designed capacity to capture 1 TPD at 90% CO2 recovery and steam consumption of less than 1.2 kg/kg.
The second and third test runs (Runs #2 and #3) were successfully conducted to capture more than 90% of CO2 from the flue gas at steam consumption of equal or less than 1.2 kg steam per kg CO2. In this turndown case (flue gas rate of 126 kg/h and solvent rate of 350 kg/h), it is possible to achieve steam consumption of less than 1.2 kg steam per kg CO2 by capturing about 0.6 TPD of CO2 from coal flue gas, which amounts to 40% turndown capacity.
The ERTF Pilot Plant can be operated at a steady‐state for reasonable time and meeting the low energy demand of RS-2® solvent. Furthermore, Delta team conducted validation study of the ERTF operating results using rate-based process simulator. The comparison to validate the steam consumptions in the three-test campaign runs (#1, 2 and 3) with the simulation prediction is provided.

11.3 (10:35-10:55) Directly-Spun Epoxy-Crosslinked PEI Chemisorption Fiber Sorbents (CHEFS) for Direct Air Capture (DAC) of CO2

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Greenhouse gas emissions have been widely recognized as the main contributor to anthropogenic climate change. Technologies for carbon capture offer great potential to reduce the atmospheric CO2 concentration. In this work, we developed a solvent-stable, epoxy-crosslinked mixed-amine sorbent for carbon capture from ambient air and post-combustion gas. The particle sorbent was further incorporated into a solid chemisorption fiber, which offers important performance benefits for industrial circles. The CO2 adsorption capacities under simulating ambient air (400 ppm CO_2 in inert gas) and simulating post-combustion gas (14% CO2 in inert gas) were studied in terms of amine size, crosslinker ratio, PEI-modifier amine type and ratio, and organics loading. The optimized sorbent presented outstanding CO2 adsorption capacities (0.89 mmol/g-sorbent under DAC conditions and 1.41 mmol/g-sorbent under post-combustion conditions), as well as enhanced adsorption kinetics compared to conventional sorbents. The new sorbent showed excellent stability in solvent during fiber formation and maintained stable CO2 uptake in cyclic adsorption-desorption operations. The resulting solid fiber sorbent showed outstanding CO_2 adsorption capacities of 0.34 mmol/g-fiber under DAC conditions and 0.82 mmol/g-fiber under post-combustion conditions compared to lower-performing solid and hollow fiber sorbents in the literature. The solvent-stable sorbent showed a high potential to effectively remove CO2 from both ambient air and post-combustion gas.

11.4 (10:55-11:15) DEVELOPING GIGATONNE SCALE CO2 STORAGE INFRASTRUCTURE IN THE U.S

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Two decades of Department of Energy, Office of Fossil Energy and Carbon Management (DOE FECM) and National Energy Technology Laboratory (NETL) directed research, development, and field demonstration, together with industry investment, and technical involvement of states and other federal organizations, have demonstrated that carbon dioxide (CO2) can be reliably transported and stored in geologic formations. These efforts include: the Regional Carbon Sequestration Partnerships (RCSPs) initiative, which completed six large-scale field projects cumulatively storing over 11 million tonnes of capture CO2; the Regional Initiative projects, which are successors to the RCSPs that accelerate efficient and equitable CCUS deployment; and the Carbon Storage Assurance Facility Enterprise (CarbonSAFE) initiative, which began in 2016 with the goal to characterize, permit, and construct commercial-scale storage facilities, each with the capacity to store 50+ million tonnes of CO2. To meet the Administration's decarbonization targets, investments in building the infrastructure for dedicated carbon storage and transport must be accelerated over the next decade. By 2030, recent studies show that geologic storage and transport infrastructure must accommodate additional storage of at least 65 million tonnes of CO2 per year, along with development of 19,000 km of pipelines. Injection of CO2 at this rate over a 30-year period will require 2 billion metric tons of commercial storage capacity by 2030 with the need for additional capacity continuing to grow over the 20 years thereafter. To spur this level of growth, DOE FECM will make key investments supported by the Infrastructure Investment and Jobs Act (IIJA). DOE FECM plans include investments in storage facilities and regional hubs that will require future intra- and inter-regional transport networks that include pipelines. Expansion of the CarbonSAFE initiative, including development of storage hubs anchored with CarbonSAFE facilities, storage facilities that are significantly larger than 50 million tonnes of CO_2, and incorporating diverse types of CO2 sources, will help to catalyze the rapid deployment of carbon storage necessary to meet decarbonization goals. Underpinning the infrastructure development is the development of enabling technologies to improve performance and reduce the cost of gigatonne scale carbon storage. The SMART-CS initiative focuses on enhancing real-time visualization and forecasting and virtual learning capabilities to improve project performance and inform decision making. NRAP's tools and workflows offer the means to demonstrate that risks associated with geologic storage are manageable for carefully selected and well-characterized storage sites, leading to an increase in operator, regulator, and public confidence. The SMART-CS and NRAP projects leverage the FECM Energy Data Exchange (EDX) as a secure virtual platform to support research collaboration and curation of research data and tools.

11.5 (11:15-11:35) Pilot-scale (0.5MW) study for the alkalized alumina sorbent based post-combustion CO2 capture

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TDA Research, Inc. is developing an alkalized alumina sorbent based post-combustion CO2 capture technology. A pilot-scale skid, using a slipstream of the flue gas, was installed and tested at National Carbon Capture Center. It was designed to process coal derived flue gas equivalent to 0.5 MWe of power generation. The pilot test data shows that TDA's process can achieve 90% capture rate and 95% CO2 purity for both coal and natural gas flue gases. For coal flue gas, the system met its performance target even when processing 24% more flue gas than its design capacity. After the 3-month test, TDA sorbent still maintained 91% capture capacity and the degradation reached a plateau.

> ## SESSION 12 (9:55-11:35)
> ## VALUE-ADDED PRODUCTS FROM COAL - 2
> *Dick Winschel and Atushi Ishihara*

12.1 (9:55-10:15) Design for Carbon Conversion Product Pathways with Nuclear Power Plant Integration

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Coal is a globally abundant resource that historically has been used for power generation via combustion. As the power industry replaces coal with cleaner methods of generation, energy rich coal could be used in other chemical and fuel applications. This study presents a coal utilization option in which coal combustion is replaced with a carbon-free nuclear power plant and the coal is upgraded to valuable products for a variety of markets. Coal is prepared for conversion first by the pyrolysis process, which will optimize solid, liquid, and gaseous products based on the market size and potential product value, maximizing the monetary value of coal. This process is designed using bituminous coal from the Appalachian region as a basis to provide a pathway to preserve or transition coal-related jobs and create new jobs associated with the clean energy transition. Process modeling will be used to determine each component's sensitivities, costs, inputs, and outputs, which will be transferred to the Framework for the Optimization of Resources and Economics (FORCE) toolset for dynamic modeling and economic analysis, using for example, an intermittent production of hydrogen and operation of process units that interact with the grid using demand response. Advanced and light-water reactors are considerations to supply the heat, steam, and electricity to the process. Product pathways are focused on activated carbon, tar for construction purposes, and methanol synthesis for further upgrading to marketable chemical and polymer products.

12.2 (10:15-10:35) Status of NETL's Carbon Ore Processing Program

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The Carbon Ore Processing Program, conducted under the U.S. Department of Energy's Office of Fossil Energy and Carbon Management (FECM) and the National Energy Technology Laboratory (NETL), is developing advanced technologies by supporting R&D to transform coal and coal wastes into products outside of traditional thermal and metallurgical markets. Supported R&D will lead to a range of products covering the entire value spectrum, from high volume through high value.

Recent activity includes cost-shared research and development of high-value carbon materials and carbon metal composites. These could have applications for computer memory devices, electromechanical applications (e.g., BEV motors), filtration, and vehicle light weighting. Additional activity includes the development of carbon materials for building and infrastructure applications that can foster new uses for domestic coal resources. The program has also announced plans to support the design, validation, and fabrication of a prototype carbon-based building. The envisioned prototype building will demonstrate the technical and economic viability of carbon-based building materials by assessing properties including flexural strength, thermal stability and water adsorption where such materials offer opportunities for economically and environmentally superior buildings. In addition, the Carbon Ore Processing Program continues to make significant progress developing other carbon products including carbon fibers, graphite for battery anodes, conductive inks, and nanomaterials. This talk will highlight the recent progress and accomplishments and the future direction of the NETL Carbon Ore Processing Program.

12.3 (10:35-10:55) Graphitic Carbons from Plasma Upgraded Coal Tars

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This paper reports graphitic quality assessment of carbons obtained from plasma-upgraded coal tars and pitches. During coal devolatilization, labile bonds break to give tar molecules in primary pyrolysis stage, which then pyrolytically decompose within the forming char if they are not liberated (secondary pyrolysis). Compared to conventional thermal pyrolysis, the rapid devolatilization under MW exposure limits charring while the reactive atmosphere can limit secondary pyrolysis/cracking reactions by capping free radicals. H Quest's MW plasma pyrolysis conducted under reactive atmospheres (such as CH_4, H_2) was shown to promote methylation and hydrogenation, thought to be promoted by methyl radicals and hydrogen atoms formed via electron impact dissociation within the highly energetic plasma. Two coals presenting different ranks and volatile content: a) Middle Kittanning (bituminous) and b) Powder River Basin (sub-bituminous) were pyrolyzed in a MW plasma under different reactive gas environments. The tars were collected and distilled at 200 °C to obtain pitches. Fourier Transform Infrared Spectroscopy is used to assess aromaticity of the products. The set of tars and pitches were carbonized at 600 °C for 3 hrs and the obtained cokes were graphitized at 2500 °C for 1 hr. The samples were analyzed at the carbonization stage using Polarized Light Microscopy for optical texture. The graphitized samples were analyzed using X-ray diffraction for lattice and crystallite parameters and Transmission Electron Microscopy for nanostructure assessment. The bulk crystallinity of these graphitic carbons is compared with graphitized needle coke, shot coke and commercial pitch.

Pennsylvania, focused on the development and commercialization of novel hydrocarbon conversion technologies. This material is based on work supported by the Dept. of Energy under DE-FOA-0001992, Prime Award No. DE-FE0031793 to H Quest Vanguard through DOE subcontract No. 207815 with Penn State.

References:
Strohm, J. J., Linehan, J. C., Roberts, B. Q., McMakin, D. L., Sheen, D. M., Griffin, J. W., & Franz, J. A. (2012). U.S. Patent Application No. 13/401,216.

12.4 (10:55-11:15) Filament Formation and Melt Spinning of Coal-Based Mesophase Pitch for Carbon Fiber Production

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High-performance carbon fibers excel as high specific strength and modulus materials, and are utilized in composites applications ranging across aerospace, automotive, energy, infrastructure, and sports equipment sectors. Compared to PAN-based carbon fiber, mesophase pitch-based carbon fiber has lower tensile strength but provides a higher modulus, higher thermal conductivity, and a lower cost potential. However, challenges in stable, continuous melt spinning processing are a serious limiting factor. Unlike typical melt spinning of long, linear chain polymers, mesophase pitch is a comprised of relatively shorter polycyclic aromatic hydrocarbons which form a liquid crystal. In its 'green' or 'as-spun' state, the fibers are very fragile. Moreover, its temperature of processing is quite high, often approaching 400ºC. Complex flow dynamics combined with short length and time scale heat transfer render its melt spinning a formidable processing challenge. Improved understanding of the root causes for nascent filament breakage and spinning instabilities are needed. This work aims to determine fundamental phenomena that govern mesophase pitch filament formation by comparison of required draw force and uninterrupted spinning minutes with applied draw down ratio. The effect of perturbations on spinning stability are analyzed using capillary rheometry, microscopy of elongating filaments, and filtration.

12.5 (11:15-11:35) Optimization of Direct Coal Liquefaction Conditions for the Production of Mesophase Pitch

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The Coal-to-Products area has experienced renewed interest due to reduced coal demand for energy generation. Simultaneously, coal tar from metallurgical coal coking has been investigated as a precursor for carbon fiber production, potentially offering a lower-cost alternative to traditional PAN precursors. Apart from coking coals, direct coal liquefaction through mild solvent extraction produces various heavy liquids, which can be distilled to pitch. This work explores converting coal to liquid by direct coal liquefaction for downstream production of mesophase pitch. Four different coals of various rank were explored along with two different by-products from the coal and petroleum industries which were used as solvents in the digestion process. Coal slurries

included each coal and solvent combination in a 1:3 coal-to-solvent mass ratio. Slurries were digested at temperatures between 350-450 °C and for residence times between 30-120 minutes. Each sample was analyzed for quinoline insoluble content which was used to calculate coal conversion on a dry, ash-free basis, and optical microscopy images were taken to observe particle content in the resulting liquids. Generally, higher temperatures (450 °C) were unfavorable conditions for digestion. A marked difference was found in quinoline insoluble content and coal conversion between different ranks of coals. The lowest rank coal, sub-bituminous, generally resulted in the highest quinoline insoluble content and lowest coal conversions. The results of this study will be used to guide further research in coal liquefaction for the production of mesophase pitch.

SESSION 13 (12:35 – 14:15)
CARBON MANAGEMENT – 3
Nick Siefert and Bingyun Li

13.1 (12:35-12:55) Advanced Ceramic Membranes/Modules for Ultra Efficient Hydrogen (H2) Production/Carbon Dioxide (CO2) Capture for Coal-Based Polygeneration Plants: Fabrication, Testing and CFD Modeling

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Inorganic membrane-based systems are a promising technology for precombustion CO2 capture with simultaneous H2 production. State-of-the-art packages for high temperature and pressure service consist of multiple tube membrane bundles prepared in a "candle filter" configuration, in which the membrane tubes are open at one end and sealed at the other. This configuration is used for practical reasons, specifically the need to minimize problems due to thermal expansion mismatch between the ceramic tube bundle and the steel housing. However, the primary technical problem with the candle filter format for commercial-scale installations is the inability to purge the tube side (typically the permeate side), a feature that is crucial for high H2 recovery. In this study, the focus is to design and fabricate the first dual end open full ceramic multiple tube membrane bundle that enables tube side (permeate) purge for gas separation applications. An additional key feature of this design is the simplified module layout, as the membrane bundles can be installed end-to-end with tube side (permeate) flow directly from one bundle to the next. This layout simplifies membrane to housing seals and yields significant improvement in membrane packing density. Detailed focus areas in our studies include: (i) Materials development and preparation of the tube-to-tube sheet potting for the dual-ended bundle; (ii) the sealing and optimal module configuration design to minimize membrane stress upon module mounting; (iii) the demonstration, via the fabrication of CMS and Pd-alloy membranes supported on full-size, dual-ended ceramic support bundles, of the first example of a purgeable ceramic membrane and module; and (iv) development of a CFD model of the membrane module for calculation of feed flow distribution, and for use in scale-up, and capital cost estimating. The CFD model was validated using experimental data with the multi-tubular membrane system, employing He/N2 as a model gas mixture (surrogate for H$_2$/CO), and has been shown to be quite accurate. Employing the model, we are able to study the effects of operating pressure and temperature, feed and sweep gas flow rates, and the choice of membrane tube configuration on system performance.

13.2 (12:55-13:15) Review of techno-economic analysis studies using physical solvents for pre-combustion CO2 capture

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Novel physical solvent absorption processes have potential to improve the efficiency and economics of pre-combustion carbon capture, which will be required to meet future CO2 emission reduction goals. Commercial physical solvent absorption process like Selexol and Rectisol have been operating for many years to remove CO2 from natural gas streams. These commercial processes use hydrophilic solvents that remove both acid gases and water vapor from the gas stream and must be operated at low temperatures. For high pressure hydrogen rich gas applications such as IGCC-CCS and blue hydrogen production, there are processing and economic benefits to not removing water with the acid gases and operating the physical solvent absorption and regeneration processes at higher temperatures and pressures. To meet the needs of these newer applications, novel physical solvents including ionic liquids and hydrophobic solvents have been proposed for CO2 removal from high pressure syngas streams. However, to fully realize the technical benefits of these novel physical solvent processes, the economics must also be considered. Therefore, the aim of this presentation is to review the methods, assumptions and models used in techno-economic analysis (TEA) studies for CO2 removal from high pressure syngas streams using physical solvents.

When reviewing the literature for technical performance of novel solvents, it was found that although some physical solvents show promising performance at bench scale (e.g., high CO2 loading and low vapor pressure), other issues such as solvent viscosity or solvent cost may limit industrial implementation. Process simulations were found to be useful tools for modeling the technical performance, however, the predictions were only reliable when validated with representative experimental data. Additionally, it was found that more accurate baseline models are required for fair comparison among physical solvents. The key inputs and assumptions used for economic analysis were also summarized and found to vary significantly between studies making direct economic comparisons challenging. To improve confidence, more in-depth TEAs are required that use validated process models, transparent economic assumptions, and conduct comparisons to baseline technologies. These steps will be important for advancing the development of CO2 removal from hydrogen rich syngas as understanding both the technical and economic performance is an essential step for future demonstration and commercialization of novel pre-combustion carbon capture solvent processes.

13.3 (13:15-13:35) Investigation of potential cycling reaction mechanisms in CO2 solvents

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With the increase of carbon dioxide (CO$_2$) concentration in air, as well as the rising of global average surface temperature, it is critical to capture CO2 either from point sources (like power plants) or directly from air, since the complete elimination of fossil fuel consumption seems to be impossible in the foreseeable future. Among the several carbon management methods, namely solvent, sorbent, membrane, chemical looping, and cryogenic distillation, chemical solvent absorption is considered as the most promising technology for large scale deployment of CO2 capture. Amino acid salt (AAS) solvents were studied for CO2 capture due to their environmental friendliness, low volatility because of their ionic status, and excellent oxygen and thermal stability. Amino acids (AAs) dissolving in water generally need to be added with equimolar amount of alkaline substances (e.g., KOH) to deprotonate the -NH3+, making them reactive with CO2 in a manner similar to alkanolamines. However, very little is known about the reactions when more base is applied. This study determined the reaction mechanisms of AAS solvents

with base to AA ratio over equimolar and the potential benefits of such solvents for CO2 absorption. The CO2 loading capacity was found to be dictated by the molar concentration of the base and was approximately half of the base applied. The reaction mechanisms were investigated based on the compositions of carbamate, carbonate/bicarbonate, and AA using nuclear magnetic resonance. An innovative cycling reaction mechanism of CO2 absorption was proposed and experimentally confirmed for AAS solvents with base/AA > 1. Besides all steps of the current widely accepted Zwitterion mechanism, this reaction pathway also contains two cycles: 1) The extra base (i.e., OH-) reacts with the protonated AA generated during CO2 absorption to form deprotonated AA which further absorbs CO_2 to form more carbamate. 2) The carbamate, as a product of reaction cycle 1, undergoes hydrolysis to yield bicarbonate and deprotonated AA, which further absorbs CO_2. As a result, high CO2 loadings were achieved. Compared to the use of alkaline solutions like KOH alone for CO2 absorption, AAS solvents with base to AA ratio over equimolar resulted in lower pH and temperature while maintaining high CO2 loading. These innovative cyclic mechanisms will enable advanced CO2 management approaches using AAS solvents with base/AA > 1. The cycling reaction mechanism may also be applicable to other solvents like monoethanolamine (MEA).

13.4 (13:35-13:55) Pilot plant performance and process simulation of a hydrophobic physical solvent for pre-combustion CO2 capture

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Pre-combustion carbon capture using physical solvent absorption has been investigated at pilot scale with syngas produced from a fluidized bed coal gasifier at the University of North Dakota's Energy and Environmental Research Center. Two physical solvents were tested in the packed bed absorption column including polyethylene glycol dimethyl ether, or PEGDME, which is a hydrophilic physical solvent analog for the commercial process SelexolTM and diethyl sebacate, known as CASSH-1, which is a novel hydrophobic physical solvent developed by the National Energy Technology Laboratory (NETL). Hydrophobic solvents such as CASSH-1 have been shown to have favorable physical properties and good CO2 absorption performance while absorbing less water than traditional hydrophilic physical solvents. Additionally, thermodynamic efficiency and costs can be improved with hydrophobic solvents due to the potential to operate at or above room temperature which reduces the need to cool the syngas and allows regeneration of the solvent using waste heat rather than pressure swing. In this presentation, we will present solvent absorption performance results and process simulation outcomes from ten days of pilot plant operation at a solvent temperature of 25°C. The hydrophobic solvent CASSH-1 was found to absorb less water but had comparable CO2 absorption performance compared to the hydrophilic solvent PEGDME. The limited water uptake of CASSH-1 alleviates corrosion concerns and the general decline in selectivity observed with increased water absorption. An Aspen Plus process simulation developed with measured bench scale equilibrium data was validated with the plant performance data using both PEGDME and CASSH-1. This validated process model will be an important tool for further optimization and scale-up of hydrophobic solvent processes which have shown promise for lower cost carbon capture from high pressure gas applications.

13.5 (13:55-14:15) Techno-Economic Analysis of The Pre-Combustion CO2 Capture Process using Artificial Neural Network

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An artificial neural network (ANN) is developed to perform a techno-economic analysis (TEA) for pre-combustion CO2 capture applications. The ANN predicts the CAPEX, OPEX, and LCOC using properties of the solvent used, the plant power capacity, and the operating temperature. The ANN consists of 1 input layer consisting of 11 nodes, 2 hidden layers consisting of 10 nodes each, and 1 output layer consisting of 3 nodes. The ANN utilized data from previous works 1–4 to develop the weights and bias of the nodes. The hidden layers' nodes use the sigmoid transfer function while the output layer nodes use a linear transfer function. The parameters input to the ANN were normalized using the minimum and maximum values of each input that were obtained from previous works. The data was split randomly into training data and testing data, and it was found that the ANN can perform the TEA with a coefficient of determination (R^2) of 0.9961, 0.9994, 0.9995 for the CAPEX, OPEX, and LCOC, respectively.

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14.1 (12:35-12:55) Application and Development of X-MAT® Carbon Core Composites for Building Components

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The drastic reduction in quantities of coal feedstocks for electric power generation has caused economic hardship in coal-producing communities. There is particular concern with respect to the generation of carbon dioxide in the combustion of coal to produce electric power. Additional amounts of greenhouse gases such as carbon dioxide have been linked by some to climate change events.

X-MAT Research and Development activities with coal have been concentrated on usage of coal as a carbon feedstock for carbon conversion building products. There are several advantages of the X-MAT process over the traditional use of coal as a power source. The carbon conversion product, which uses up to 70% by mass raw coal powders, is a Carbon Core Composite which does not burn in an open flame due to the ceramic transformation process. Carbon Core Composites also have key advantages in terms of weight, durability, and strength over conventional alternatives.

The Department of Energy National Energy Technology Laboratory (NETL) awarded X-MAT CCC a Phase 1 Research contract to design a prototype structure using carbon conversion projects. Moreover, X-MAT CCC has recently won a NETL Phase 2 contract to build a prototype building section including two walls, a partial foundation, and partial roof. This building demonstration project will use carbon conversion products such as roof tiles, bricks, blocks, mortar, facades, panels, and insulation materials that are 50% derived from carbon from coal or coal waste. This talk will highlight the current status of the project.

14.2 (12:55-13:15) Manufacture of Carbon Foam in Continuous Process at Atmospheric Pressure

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

14.3 (13:15-13:35) Development of Competitive Supercapacitor Electrodes of Diverse Compositions from Coal Extract

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Recent demand for coal as a thermal energy source has decreased significantly and will likely continue to decrease as renewable sources of energy become more available and environmental concern and cost from burning coal makes it more costly than renewables. Given that Powder River Basin (PRB) coal in Wyoming has relatively low thermal energy, it is critical for Wyoming to employ coal in other capacities at the current energy transition period in history. Among many potential non-thermal applications, PRB coal can be utilized for membrane and electrode applications through the formation of carbon fibers. Coal-derived membranes can become low-cost, conductive membranes for use in electrodialysis separation processes. Carbon fiber derived electrodes have been shown be a cost-effective alternative to typical electrode materials that can meet or exceed the performance of current carbon electrode materials.

In this talk, we demonstrate the manufacture of supercapacitor electrodes from Powder River Basin (PRB) coal-derived precursors. Specifically, PRB coal was treated in cheap solvents and partitioned into liquid extract and solid residue. An electrospinning process has been developed that can convert either the liquid extract or the solid residue into carbon fiber mats. The electrospinning process is versatile with many tunable process parameters to achieve desirable physiochemical properties. For example, the coal residue can be manipulated by additional heat treatment, or by adding binders, salts, or surfactants to create a solution that can be electrospun into advanced carbon electrodes with desirable structural and surface properties. Similarly, some of the liquid extract (tar fraction) can be subsequently reacted with toluene diisocyanate to create resinous coal-derived polyurethane (PUs) as a spinnable ink. Carbon nanofiber mats made from our proprietary electrospinning process were further carbonized at temperature ranging from 700°C to 900°C before they are used as electrodes in supercapacitors. Galvanostatic charge-discharge (GCD) results show that the best performing PU fiber mats can deliver a specific capacitance of 604 F g-1 at the current density of 1 A g-1. A carbon fiber mat from a different solvent extraction residue also delivered the specific capacitance of 508 F g-1. These specific capacitance values are comparable to or better than commercial activated carbons, demonstrating the viability of manufacturing carbon nanofiber electrodes from coal without the use of a commercial polymer as binder in the spinning ink.

14.4 (13:35-13:55) Developing a Coal to Products Technology Portfolio

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At Ramaco Carbon we are working to bring into existence a new carbon economy with the mottos "coal is too valuable to burn" and "no molecule left behind." Our research focus is using coal (carbon ore) as a feedstock for a variety of high-value carbon products. We have developed a process and manufacturing technology portfolio including carbon fiber, porous carbons, nano-structured carbons (bulk graphene), building products, monolayer graphene, and rare earth elements (REEs). A review of these product lines, the associated processes, and economics will provide insight into the value of carbon ore as a feedstock for high-value and specialty products. We will present our current progress in manufacturing and tailoring the properties of porous carbons and nano-structured carbon to enhance existing products and produce novel products. Included is a discussion of the properties of carbon fiber derived from direct liquefaction of sub-bituminous coal, and from pitches produced by pyrolysis and solvation by supercritical CO2. New processes for converting carbon ore into structural building materials and monolayer graphene and the evaluation of REE deposits in a Powder River Basin thermal coal reserve will also be described. The presentation will provide a review of our carbon ore to products technology portfolio and the economic advantages of using carbon ore as a feedstock for advanced carbon products and several associated end use applications.

14.5 (13:55-14:15) Understanding the molecular architecture of mesophase pitches to generate a better carbon fiber precursor

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Coal is an abundant natural resource available across the world with high levels of reserves in the United States. Although coal has been used in large quantities as a fuel source, the chemical makeup of coal is well suited for higher-value uses. Coal-based materials are employed as precursors for advanced carbon materials, such as fibers, foams, and composites. Several methods have been investigated to extract the desired alkyl-aromatic compositions from coal. Direct coal liquefaction into gases and liquids has gained ground in the last half century. Pitches, the name given to the distribution of hydrocarbons, are classified into isotropic and anisotropic (mesophase). Isotropic pitches are composed of low molecular weight aromatics in mass range below 500 amu and significant amounts of aliphatic components. Mesophase pitches on the other hand are made of poly condensed aromatic molecules with greater than twelve aromatic rings. These planar aromatics align themselves to form an oriented structure, that make mesophase pitch the most sought-after precursor for high strength materials such as carbon fibers. However, the process of mesophase pitch preparation is guided by a multitude of factors such as extraction process, thermal history, source material and processing conditions of precursor material. Therefore, in this work, efforts were focused on understanding the chemical architecture along with physical characteristics of mesophase pitches obtained from three different precursor materials: coal, decant oil and naphthalene-based pitch. Optical imaging of pitches revealed that while decant oil-based pitch is composed of broader flow domains, coal based mesophase is made of finer mesophase domains. Infra-red spectral data showed a linear, alkyl substituted pitch from decant oil and naphthalene-based pitch. While coal-based pitch is made of peri-condensed aromatics. 13Carbon and proton Nuclear Magnetic Resonance (NMR) data also revealed a higher proportion of alkyl substituents in naphthalene based and decant oil-based pitches with lesser number of peri-condensed aromatics. Molecular stacking parameter obtained from combination of crystal size and d-spacing form X-ray diffraction analyses showed that decant oil and naphthalene-based pitches are composed of higher number (> 10) molecular layers resulting in a good quality mesophase. A systematic study using a suite of techniques at multiple length scales is ideal to generate a wholesome picture of mesophase. By performing such detailed study, we aim at establishing suitable synthetic pathways for generating a superior quality mesophase for high functional carbon materials.

SESSION 15a (14:25-14:45)
CARBON MANAGEMENT - 4
Nick Siefert and Bingyun Li

15a.1 (14:25-14:45) TEA OF A UNIQUE TWO-PATHWAYS PROCESS FOR CO2 CAPTURE FROM POST-COMBUSTION APPLICATIONS USING TWO AMINO ACID SALTS

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A unique process using two different amino acid salts (aqueous sodium glycinate solutions (SGS) and potassium glycinate solutions (PGS) for CO_2 capture from a split post-combustion flue gas stream from the 780 MWe Longview coal power plant, was developed in Aspen Plus v.10 using the rate-based model. The raw flue gas flow rate used for both solvents was 60.78 ton/h; and it contained 0.0033 mol% SO_2, 0.0035 mol% NO_2 and 12.02 mol% CO_2. The overall process was designed to remove all SO_2 and NO_2 and capture at least 90 mol% of the CO_2 in the flue gas stream. The chemical reactions between CO_2 and SGS and PGS leads to a phase change, including solid bicarbonate nanomaterials suspended in aqueous glycine solution.

The developed process includes four main units: washing unit (WU) for removing SO_2 and NO_2 from the split flue gas stream, CO_2 absorption unit (CAU) for CO_2 capture using SGS or PGS, ultrafiltration unit (UFU) for separating the solid bicarbonate nanomaterials produced, and reverse osmosis unit (ROU) for removing the dissolved ions from the washing liquid, deionized water (DIW). The WU and CAU were fixed-bed reactors containing Mellapak 250Y as packing. The constraints imposed on the process were: (1) complete removal of SO_2 and NO_2 and at least 90 mol% of CO_2 capture from the plant flue gas, (2) no flooding in the WU and CAU, (3) the ratio between the packing height to the reactor inside diameter (ID) should be greater than or equal 6 to avoid liquid and gas phases channeling and segregation in the fixed beds, and (4) the water content in the CO_2 stream intended for sequestration must be less than 600 ppm to avoid the formation for ice-like CO_2 hydrates in the transportation pipelines.

The process operates as follows: the raw flue gas enters from the bottom and the DIW enters from the top of the WU. The ions dissolved in the DIW are removed in the ROU and he polished (SO_2 and NO_2 free) flue gas directed to the bottom of the CAU to react with the amino acid solvent which enters from the top of the CA. The clean gas stream exiting the top of the CAU is continuously vented to the atmosphere, while the solvent CO_2-rich stream coming from the bottom of the CAU is further processed in two different pathways, pathway (i) the CO2-rich stream is regenerated in a stripper and the released CO_2 is compressed for subsequent sequestration in geological formation and the liquor is recycled back to the CAU; and pathway (ii) the solid nanomaterials in the CO2-rich stream are separated in the UFU and sold as high-value products to offset the cost of the overall CO_2 capture process.

At steady-state, Aspen Plus v.10 was used to calculate the hydraulics (flooding two-phase pressure drop, and liquid holdup) and mass transfer characteristics (gas-side and liquid-side mass transfer coefficients and the packing specific wetted surface area) in the WU and CAU. Also, techno-economic analysis (TEA) for the two pathways for each solvent, in terms of capital expenditure (CAPEX), operating expenditure (OPEX), and the Levelized cost of CO2 captured (LCOC), were calculated and compared. These calculations were made for a 15.6 MWe post-combustion power plant assuming a lifetime of 30 years, a discount rate of 10%, a capacity factor of 0.8, a capital recovery factor of 0.106, and an annual operating and maintenance (O&M) cost of 4% of the total CAPEX. It should be noted that the plant power plant was assumed to be directly proportional to the rate of the flue gas emitted.

The calculated hydraulics for the flue gas-solvent systems used indicated no flooding in the WU and CAU, and the gas-side mass transfer coefficients for CO2 in both solvents were orders of magnitude greater than the liquid-side mass transfer coefficients, indicating that the resistance to mass transfer is located in the liquid film. The pressure drops associated with the two-phase flow in the WU and CAU were 0.055 and 0.007 bar, respectively, and the behaviors of the liquid holdup and the packing specific wetted surface area were similar in both units.

For pathway (i), CO2 capture and sequestration, the calculated CAPEX, OPEX, and LCOC for SGS were ($12,413,127), (8,424 $/day), and (55.77 $/ton-CO2 captured) for SGS, and ($11,413,127), (8,088 $/day), and (51.51 $/ton-CO2 captured) for PGS. For pathway (ii), separating and selling solid bicarbonates, the calculated CAPEX, OPEX, and LCOC pathway (ii) were ($5,905,493), (6,472 $/day), and (37.11 $/ton-CO2 captured) for SGS, and ($5,853,103), (4,320 $/day), and (27.59 $/ton-CO2 captured) for PGS.

Comparing the two pathways for both SGS and PGS solvents showed: (a) the CAPEX values of pathway (i) were greater than that of pathways (ii) due to the former's costs associated with the need for a stripper, heat exchangers, and rotating equipment; and (b) the OPEX values of pathway (i) were also greater than that of pathways (ii) due to the former's higher O&M cost, and greater reboiler duty for solvent regeneration.

Comparing SGS and PGS solvents for pathways (i) and (ii) revealed: (a) the ratio between NaHCO3 produced (18.45 ton/h) and CO2 captured (9.67 ton/h) is 1.907 for SGS, and the ratio between KHCO3 produced (22.14 ton/h) and CO2 captured (9.73 ton/h) is 2.275 for PGS, (b) the CO2 reaction kinetics with PGS were faster than those with SGS, and subsequently lower solvent flow rates were required for PGS than SGS to meet the process constraint of capturing more than 90% of CO2 in the flue gas stream, leading to less reboiler and pumping duties, and smaller heat exchanger. In addition, the calculated LCOC values for both solvents in the two pathways indicted that LCOC values using PGS in pathway (ii) were the lowest, making it the most cost-effective pathway for CO2 capture from the Longview post-combustion power plant using these two amino acid salts.

SESSION 15b (14:45-16:05)
COAL ASH MANAGEMENT
Eric Grol and Allan Kolker

15b.1 (14:45-15:05) Spectroscopy-based Analysis of Fly Ash Interaction with Air-entraining Agents in Concrete

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Fly ash (FA), a coal-combustion residual (CCR) and a by-product from power generation facilities, has been extensively used as a supplementary cementitious material (SCM). However, fly ash tends to interfere with the use of air-entrainment agents (AEAs), which are important chemical admixtures used to increase air content (to about 6%) in concrete. A relatively new spectroscopy-based analysis will be presented on the adsorption properties of various fly ash materials when used with commercial AEAs. Furthermore, a quantitative study of AEA precipitate formation when used with ion-rich water and materials will be presented, along with a correlation between soluble AEA loss and foam index numbers. The relationship between AEA dosage and air content in concrete will also be discussed.

15b.2 (15:05-15:25) Development of Sorbents for Boron Capture from Coal Combustion Impoundment Leachates

John Findley, Jan Steckel, Evan Granite

In the United States, where approximately half of the generated coal combustion residuals (CCRs) are not used, there are about 300 active on-site landfills at coal-fired power plants. CCR landfills in the U.S. must monitor groundwater and control runoff. Impoundments can lead to elevated contaminant concentrations, particularly of arsenic, boron, barium, selenium, and strontium.

Zeolites can be readily synthesized from materials contained within the coal combustion ash impoundments and can be promoted or cation-exchanged to enhance adsorption capacity and reactivity. However, when the number of possible zeolite topologies, Si to Al ratios and number/type of cations are considered, the optimization of this material for maximum uptake of a pollutant becomes a daunting task. Molecular simulations provide methods that give physical insight into the adsorption process and can help guide the design of zeolite sorbents for contaminant removal. This work focuses on the development of models that can predict adsorption of boric acid in zeolites. Because of

the lack of experimental boric acid adsorption data available in the literature, boric acid and water model potentials were parametrized based on first-principles calculations for Na, K, Ca, Mn, and Fe-exchanged zeolites. These models were used to predict adsorption of boric acid from aqueous solutions, with boric acid concentrations that are comparable to those at CCR impoundment sites. The generated database was combined with machine learning methodologies to optimize the sorbent for boron uptake.

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15b.3 (15:25-15:45) Adsorption Properties of Functional Coal Combustion Residuals as Environmental & Energy Catalysts

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Maximizing the surface area of catalysts and their corresponding templates while minimizing the quantity of exotic and expensive materials used are important criteria in the manufacturing of large-scale catalytic devices. Instead of the traditional ceramic or metal substrates used for catalysts/supports, fly ashes and other CCR materials as catalysts/supports for environmental & energy catalysis applications could significantly expand their beneficial use in new markets involving a wide range of environmental remediation and energy harvesting technologies as well as existing concrete, mortar, or other cementitious applications. In this presentation, we will discuss the adsorption properties of fly ash systems with a wide range of carbon contents (e.g., 0-15%), including adsorption isotherm, adsorption kinetics, and adsorption capacity for different chemicals, including hazardous ones such as methylene blue. A new strategy for screening and developing suitable CCR materials with potential to be used as catalysts/supports will be proposed

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SESSION 16 (14:25-16:25)
RARE EARTH ELEMENT
Evan Granite and Allan Kolker

16.1 (14:25-14:45) Preliminary Review of Rare Earth Element (REE) Contents of Coal of the Southern Appalachian Basin

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Previous studies have shown that coal, as well as its enveloping sediments (underclays, roof strata, and shale interbeds) and waste materials, are promising sources of critical minerals and rare earth elements (CM-REE). While significant study is being conducted to evaluate the feasibility of coal and its associated sediments and waste materials as potential feedstock materials for these strategic elements, a thorough assessment of resources within the Southern Appalachian (SoApp) Basin (AL, TN, and GA) has not yet been undertaken. In this study, a comprehensive search of Geological Survey of Alabama (GSA) publications, the United States Geological Survey (USGS) CoalQual database, the DOE/NETL Energy Data eXchange (EDX) website, unpublished coal mining company records, and the published literature has been conducted and REE data

for coal resources have been compiled. For Alabama, Georgia and Tennessee, 1045, 44 and 22 REE data records were retrieved, respectively, for coal and its associated sediments or wastes.

The total REE+Y+Sc (REE+) concentrations of the retrieved sample records ranged between 4 ppm and 654.86 ppm, with an average of 98 ppm. The Gholson Coal bed, located in Shelby County, Alabama, recorded the highest total REE+ concentration (654 ppm), while the Mingo Coal seam, located in Claiborne County, Tennessee, recorded the lowest concentration (4ppm). Generally, coal samples from Tennessee recorded the lowest total REE+ concentrations. The concentration range, for each REE+ are as follows: Cerium 196.6-2.2 ppm; Dysprosium 25.4-0.28 ppm, ; Erbium 24-0.052 ppm; Europium 5-0.061 ppm; Gadolium 32.8-0.17 ppm; Holmium 26-0.081 ppm; Lanthanum 591–1 ppm; Lutetium 8-0.015 ppm; Neodymium 91.8-0.47 ppm; Praseodymium 73-0.92 ppm; Scandium 62-0.37 ppm; Samarium 26.5-0.21 ppm; Terbium 15-0.026 ppm; Thulium 11-0.045 ppm; Yttrium 136-0.25 ppm; and Ytterbium 13-0.1 ppm. Of these elements, Cerium, Lanthanum, Neodymium and Yttrium were present at the highest average concentrations (>10 ppm), while Ytterbium, Lutetium, Terbium, Europium & Thulium were present at the lowest average concentrations (<1 ppm).

This preliminary review of existing CM-REE data for the SoApp Basin has allowed identification of critical knowledge gaps. Evaluation of the compiled data reveals that bituminous coal is the primary characterized sample type and that only limited CM-REE data are available for coal-associated sediments and waste materials. This finding suggests that SoApp Basin coal resources are under-evaluated as potential sources of these strategic elements. Hence, additional work needs to be conducted to collect and characterize samples of coal-associated sediments and wastes of the SoApp Basin.

16.2 (14:45-15:05) The Department of Energy's Advances Towards a Sustainable CM/REE Supply Chain

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The US is import-dependent (>50% from foreign source) on 32 of the 35 critical minerals and import-reliant (100% from foreign source) for at least 14 critical minerals. The DOE established the Division of Minerals Sustainability to help address this problem as we move into a future with an increasing mix of clean energy technologies. The Division of Minerals Sustainability's vision and mission are focused on producing unconventional and secondary feedstocks containing critical minerals and carbon ore derived from previous mining operations, as well as other fossil energy-related byproduct streams, such as produced water from natural gas and oil operations. This approach will augment recycling efforts, which are projected to relieve the pressure on primary critical mineral supply but will not be sufficient to meet the demand required for electric vehicle and battery materials. Since 2014, the U.S. Department of Energy (DOE) Office of Fossil Energy and Carbon Management (FECM) and its national lab, National Energy Technology Laboratory (NETL), have been developing technologies to diversify the domestic supply and enable the reuse of coal waste and byproducts, particularly in the manufacturing of high value carbon products. These carbon products may include graphene, graphite, and carbon fibers. FECM and NETL launched the CORE-CM (Carbon Ore, Rare Earth, and Critical Minerals) initiative last year, aimed at catalyzing regional economic growth and job creation by addressing the upstream and midstream CM supply chain and downstream manufacturing of nonfuel, carbon-based products, to accelerate the realization of full potential for carbon ores and CMs within the U.S basins. 13 CORE-CM awardees across the US are currently working in their respective basins to regionally characterize their CM resource potential. FECM's RDD&D program activities for critical mineral production have demonstrated successful recovery of CMs from unconventional and secondary sources. Researchers have identified localities across the United States where coal by-products yield concentrations of rare earth elements deemed to be economically producible. The RDD&D program has identified opportunities for creating new critical mineral supply chains through upgrades to feedstock extraction, concentration, extractive metallurgy, reduction, and alloying. This includes three pilot-scale REE separation facilities that are producing kilograms of high-purity (~98%) Mixed Rare Earth Oxides (MREO). It also includes the pre-FEED studies for facilities designed to produce 1-3 metric tons/day of high-purity MREO. Over the next several years FECM will focus its efforts on building and strengthening sustainable critical mineral supply chains through unconventional and secondary sources that contain CMs and carbon ore. These efforts will work synchronously with strategies to support the commercialization of high-value carbon ore products to advance domestic clean energy manufacturing.

16.3 (15:05-15:25) Multi-bed Adsorption Study for the Fractionation of Critical Metals from Acid Mine Drainage

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Critical metals (CM), including rare earth elements (REEs), aluminum, manganese, cobalt, and others outlined by the U.S. Department of the Interior's Geological Survey (USGS), are essential to the national and economic security of the U.S. The reported >50% net import reliance of the U.S. on CM in 2020 by the USGS highlights that potential supply chain disruptions be mitigated with a domestic CM source. Because of the negative environmental impacts inherent with the conventional mining and processing of solid ores for CMs, adsorption-based recovery of naturally dissolved species from coal wastewaters is appealing. Acid mine drainage remains a relatively untapped source that can be rich in REEs, and especially in Al, Mn, and other CMs. Our work herein showcases a multi-packed bed reactor set-up for the removal and fractionation of different CM (and REEs) across eight Basic Immobilized Amine Sorbent (BIAS) beds in series from authentic aluminum-rich (~11 ppm) acid mine drainage (AMD). Lab-scale tests were performed to assess the effects of both treated AMD volume/BIAS ratio and AMD weighted hourly space velocity (WHSV) on the wt% uptake and % purity of different CM distributed across each of 8, 0.5 g sorbent beds. Results showed that a ratio of 3 L AMD/4 g BIAS and a WHSV of 0.1 min^{-1} gave 3.2 wt% Al uptake at >90% purity across multiple beds and 0.16 wt% Mn at 63% purity on separate beds. Meanwhile, iron was essentially eliminated in the first two or three beds. Increasing the WHSV to a practical 16 min-1 gave about 1 wt% Al uptake at >90% purity, whereafter elution with HCl gave an 80-89% pure Al stream. Translating these AMD/sorbent ratios and WHSV parameters to a field test at the Pittsburgh Botanic Garden (PBG), using 140 g of BIAS to treat 90-100 L of AMD in an eight-bed setup, gave 0.45 wt% Al uptake at >80% purity. Subsequent elution of the Al (lab-scale sample) gave a >70% pure Al stream, whose pH could be raised to precipitate Al(OH)3 that can be filtered and recovered as a solid. Ongoing work aims to find alternative AMD sites enriched with either REEs or other CM, and to perform additional field tests at these sites. Overall, our work shows the viability of recovering CMs from AMD and other coal waste streams, using a multi-bed adsorption system that can also employ a selective elution technique to achieve highly purified metal resources.

16.4 (15:25-15:45) NdFeB Permanent Magnets: Sector Usage Translated to Rare Earth Oxide Demand

Randy Vander Wal, Professor, Penn State University, USA

Across consumer, defense, manufacturing and power generation sectors, rare earth based permanent magnets are prevalent for their superior coercivity. Nominally referred to as NdFeB magnets, the short acronym misses the Praseodymium, Pr and Dysprosium, Dy content, and occasional inclusion of Terbium, Tb. The supply of Neodymium, Nd is limited with the US having no domestic production of rare earths and little permanent magnet manufacture. Hence imports in the form of the REE oxide, intermediate and end products are essential to fulfilling demand. Unfortunately, this results in missed manufacturing and economic opportunity. This presentation relates permanent magnet consumption to specific rare earth quantities required across major demand sectors. The distribution of Nd and Dy across application sectors is shown in Fig. 1 [1]. With exception of a couple material uses for Dy (glass, ceramics, catalyst), their applications are identical – underscoring their common usage in NdFeB magnets.
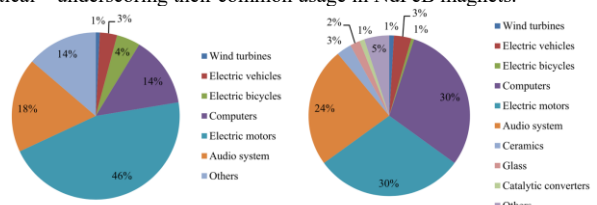

Figure 1. Share of end-use sectors for Nd (right) and Dy (left). Source reference [1]

Consumer electronics, including computers encompasses a broad category of computer, CD and DVD hard drives in addition to the ubiquitous cell phones. Though the nominal NdFeB magnet content in consumer electronics, e.g., computer hard drives, cell phones, speakers, etc. is small, nevertheless for this sector the global market share is 29% of NdFeB demand, a testament to the global consumer base which continues to increase. For wind, differentiation is made between gear-box versus direct drive and on-shore versus off-shore siting, the latter using preferentially using permanent magnets. The Global Wind Energy Council estimates roughly 75 GW on-shore and 6 GW off-shore capacity will be added annually, through 2026 [2]. Electric vehicles (EVs) equipped with permanent magnet motors and electric bicycles comprise the transportation contribution. For electric vehicles, permanent magnet motors have gained nearly 100% market share among vehicle manufacturers worldwide as the leading technology. Industrial, professional service and personal robots, most using permanent magnets are also included in the projected global need for Nd and Dy. The international robotics federation (IFR) projects significant growth across robotic categories with the industrial annual growth rate, AGR at 9%, service at 10% and consumer robots at 12%. Across these sectors, Nd and Dy future demand through 2050 is calculated using a compounded annual growth rate coupled with magnet weight and rare earth content. Uncertainties in the estimates are considered such as true global production of Nd, fragmented markets in each sector, varied magnet compositions and range of usage for any end use product or unit scale. Figure 2 illustrates the aggregate NdFeB demand across multiple end use applications through 2030 by our initial analyses.

With total rare earth oxide (TREO) production in 2020 estimated at 240,000 tons, the Nd/Pr oxide amount of 46,000 tons is consistent with an overall ore fraction of ~ 19%. For the sectors evaluated in the analysis, wind turbines (on- and off-shore), electric vehicles, electric bicycles (EBs) and scooters, global cell phone and consumer electronics, industrial and service robots, industrial motors, the cumulative Nd/Pr demand across all these sectors is 49,924 tons, within 10% of the USGS estimate for TREO in 2020. Notably the fastest growth opportunities are the permanent magnets in industrial robots and consumer electronics followed by wind turbines. These preliminary analyses used an AGR for on-shore wind of 6.1% and off-shore of 8.3% and a 10% blended AGR across all robotic sectors. Surprisingly, electric vehicles are not the dominant driver for increased Nd/Pr oxide (using a modest AGR of ~ 5%). Partially accounting for this is that current light vehicles already use rare earth permanent magnets for power steering, power door locks, power window lifts, cruise control, power steering, automatic mirror positioning, fluid pumps and sensors, electric brake actuators, and power seats among many others. As most of these uses are likely to carry over into electric vehicles their contribution to permanent magnet demand is effectively constant as declining gasoline/diesel passenger vehicles are offset by corresponding increasing EV sales.
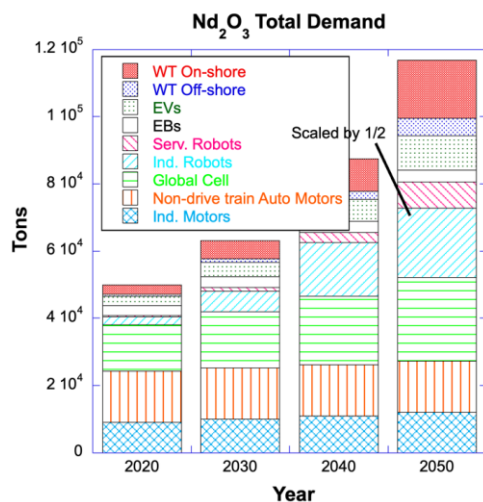
Figure 2. NdFeB magnet demand by application for the indicated market sectors.

While rare earths used for magnets (neodymium, praseodymium, dysprosium, and terbium) constitute only 25% of the total rare earths production volume, they represent 80% to 90% of the total rare earths market value. More than 90% of rare earth magnets are produced in China today. In China, the rare earth value chain is a highly strategic asset to secure a growing market share in major downstream industrial ecosystems. In 2020, an estimated 122,000 t of rare earth permanent magnets (NdFeB) were produced worldwide [3] which corresponds to a market volume of about $14.4 billion [4]. Roughly 93% of these magnets were produced in China, reflecting a very high production concentration (which is, in fact, found across all rare earth value chain steps, from mining to recycling). In addition, rare earth magnets are increasingly imported as part of motors and generator assemblies and products.

Lately, this has been demonstrated by the new Chinese "Export Control Law", effective since December 2020. The largest rare earths mining and processing companies are

state-owned and are sustained by various direct and indirect state subsidies. The combination of a lack of diversified rare earths supply chains and the exponential growth in the demand for high performance permanent magnets, particularly in automotive and renewables, creates the perfect conditions for supply chain disruptions. Whilst the rare earth permanent magnet market itself is relatively small – about $14.4 billion – its downstream leverage is enormous. In addition, there is the strategic importance of rare earths for defense applications. A circular economy around rare earths needs to be created by advancing recycling and substitution, as well as exploration, mining, processing, separation, metal making, alloying, magnet making, and motor design.

The economic importance of the rare earths value chain becomes obvious by looking at the emerging electric vehicle market: over the last decade, the evolution of technology has resulted in 95% of EVs using permanent magnet motors by 2019, particularly because they provide the highest energy efficiency which translates into drive range. In 2019, about 5,000 t of rare earth permanent magnets were used in EVs worldwide. By 2030, the number may rise to between 40,000 and 70,000 t on a global level, depending on the anticipated growth scenario. A global EV market worth of about $600-900 billion would depend on securing access to sustainably produced rare earth magnets – a comparatively small but specialized market of about $2-3 billion (value corresponding to magnet volume share needed in the EV sector). (Assumptions for the calculation are that the global electric vehicle market will have grown to 20-30 million cars per year by 2030, including battery electric and plug-in hybrid electric passenger, light duty vehicles; average price per car is $30,000; NdFeB use per EV is 2 kg; average NdFeB price is $50/kg.) As indicated above, this pattern is reflected in other industrial ecosystems: energy efficient electric motors are also needed in fuel cell electric vehicles and domestic appliances, like energy efficient refrigerators, washing machines, and dishwashers; rare earth containing wind turbines are gaining market share, particularly in offshore wind farms due to their robustness and efficiency; all speakers of mobile devices use rare earth magnets due to the need for miniaturization.

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1. K. Habib, H. Wenzel / Journal of Cleaner Production 84 (2014) 348-359.
2. Global Wind Report 2022. https://gwec.net/global-wind-report-2022/
3. Estimates based on Roskill 2018 and consolidated reports by REIA 2021.
4. The $14.4 Billion Worldwide Rare Earth Magnet Industry to 2026, ResearchAndMarkets.com

16.5 (15:45-16:05) Yampa Coal Field Revisited – Rare Earth Elements and Critical Minerals

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Our 2019 PCC abstract (Kolker et al., abstract 9.1), noted the possible occurrence of rare earth element (REE)-enriched coals in the Yampa coal field, northwestern Colorado, USA, as a geologic analogue to the Appalachian Basin Fire Clay coal. In both coals, airfall deposition of volcanic ash occurred during the coal-forming sequence. The Yampa coal field contains a prominent, regionally extensive tonstein, the Yampa Bed, within the Upper Cretaceous Mesaverde Group. Reconnaissance sampling included Yampa Bed core, and two benches of the overlying, actively mined Wolf Creek coal interval, which also contains volcanic ash. For coal samples, float/sink gravity separates were prepared at a density of 1.5 g/cm3 to investigate critical mineral (CM) element partitioning between raw coal, prepared coal, and inorganic-enriched waste products from coal preparation.

REE contents for the Yampa Bed, including Y and Sc, are 77-81% of the 300 ppm U.S. Dept. of Energy (DOE) interest level, with near upper continental crust (UCC) distributions for middle and heavy rare earth elements (MREE, HREE), and pronounced enrichment in light rare earth elements (LREE; Figure). Conversely, a black shale underlying the Yampa Bed has near-UCC LREE and MREE, and relative enrichment in HREE. Non-REE CMs Zr, Nb, Cs, and Hf show enrichment at near-UCC levels, like that of the REEs. Coal sink fractions show enrichment in both REEs and CMs. While total REEs in the Yampa Bed and associated coals are below DOE interest levels, this may be offset by the tendency for REEs in western coals and their ashes to be readily extractible.
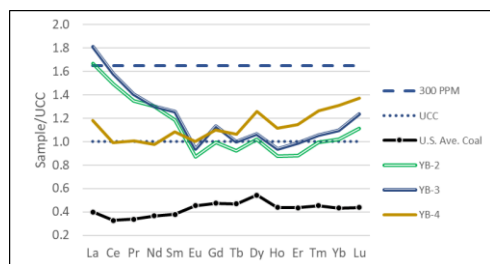
Figure. Lanthanide REEs in the Yampa Bed tonstein (YB-2 and YB-3) and underlying black shale (YB-4), normalized to upper continental crust (UCC). Reference 300 ppm DOE interest level shown assumes a UCC element distribution. U.S. average coal from Finkelman, 1993; UCC from McLennan, 2001.

16.6 (16:05-16:25) Material Intensities and Growth Rates versus Supply Chain Constraints

Randy Vander Wal, Professor, Penn State University, USA

Low-carbon power generation to meet climate goals requires substantial increase in REEs and CMs. The rising demand is offsetting decreasing production costs. Developing new supplies is challenging; on average over 16 years is required to move mining projects from discovery to first production.

An energy system powered by clean energy technologies differs profoundly from one fueled by traditional hydrocarbon resources The transition to clean energy means a shift from a fuel-intensive to a material-intensive system. The types of mineral resources used vary by technology. Lithium, cobalt, and nickel play a central role in giving batteries greater performance, longevity, and higher energy density. Rare earth elements are used to make powerful magnets that are vital for wind turbines and electric vehicles, EVs.

These characteristics of a clean energy system imply a significant increase in demand for minerals as more batteries, solar panels, wind turbines and networks are deployed. It also means that the energy sector is set to emerge as a major force in driving demand growth for many minerals, highlighting the strengthening linkages between minerals and clean energy technologies.

Recent studies have projected the REE and CM demand for renewable energy (solar and wind) and "clean" technologies such as electric vehicles to meet particular climate scenarios based on current climate models. Most notably are those by the IEA with results shown in Fig. 1 for the role of critical minerals in clean energy transitions [1]. The relative demand growth is particularly high for battery-related minerals. Yet the material intensity factors are not reported, instead there is an extensive annex of references. Even with these, the question is what end-product types and blend have been included in the calculation. And what scale of power generation or displaced energy consumption underlies the net element or mineral projection? Elsewhere the number of units (EVs, solar panels or wind turbines) is not given, only total element and mineral tonnage requirements.

For such changes in energy supply and transportation to be realized, the supply chain must be expanded or for many REE and CMs in the U.S., will need to be created. Therein comparison should also include relative economic value. Market growth rates need to be adjustable to reflect physical constraints along the supply chain, market factors, and overlapping elemental and mineral requirements across these end-use sectors. Thus, detailed knowledge of material intensities, intermediate or subcomponents and required supplies under different demand / growth scenarios is necessary. This presentation will survey these values for the listed clean-tech areas.

Figure 1 – Relative growth in demand for selected minerals for clean energy technologies in 2040 relative to 2020 levels [1].

Reference
1. IEA Report, The Role of Critical Minerals in Clean Energy Transitions. p. 50, (2021).

17.1 (8:05-8:25) Study on mineral transformation during the thermal conversion of Zhundong high-alkali coal via FactSage software

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The information about the mineral transformation is of great importance to solve the ash-related issues, which contributes to the large-scale utilization of Zhundong high-alkali coal. Although lots of related work has been carried out by many researchers, their studies usually have been restricted to serval specific coals. Given the fact that Zhundong coals are significantly different in ash composition, universal knowledge of mineral transformation that applies to more kinds of Zhundong coal is required. In our previous work, the ash compositions of over 250 Zhundong coal samples were collected, and then the range and average of each composition were obtained. Based on the statistical data, the FactSage software was employed in the present research to study the mineral transformation with the temperature varying from 500 oC to 1500 oC. The simulation results show that melilite (Ca2MgSi2O7) accounts for a large part with 1% Na2O, while merwinite (Ca3MgSi2O8) is the main mineral when the Na2O content increases (1-13%) and some minerals with low melting points like nepheline (NaAlSiO4) are obviously observed. Nepheline is the main mineral in the cases of 2-16% CaO, but its proportion decreases with a rise in CaO content (16-40%) and merwinite becomes more. The content of merwinite with high melting point decreases when the Fe2O3 content rises from 0 to 30%, implying that Fe2O3 leads to the decline of ash fusion temperature. More silicates and aluminosilicates are found with the increasing SiO2 content (5-50%). When the Al2O3 content increases (5-35%), the production of merwinite is suppressed while gehlenite (Ca2Al2SiO7) becomes more. The reactions among basic oxides (Na2O, CaO, Fe2O3), SiO2, and Al2O3 were also investigated using ternary phase diagrams. The present study could provide more general information about mineral transformation, which helps to alleviate the ash-related issues and promotes the utilization of Zhundong coal cleanly and safely.

17.2 (8:25-8:45) Evaluation on physicochemical properties of BRDF for utilization as fuel in thermal power plant

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Biomass is an important energy source in the power generation sector. Biomass is considered as one of the solutions to reduce greenhouse gas emissions in the energy sector. Recently, a 125 MW biomass power plant in South Korea is operating using 600,000 tons of wood pellets annually as fuel for power generation. This waste generated during the power generation process is called biomass refuse derived fuel (BRDF). In

this study, considered applicability with BRDF as a fuel in thermal power plants. These BRDFs are large biomass particles that are difficult to burn completely and are disposed of in a bottom ash hopper during generating process. To evaluate the recyclability and applicability of this BRDF, this study investigated the fuel properties compared to other fuels through physicochemical analysis. The fuel characteristics of the raw wood pellet and torrefied wood pellets used as fuel were compared with BRDF. In this study, physicochemical properties of each sample were analyzed and compared through thermally treated biomass grindability index (TTBGI), Fourier transform infrared spectroscopy (FT-IR), and thermogravimetric analysis (TGA). TTBGI method modifies the HGI test to consider the low bulk density of biomass and is calibrated to the same scale with HGI. In the TTBGI method, the powder of biomass sieved between 0.6 and 1.18 mm is ground and the mass fraction below 500 μm is determined using a sieve for the sizing. TGA pyrolysis experiments were conducted under N2 atmosphere with the heating rate of 10 K/min, and the temperature at the range of 300 - 1073K. In addition, a TGA combustion experiments were performed at the same temperature range and heating rate as the pyrolysis experiment in a 21% O2/ 79% N2 atmosphere. As a result of the proximate analysis, the fixed carbon amount of BRDF increased compared to the raw wood pellet, and the volatile matter content decreased. The carbon content of fuel after torrefaction increased by 10% and BRDF increased by 40% in the ultimate analysis. Whereas the oxygen content of fuel after torrefaction decreased by 10% and BRDF decreased by 40%. As a result of grindability and calorific value analysis, it showed increase than that of the raw wood pellet. TGA experiment showed that the lignin fraction of the raw wood pellet at 19% and the BRDF lignin fraction increased by 92%. It was predicted that combustibility would deteriorate. However, the experimental results through TGA showed combustion characteristics similar to those of raw wood pellets. This is due to the alteration in properties as the specific surface area of the sample increases. Therefore, the study results suggest that the BRDF is usable as a fuel in thermal power plant.

17.3 (8:45-9:05) Overview on Mercury Control Options for Coal-Burning Power Plants

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With the USEPA issuing a national regulation requiring high levels of mercury capture, the need exists for low-cost removal techniques that can be applied to coal-burning power plants. The injection of powdered activated carbon into the ductwork upstream of the particulate control device is the most developed technology for mercury capture. Alternative techniques for mercury capture also play a role because of the numerous configurations of air pollution control devices present within the power plants, as well as the many different coals and coal-blends being burned. These methods employ sorbents, catalysts, scrubber liquors, flue gas or coal additives, combustion modification, flue gas cooling, barrier discharges, and ultraviolet radiation for the removal of mercury from flue gas streams. The DOE Mercury Program was an enormous success, spurring continuing development, demonstration, and commercialization of many technologies for the capture of mercury.

An overview of current and alternative technologies for mercury capture from coal-derived flue gas will be provided. In addition, six methods for mercury control within coal-derived flue and fuel gases have been recently developed at NETL and will be discussed. The on-going research needs for mercury control include improved sorbent-flue gas contact, development of poison-resistant sorbents and catalysts, novel sorbent promoters, new scrubber additives for retention of mercury within wet FGD systems, concrete-friendly activated carbons, new continuous measurement methods, benign coal additives, byproducts research, and exploration of international markets.

17.4 (9:05-9:25) Mitigation of Aerosol Impacts from Coal Combustion processes

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Combustion of fuels with high levels of alkali species can result in significant fouling of heat-transfer surfaces, reducing boiler efficiency and increasing maintenance costs. The formation of sulfur-based compounds with alkali elements has been identified as a major fouling contributor, by acting as a bonding medium for coal ash leading to deposit growth on heat-transfer surfaces. Methods such as fuel blending/ switching and extensive combustion monitoring are currently employed to mitigate these types of fouling. However, targeted solutions that eliminate alkali vapors from the combustion process can be a viable solution to mitigating these deposit growths. This paper describes laboratory scale experiments on a 10-kW down-fired combustor to demonstrate the effectiveness of using low-cost alkali sorbents to capture vaporized alkali species released during the combustion of high sodium fuels. Size-segregated ash samples are collected using gravimetric impactors and analyzed to determine the ash chemical composition, size distribution and fate of the alkali species, as these correlate with their propensity to act as fouling agents.

17.5 (9:25-9:45) CFD study of a 100-kW flame burning coal water slurry made from fine coal

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TDA Research, Inc. is developing a process to directly combust the fine coal from coal waste. The technology has been demonstrated in a 19-kW combustor and will soon be tested in a 100-kW combustor. CFD simulations has been conducted for the 100-kW burner to show stable flames can be maintained for coal water slurry by the strong external recirculation. Multiple Rosin-Rammler (R-R) distributions were assumed for the droplets in the model with the mean diameter of 65 μm. The char burnout reduces as the spread parameter reduces, which indicates a wider distribution of particle size in the R-R distribution. Two cases with different atomization flow rates were compared. The char burnout for the case with lower atomization flow is higher.

SESSION 18 (8:05-9:25) CLEAN COAL AND GAS TO FUEL
Dan Connell and Andreas Ritcher

18.1 (8:05-8:25) Phenanthrene Hydrogenation Saturation over Ni-Co/NiAl2O4 Catalyst

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There are about 4~6wt% phenanthrene existing in high-temperature coal tar, and they are not well utilized in recent years. One of the promising utilizations of phenanthrene is to prepare perhydrophenanthrene via hydrogenation saturation. Perhydrophenanthrene is an ideal component of jet fuel because of its high density and high energy, furthermore, perhydrophenanthrene can be isomerized to produce adamantane with better performance fuel. However, hydrogenation of phenanthrene to perhydrophenanthrene is difficult, especially the hydrogenation of symmetrical octahydrophenanthrene is the rate-control step of phenanthrene to perhydrophenanthrene, which was ascribed to the large steric hindrance of symmetrical octahydrophenanthrene, resulting in the difficulty in absorbing and activating on the surface of catalyst. In order to solve this problem, the key point is to develop a kind of saturation catalysts with high activity, which can overcome the steric hindrance and promote the hydrogenation of symmetric octahydrophenanthrene. Traditional transition metal sulfide catalysts had strong sulfur resistance, while its hydrogenation saturation capacity was weak. Noble metal catalyst had the advantage of strong hydrogenation saturation capacity, while their high cost limited their application. Compared to single metal component catalysts, bimetallic catalysts exhibit superior catalytic reaction performance due to their synergistic effect. In this work, a series of Ni-Co/NiAl2O4 catalysts with different Co loading were prepared by impregnation method. By evaluated at 300 °C, hydrogen pressure of 5 MPa, WHSV of 52 h-1, the Ni-2Co/NiAl2O4 catalyst

(Co doping content was 2 wt.%) obtained the phenanthrene conversion of 9.0 mmol·g-1 active component·h-1, and the maximum selectivity of perhydrophenanthrene was up to 91%, which was higher than that of Ni/NiAl2O4 (the maximum selectivity of perhydrophenanthrene was about 80%). According to the analysis of catalyst structure, it is found that the formed NiCo greatly contributed to the superior hydrogenation performance. Co doping promotes the reduction of Ni and provides more active sites. The unique electronic characteristics of NiCo alloy could strengthen aromatics adsorption, and finally enhanced the hydrogenation saturation performance of the catalyst.

18.2 (8:25-8:45) Effect of pore structure on Ni2P/Al2O3 catalyst for hydrogenation saturation of phenanthrene

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Phenanthrene, a typical polycyclic aromatic hydrocarbon in coal tar, has an annual output of 900,000 tons. It is usually used to produce carbon black materials, which has not been reasonably used, thus reducing the added value of phenanthrene. Perhydrophenanthrene, the product of hydrogenation saturation of phenanthrene, can be used as an ideal component of jet fuel enhancing the utilization of phenanthrene. Ni2P catalyst has attracted extensive attention in the hydrogenation field because of its strong sulfur and nitrogen resistance and excellent hydrogenation activity. It is known that the properties of the support strongly affect the catalytic active components, and then affect the catalytic performance of the catalyst. In this work, three Al2O3 supports with different pore sizes (9.6 nm, 23.1 nm, 36.3 nm) were selected to prepare Ni2P/Al2O3 catalysts via the thermal decomposition of hypophosphite. Based on the exclusion of internal and external diffusion, the effect of pore structure on the catalytic performance of Ni2P/Al2O3 catalysts for hydrogenation saturation of phenanthrene was investigated. At the temperature of 320 □C, pressure of 5MPa, hydrogen oil ratio of 600, weight space velocity of 52.4h-1, Ni2P/Al2O3 catalyst with a pore size of 23.1 nm displayed superior hydrogenation activity with the phenanthrene conversion of 99% and the perhydrophenanthrene selectivity of 42%. The catalysts were characterized by N2 physisorption, NH3-TPD, CO chemisorption. It is found that all catalysts had almost the same physicochemical properties, such as the specific surface area (162.02 m2/g, 155.43 m2/g, 152.78 m2/g), apparent morphology, microstructure, acidity, and only different in the pore size. The results of CO chemisorption showed that when the pore size of Al2O3 ranged from 9.6 to 23.1nm, the CO adsorption capacity of the catalyst increased from 4.53 □mol/g.cat to 12.21 □mol/g.cat. With the further increase of pore size to 36.3 nm, the CO adsorption capacity of the catalyst decreased to 6.08 □mol/g.cat, indicating that Ni2P/Al2O3 catalyst with a pore size of 23.1 nm had the most active sites. Furthermore, Ni2P/Al2O3 catalyst with a pore size of 23.1 nm obtained the highest metal dispersion (1.64%). It can be concluded that appropriate pore size can promote the dispersion of active sites and influence the amount of active sites, finally improve the hydrogenation activity of Ni2P/Al2O3 catalyst.

Keywords: nickel phosphide; phenanthrene hydrogenation; pore size; active sites

18.3 (8:45-9:05) Road Map for Producing SNG from Thar Coal in Pakistan

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Pakistan has a state-of-the-art Natural Gas transmission and distribution network that covers the entire land. After the discovery of huge gas reserves (12 TCF) in the year 1952 the nation remained energy surplus. However due to mismanagement and lack of new discoveries the country now faces serious shortages (2000 mmcfd) which is being met through imported LNG (Liquified Natural Gas). After the natural gas find in 1952, Pakistan has now discovered a massive coal reserve at Thar (175 billion Tons). An integrated system has been prepared to ensure Energy Security; Road Map has been prepared to produce SNG (Synthetic/Substitute Natural Gas) from the available 'Black Gold'. The Dakota Gasification Company model is being followed. Bench studies will be conducted in South Africa followed by Pilot Plant (100 mmcfd) at Karachi the

commercial hub of the country. To ensure autarky in this vital area the indigenously produced SNG can replace the imported LNG.

18.4 (9:05-9:25) Thermo-catalytic Decomposition of Methane to Produce Hydrogen Fuel Using Carbon as Catalyst

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Thermo-catalytic decomposition (TCD) is well-suited for the generation of hydrogen from natural gas. In this decarbonization process for natural gas—solid carbon is produced, with potential commercial use as energy storage media. TCD rates and carbon catalyst stability vary widely across carbons. Regeneration remains rarely investigated but does appear necessary to maintain long-term TCD activity in a cyclic TCD–partial oxidation sequence. Presently, there are no studies that have made fundamental connections between active sites and deposition rates. Accordingly, TCD measurements were performed using a hot wall reactor with silicon and quartz deposition substrates. The test matrix encompassed a series of temperatures (700 – 1,100 ℃) and reaction durations Deposition rates were measured periodically for determination of deposition rate by deposit thickness, using scanning electron microscopy (SEM). The nanostructure of the deposit was evaluated using transmission electron microscopy (TEM). At selected stages during TCD, samples were subjected to activated chemisorption in preparation of active site measurement. Active sites were quantified by X-ray photoelectron spectroscopy (XPS).

Keywords: Thermo-catalytic decomposition, pyrolytic carbon, hydrogen, active sites, nanostructure

Thermo-catalytic decomposition (TCD) of methane is an attractive alternative for hydrogen production in relation to conventional steam reforming. In addition to generating clean hydrogen, TCD does not produce CO/CO2 by-products or consume water resources. Moreover, the energy requirement for methane cracking (37.8 kJ/mole of H2) is less than that of steam reforming (75.6 kJ/mole of CH4) [1,2]. TCD offers several technical and societal benefits, including the decarbonization of fossil fuels, providing a bridge to the H_2 economy and allowing for the coupling/storage of renewable energy into chemical bond energy. Beneficially TCD produces elemental carbon, negating the need for CO_2 capture storage with potential to realize at-scale carbon sequestration. Moreover, the solid carbon has commercial value as energy storage media or adsorbent material.

Although TCD is suitable for production of hydrogen from natural gas, at present, the primary barrier for TCD is the inability to maintain long-term carbon catalyst activity. Muradov et al. examined several types of carbons such as carbon blacks, activated carbons, and carbon allotropes. Their studies showed that the activity of the carbons depended on the degree of disorder inherent to each carbon form. More disordered forms of carbon showed higher activity compared to ordered ones. Yet regardless of the initial activity, the TCD activity of these carbons decays with time-on-stream. [2].

Given the ever-present declining rates in TCD, regeneration by partial oxidation is a potential solution decreasing activity. If active site loss is responsible for decreasing TCD rate, then active site gain by partial oxidation should increase the subsequent TCD rate in a cyclic process. Key to testing this hypothesized correlation and assessing the relation between rate and active sites is the measurement of active site number. For this we have chosen XPS rather than temperature programmed desorption (TPD). XPS has three key advantages for active site determination when coupled with chemisorption, compared to thermal programmed desorption using thermal conductivity detection – the commonly used technique. First, XPS is quantitative for oxygen content (at. %), second, XPS has better sensitivity (~ 0.1%) and third, XPS directly measures chemisorbed oxygen rather than derivative reaction products (CO and CO₂) as in TPD. Therein it also differentiates oxygen groups, which otherwise can be scrambled by interconversion during the high temperature ramp used in TPD. Before applying chemisorption – XPS analysis to measure active site loss in TCD, we are testing the methodology against partially oxidized carbons – for which active sites are known to increase upon partial oxidation. Here carbon blacks with well characterized nanostructure and oxidation behaviors are used as model materials and surrogates for TCD carbon deposits, as prepared via a chemical vapor deposition process.

TCD measurements were performed using a hot wall reactor using flat quartz substrates as deposition substrates. Deposition rates were measured periodically for determination of carbon deposition rate by deposit thickness, using scanning SEM. Methane diluted in an argon carrier served as the initial feed. At selected durations in the deposition process, the reaction was stopped for active site measurements through XPS.

As kinetic rates are mapped, they are related to active site number for each of the two processes. Nanostructure is also being assessed to identify correlations with kinetic rates. Nanostructure is an easier metric with which to gauge carbon catalyst activity and deposition rate, in comparison to chemisorption followed by XPS, an approach requiring two techniques and more definitive than TPD. For reference there is considerable literature precedence using nanostructure for interpretation of soot oxidative reactivity [4-6]. Here nanostructure is used to gauge the efficacy of carbon catalysts prior to TCD testing.

TCD provides a pathway to the hydrogen economy, as provides a bridge from fossil fuel to renewable hydrogen energy systems. In a decarbonization process for fossil fuel—pre-combustion—solid carbon is produced, with potential commercial uses including energy storage.

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SESSION 19 (9:55 – 10:15)
COMBUSTION TECHNOLOGIES – 2
Alberto Pettinau and Evan Granite

19.1 (10:35-10:55) Influence of various conditioning agents on the fly ash resistivity of South African power plant fly ashes.

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South Africa operates an energy intensive economy with coal contributing around 80% the country's energy mix. Increasingly stringent particulate matter (PM) minimum emissions standards as promulgated by the National Environmental Management: Ambient Air Quality Act (Act no. 39 of 2004), necessitates performance improvements of current particulate matter (PM) emissions abatement technologies at South African coal-fired power stations. Electrostatic precipitators (ESPs) are used at many of the South African coal-fired power stations, and the resistivity of the fly ash is one important factor that impacts the efficiency of ESPs. The chemical composition of fly ashes has been found to highly influence the resistivity of the fly ash, which can be controlled by the introduction of conditioning agents such as moisture, sulphur trioxide (SO_3), and brine injection into the flue gas upstream of the ESP.
In this study, the effect of injecting different conditioning agents on the resistivity of fly ash sampled at various South African power stations using ESP as PM abatement technology were investigated. Fly ashes from these power stations were treated with various conditioning agents, including doping with a synthetic brine solution with composition similar of that used at one of the coal-fired power stations. Additionally, the ambient moisture concentration was varied to characterise the combined effect of moisture and other conditioning agents on the fly ash resistivity as a function of temperature. A comparison of the individual and synergistic effect of these conditioning agents on the fly ash resistivity was conducted and presented.
All three fly ash conditioning agents resulted in the reduction of the fly ash resistivity within the surface resistivity region (< 200 ℃) which was more significant for the SO_3 injection conditioning method. The determination and quantification of the influence of these conditioning agents under varying levels of moisture were also conducted and reported. The elemental composition of the sampled ashes was also used, along with the standard Bickelhaupt predictive model to determine the theoretical resistivity values. The standard Bickelhaupt model showed deviations of several order of magnitude

between the experimental and theoretical resistivity values, with the model overestimating the resistivity. Modifications were proposed to the volume and surface resistivity term of the Bickelhaupt model to better account for the unique chemistry of South African ashes. These modifications improved the predictive accuracy of the model significantly and deviations smaller than a factor of 2.5, a ratio commonly considered acceptable for between-laboratory repeatability by the IEEE was obtained.

SESSION 20a (9:55-10:35)
SUSTAINABILITY AND THE ENVIRONMENT
Massood Ramezan and Richard Bajura

20a.1 (9:55-10:15) Manufacturing and Life Cycle Assessment of Char-based Concrete Bricks

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Pyrolyzed char, derived from Wyoming coal, was used to fabricate new ecofriendly and sustainable building materials, including char-based concrete brick, carbon-based structural unit, and insulation panel at laboratory-scale. To advance the technology readiness level from laboratory-scale to full-scale and to produce transformational and scalable manufacturing building materials, it is necessary to conduct life cycle assessment (LCA) for assessing the impacts associated with a building material over its life cycle. In this study, LCA was conducted to investigate factors affecting the life cycle cost and life span of the char-based concrete bricks (CCBs). Different manufacturing methods of CCBs were discussed. Two reduced-scale demonstration houses were built to compare their performances using the new CCBs and conventional building materials (concrete and building bricks) as well as to understand factors affecting the durability and life span of the CCBs. These buildings are currently subject to performance testing over a full season to assess energy efficiency and weathering characteristics. Compared with conventional building materials, the new CCBs show advantages of low cost, high engineering performance, weight saving, high compressive strength, and low thermal conductivity and are manufactured in sustainable ways that avoid release of anthropogenic CO2. These advantageous features, lead to reduced life cycle cost, lower overall design and construction costs and improve the life span of a building, ultimately, facilitating the acceptance and application of new and sustainable CCBs in the building industry.

20a.2 (10:15-10:35) Heat treatment of pyrite from southern Brazil to produce pyrrhotite – Coal Valorization Project of Santa Catarina State Research Funding Agency (FAPESC)

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Mineral coal in Brazil and in the world has marked decisive moments in world history. Since its discovery, probably in the chipped stone age, when it was used to heat the first inhabitants of the planet in caves, mineral coal has been gaining space and recognition. Mineral coal has been used in Brazil since 1827 and continues to heat the national industry. In 1827 an English company was already extracting coal from mines located in Santa Catarina. However, officially, the first coal mine in Brazil was opened in 1855, in Arroio dos Ratos. Currently the largest concentration of coal mining in Brazil is located in the southern region. The main coal reserves already identified are in the states of Santa Catarina, Paraná, Rio Grande do Sul, Minas Gerais, São Paulo and Bahia. The mineral coal in Brazil supplies the economy, especially the thermoelectric plants that consume about 85% of the production.

The state of Santa Catarina was quite used and exploited for many years in relation to coal mining and for about 20 years the region has been following an environmental recovery schedule for the compensation of environmental damage, this awareness of environmental recovery is very important because coal is an important mineral that promotes the means of production but on the other hand this same mineral causes significant environmental impacts. The extraction of coal can pollute underground water resources, soil, and rivers, causing fish mortality and the escape of wild animals. This type of exploitation also generates air pollution and causes deformities in the relief.

Brazilian mineral coal contains high levels of impurities (pyrite and sedimentary rock minerals), making its beneficiation necessary. Pyrite is a solid residue from coal extraction that, when exposed to the environment, can react with oxygen and water producing sulfuric acid and leaching the soil, forming a rusty aqueous solution, known as acid mine drainage. Therefore, the conscious management of this waste is essential. In order to find an environmental solution for pyrite, pyrite samples of the southern Santa Catarina State, located at the city of Treviso were calcined with argon at 750°C to obtain pyrrhotite and eliminate sulfur. Soon after, the sample obtained was taken for simultaneous thermal analysis with coupled infrared to analyze the gases released during the reaction and better understand the thermal treatment performed and its results. XRF, XRD, FTIR and CHNS were used as complementary characterizations for the pyrite.

The Project was funded by FAPESC - Fundação de Amparo a Pesquisa de Santa Catarina - Santa Catarina State Research Funding Agency and the aim of this project is to develop nano pyrites with semiconductor characteristics. The use of pyrite is very important to reduce the environmental degradation caused by the coal waste disposition.

SESSION 20b (10:35-11:35)
COAL MINING, PREPARATION AND HANDLING
Dick Winschel and Guven Onal

20b.1 (10:55-11:15) DYNAMIC SIMULATION TO OPTIMIZE THE DM CYCLONE PRODUCTION SYSTEM WITH IDEAS

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Taking Fangezhuang coal preparation plant of Kailuan Group as an example, the entire production system of the gravity-feed three-product dense medium (DM) cyclone for fine coal is reconstructed with the help of IDEAS software. Taking the raw coal characteristics, suspension characteristics, cyclone geometry and external operating conditions as the initial parameters, the production system of DM cyclone is dynamically simulated to verify the reliability of the selected model and the accuracy of the initial parameters. Based on the selected model and initial parameters, the existing production system is optimized, and the transformation content is determined. Compared with that before the rectification, the ash content of clean coal of cyclone is 10.36%, the loss of -1.4 g/cm3 coal in middlings is 7.17% (reduced by 18.05%), and the loss of -1.8g/cm3 coal in reject is 2.86% (reduced by 12.17%); The EP value of the first section of the DM cyclone is 0.050, the EP value of the second section of the DM cyclone is 0.055 (reduced by 0.075), the quantity efficiency is 92.19% (increased by 12.34%), and all indexes meet the expected requirements. After rectification, the theoretical clean coal recovery rate is calculated as 40%, the clean coal recovery rate can be increased by 40%×12.34%=4.95%, the amount of fine coal is calculated as 2.70Mt/a, then the clean coal output can be increased by 2.70Mt/a×4.95%=0.13 Mt/a, which can bring significant economic benefits to the coal preparation plant.

20b.2 (11:15-11:35) A coupled flow - geomechanics study on the effectiveness of methane drainage in multi-seam coal mine with the use of long-reach directional drilling

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Coal Mine Methane (CMM) is the gas released into mining excavations during coal mining activity, captured through methane drainage or discharged in the ventilation air. Due to the hazards associated with methane emissions during mining processes, the drainage of this gas, in addition to being a source of cleaner energy, also constitute a critical element of methane hazards management in the coal mines in Poland. Methane explosion hazards are controlled with the use of the methane drainage systems involving drilling boreholes from the surface or from the underground to access the disturbed zone above and sometimes below the excavated coal seams. This study aims to assess the effectiveness of the coal mine methane drainage in the multi–seam coal mine situated within the Upper Silesian Coal Basin (USCB) in Poland using the long reach horizontal boreholes and cross measure boreholes. Determination of the effectiveness of the CMM drainage is carried out using numerical methods coupling geomechanics with the modeling of the reservoir fluid flow. The basis of both geomechanical and fluid flow models are developed structural and geological parametric models of the coal seams and surrounding rocks. As a result of a comprehensive analysis and data integration, a structural model of one of the Polish hard coal mines from the USCB was developed, in which the effectiveness of methane drainage from the approx. 45 m thick zone above coal seams deposited at a depth of approx. 600 m below sea level is investigated. The data used for model construction included structural maps of coal seams bottoms, geological cross-sections, and borehole data from drillings from underground roadways as well as deep research boreholes drilled from the ground surface. For the purposes of geomechanical and petrophysical modeling, based on the available lithological profiles and point data, a lithotype model was developed, which allowed for the correct parameterization of mechanical and petrophysical properties characterizing particular lithotype occurring in the coal mine. The spatial distributions of these parameters were developed based on the well log data from the reference borehole as well as laboratory measurements, carried out on coal samples collected from the degassed seam. The investigated area's reservoir fluid flow model was constructed based on the developed

geological model and including a drainage system consisting of long reach horizontal boreholes and cross measure boreholes. For this purpose, the base model was supplemented with properties describing the transport and retention of reservoir fluids dual porosity system present in coal, i.e., matrix and fractures. These properties included the characteristics of the viscous flows in the fractures and the phenomena of desorption and diffusion in the matrix. For the model defined in this way, coupled geomechanical and flow simulations were performed. Results of the geomechanical simulations showed the influence of individual elements of the drainage system on the geomechanical condition of the seam described by the distribution of stress and strain tensors and the extent of damage areas. These quantities were used to determine changes in transport properties of the analyzed seam (Carman P.C., 1956, Shi J-Q, Durucan S., 2005) and implement the changes in the flow model. The modified dynamic flow model accounting for the geomechanical effects was further used to simulate the methane drainage process from the coal seam. To effectively couple the geomechanical and flow simulations, an original, non-iterative method was applied that resulted in time saving and precise calculations. The drainage process modelling, that includes both geomechanical and fluid flow effects, provides key data to asses effectiveness of the proposed method of methane drainage with the use of long-reach directional drilling. In addition, quantitative results of the corresponding simulations estimate the dependence of the drainage process characteristics upon the basic technological parameters of the methane drainage.

20b.3 (11:35-11:55) COAL RECOVERY FROM SLURRY RESIDUE IN TKI ÖMERLER WASHING PLANT

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The research about Recovery of Coal in the coal slurry of GLI Ömerler Washing Plant is called as "Enrichment of the lignite via shaking table, Multi-gravity Separator (MGS), and the flotation methods for Clean Fuel Technology" was funded by TUBITAK. This research was conducted jointly by TKI, MTA, and the equipment was brought after the results of the studies carried out by the labs of MTA and operated in June 2010 with the technical team and the workers of Ömerler Coal Washing Plant.

During the washing process in the plant which has 800 m3 /hour coal slurry includes 10-15% solid material, is collected and pumped to new circuit gathering tank before sending thickeners. This coal slurry is sent by pumps to the Multi Cyclone Group. (total of 48 hydro cyclones which is in 2 groups with the 24 hydro cyclones each.) Underflow of cyclone group is carried to dewatering sieve and upperflow is carried to new gathering tank which was added to this system in 2021. The second MCG is followed the same route. With the help of these cyclones; slime size classification process is applied two times to 0,5 mm below slurry material and 0,5 mm above fugitive material. According to the separation performance test, MCG separation performances ratio is found %85. Under 50-micron slurry material is taken from upper flow of secondary MCG Group and sent to thickener and +50-500-micron slurry material is taken from under flow of both MCG Groups and sent to dewatering sieve. Approximately; 19 tonnes per hour of coal slurry product is gained with the operation of full capacity of the system in washing plant. From the establishment of MCG in 2010 to the end of 2022 May, 820.000 tonnes coal slurry is gained by the system and sold as intermediate product (mixed, middling) to the Power Plants.

Keywords: Coal, Multi Cyclone Group, Washing Plant.

SESSION 21 (12:35 – 13:55)
POWER PLANTS - 1
Alberto Pettinau and Evan Granite

21.1 (12:35-12:55) Dynamic Simulation for Boiler Fault Detection and Diagnosis Using AI

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Fossil power plants are still playing a critical role in the US power system even though the share of renewable power is increasing in the past decade. Coal-fired power plants not only generate the power, but they also assume the responsibility to provide load demand support to the power grid as wind and solar power units add fluctuations to the grid system. Wear and tear of the coal-fired fleets tends to be more severe than before when the units were mainly operated at base load conditions. Thus, fault monitoring for early detection and diagnosis has become more imperative in cyclic operations of the existing coal power fleets.

GE Research has developed a novel AI learning system that is trainable end-to-end (i.e., the representations of the normal operating conditions of a complex system can be directly learned from data) for fault detection and root cause analysis. The DOE funded project is aimed at bringing the technology maturity from TRL 2 to TRL 5, with final validation performed based on data from a coal-fired power plant. In this project, operating data is provided from an operating unit in the United States. Meanwhile, dynamic simulations were planned to provide data simulating both normal cycling operations and operations with typical operating faults that impact the performance, reliability, and safety of typical coal-fired steam power plants, in particular the boiler islands.

To support the need for generating simulation data for machine learning, GE Steam Power selected a boiler dynamic model that was developed and calibrated using typical engineering design of 660MWe supercritical boiler unit as the reference. The dynamic model was built using the APROS® software from VTT and then calibrated to multiple load conditions from full load (100%TMCR) to partial loads based on internally developed steady state heat balance models at the unit level. These internal heat balance models are based on first principles and extensive engineering experiences from GE Steam Power as an OEM and a services provider.

This topical report summarizes the work done by the Steam Power team. It is organized as follows: 1) generating a list of typical faults for pulverized coal boiler operations in the field; 2) dynamic model selection and preparation for generating fault simulation data; 3) simulation data generation for normal operations with load cycling; 4) simulation data generation for unit operations with selected faults; 5) review of machine learning results using the simulation datasets and 6) conclusions and future work.

Keywords: Steam Power Plant, Boiler, Dynamic Modeling, Fault Simulation, Fault Detection and Diagnosis, Machine Learning

21.2 (12:55-13:15) HIGH-FIDELITY DYNAMIC MODELING OF A COAL-FIRED STEAM POWER PLANT

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As a result of the growth of renewables including solar and wind energy with fluctuating production, fossil fuel power plants are being required to cycle between high and low power production. This cycling is both at a greater frequency and over a wider range than in the past. In many cases, power plants are not designed for this type of cycling operation but can nonetheless endure these challenging
operation requirements under the right conditions. In this project, optimal solution for enhanced flexible operations are being investigated using model based estimation and control techniques. To support the development of model-based estimator and model-based controls at GE Research, GE Steam Power configured a dynamic model using a reference steam plant design including the boiler, turbine, and water/steam conditioning systems as well as the controls needed for plant cycling with stability and reliability. The dynamic model was built using the APROS® software from VTT, and then calibrated to multiple load conditions from full load (100%TMCR) to partial loads (75%TMCR, 50%TMCR and 25%TMCR) based on internally developed steady state heat balance models at the unit level. These internal heat balance models are based on first principles and extensive engineering experiences from GE Steam Power as an OEM and a services provider. This paper presents the structure of the unit level dynamic model, the tuning process, and representative simulation results from typical load cycling simulations using the dynamic model.

Keywords: Steam Power Plant, Dynamic Process Modeling, Model Calibration, Simulation Analysis

21.3 (13:15-13:35) Dust Control Improvements Help Winterize Your Coal Handling System

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Nearly fifteen years after OSHA issued their Combustible Dust National Emphasis Program Directive, most coal power plants have fulfilled their regulatory requirements and moved on. But, in the wake of winter storm Uri, can we take a closer look at fugitive dust generation as a symptom of larger coal handling problems? This paper will show coal handling system operators how to use dust as a leading indicator of potential weather problems, and what to do about it.

21.4 (13:35-13:55) Distributed Coaxial Cable Sensors for in-situ Condition Based Monitoring of Coal-Fired Boiler Tubes

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The increasing contributions of renewable energy sources present new challenges to the operation and maintenance of the existing coal fired power plants. One of the major operation risks is the unexpected failure of superheater boiler tubes, leading to most of the unplanned power plant outages. The boiler tube failure is difficult to predict due to the harsh operation environments. Therefore, condition-based monitoring (CBM) becomes necessary to produce meaningful assessment of the health condition of boiler tubes and their remaining lifetime. In this work, the stainless-steel and quartz coaxial cable sensor (SSQ-CCS) is proposed for in-situ distributed monitoring of the boiler tube temperatures in existing coal-fired power plants. The SSQ-CCS temperature sensor is made by using a quartz tube (1mm ID and 6mm OD) to concentrically separate a 304 stainless-steel wire (0.043-inch OD) and 304 stainless-steel tube (5/16 inch OD). Comprehensive tests have been conducted with an in-house testing facility at Clemson University to study and evaluate the sensors' performance in the temperature range of 300℃ to 600℃. The results indicated that the measurement resolution of the SSQ-CCS sensor is better than 1℃ and the drift is less than 2% over a long-period testing. Meanwhile, multi-physics finite element analysis has been conducted to evaluate the stress, strain, and temperature field of the SSQ-CCS temperature sensor under various steam temperature and flue gas temperature conditions. Based on the performance obtained in the laboratory-scale testing, a field test has been implemented at a power plant. Four SSQ-CCS temperature sensors were installed for in-situ monitoring the temperatures of a power plant's superheat tube assembles. The data acquisition system has been successfully set up and collected sensing signal for more than 3 months. The sensing signals has been postprocessed and the monitored temperature history through SSQ-CCS temperature sensor has been validated and compared with the thermal couple data.

21.5 (13:55-14:15) Use of Deposition Probe to Collect Boiler Tube Deposit

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Microbeam designed and constructed a deposit sampling probe for use in solid fuel combustion systems to study the deposition of ash-forming materials as a function of fuel properties and plant conditions. The probe was designed to represent a boiler tube and collect deposits during boiler operation. Collection of deposits for analysis is generally limited to shutdowns, however, this probe allows for real-time sampling during normal operation of the boiler. The probe has been extensively used at lignite fired power plants in North Dakota. In addition, it has been used to determine ash deposition rates and provide deposit samples for modeling of ash behavior.

Key features of the design include an enclosure for the probe outside of the boiler with rails for extension of the probe into the boiler and temperature control to allow for adjustment of temperature during operation. The ability to extend the probe into the boiler and then return the probe with the deposit into the enclosure when testing is complete protects the deposit from being lost due to pressure differences between inside and outside the boiler. The enclosure has an access door and a tray that provide the ability to photograph the deposit and collect samples along the length of the probe. The temperature control allows for the ability to replicate boiler tubes at different locations in the boiler. Thermocouples are installed on the probe to allow for remote monitoring temperature.

The deposition probe is designed to be installed in an observation port at the radiant section exit or in the convective pass of the boiler. Deposits are collected under a specific set of test conditions that are used to evaluate fuel properties, boiler load, and sampling time. During each condition the probe slides on rails into the boiler and is exposed to the particulate laden flue gas stream for selected period of time up to six hours. For each sampling period back the probe with the deposit is moved from the high temperature zone into a box that is isolated from the boiler. Once the probe is cooled the deposits are delicately collected off the probe into sample containers to be weighed and analyzed using the scanning electron microscope equipped with an x-ray microanalysis system. The probe can be used to understand the rate of deposition by performing tests at different lengths of time. The change in ash deposition rate and the materials responsible for the deposit initiation, growth, and strength development are determined.

This paper will provide results of testing performed in lignite fire power plant to determine the impact of fuel properties and boiler load.

SESSION 22 (12:35 – 13:35)
ENERGY STORAGE
Massood Ramezan and Richard Bajura

23.1 (12:35-12:55) Techno-economic Analysis of Thermal Energy Storage Systems Integrated with a Power Plant

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Coal-fired power plants are being required to ramp output up and down regularly, often to levels lower than units were originally designed for. Integrated Energy Storage improves unit flexibility (e.g., dynamic response, time-shifting peak power generation, expanded operating range, reduced load cycling, improved frequency regulation, and increased participation in Ancillary Services market) and system stability.

The main objective of this work is to analyze and compare technical and economic performance of different thermal energy storage technologies integrated with a thermo electric power plant. Techno-Economic Analysis (TEA) of four Thermal Energy Storage (TES) systems integrated with a coal-fired power plant was performed under DOE Award FE0031903. The analyzed TES systems included Low Pressure Condensate Storage, Two-Tank Molten Salt Storage, Solid State Fixed Bed TES, Liquid Air Energy Storage, and Ruths Steam Accumulator. These energy storage systems represent a range of TES designs and thermal energy storage media considered for integration with thermo-electric power plants.

TES systems were modeled, validated, and thermally integrated with a 650 MWgross Reference coal-fired power plant using Ebsilon Professional and ASPEN Plus modeling platforms to determine their performance and the effect of integrated TES system on plant performance and flexibility. TES system performance parameters included: flow

rate, temperature, and pressure of charging and discharging fluids (steam, condensate, or air), thermal storage capacity, and roundtrip efficiency. TES integration with a power plant varied depending on the type of TES, while the impact of TES on plant flexibility and performance depends on TES type and the integration strategy. The analysis was performed at full and minimum load conditions. The impact of TES charging and discharging on power plant power output, efficiency, heat rate, and other performance parameters was determined.

Economic performance of TES systems was performed for MISO (Midcontinent Independent System Operator, ISO) and PJM (Pennsylvania, New Jersey, and Maryland Regional Transmission Operator, RTO) energy trading systems by considering the effect of TES on plant revenue, including capacity, energy arbitrage, frequency regulation, and spin reserve. These results are also presented in the paper.

Key words: Energy storage, plant performance, roundtrip efficiency, energy markets

23.2 (12:55-13:15) Estimating Subsurface Hydrogen Storage Potential Across the U.S. Based on Data for Existing Natural Gas Storage Reservoirs

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Renewable energy technologies are being advanced to meet current and future energy demands while mitigating atmospheric CO2 emissions. As renewables contribute to an increasing share of the total energy supply, challenges must be addressed to accommodate intermittent supply and varying demand of energy. An option to address these challenges is to convert energy into hydrogen (H2) gas to move towards a low-carbon, and ultimately a zero-carbon energy society. H2 has been identified as having abundant benefits, can be produced by both well-established and emergent technologies, and can be applied in multiple end-use transport and energy processes. Currently, UHS is targeted in salt caverns, underground depleted reservoirs, brine aquifers, and hard rock caverns. In the U.S. an important gap, however, exists in estimating the amount of hydrogen that can be stored either as a pure gas or mixed with natural gas. There is a need to develop the capability to store large amounts of hydrogen economically and safely similar to how natural gas (NG) is stored today. In this work, we estimate the hydrogen storage capacity in existing natural gas storage reservoirs across the US. Our methodology assumes that the volume of pore space in the storage reservoir available for gas storage is equivalent regardless of the properties of the gas. Physics-based numerical approaches will provide more accurate capacity estimates of H2 and H2-CH4 mixtures in natural gas storage reservoirs. However, volumetric approaches are relatively simple to employ and are valuable for characterizing regional storage capacities, which is the goal of this study. We used the working gas volumes reported in the EIA UGS facility dataset to estimate the H2 working gas energy for existing U.S. UGS facilities. Basing our calculations on the working gas volume implicitly assumed that the fraction of the total reservoir volume that will be available for working gas will remain consistent between natural gas and H2 storage. As hydrogen storage has not been deployed on a commercial scale, accurate estimates of hydrogen storage above and below the surface are needed.

23.3 (13:15-13:35) Coal as Value-Added for Lithium Battery Anodes

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Lithium-ion batteries (LiBs) are the clear energy storage system of choice for everything from consumer electronics to electric vehicles (EVs) and will remain so for decades to come. Over the past few years there has been a significant increase in demand for LiBs, presenting a justifiable concern regarding a deficit in raw materials available to support

projected growth, particularly when the U.S. relies so heavily on foreign sources of raw materials.

For more than two years, Semplastics has worked on developing a novel material system that integrates coal with a proprietary Polymer Derived Ceramic (PDC) technology to form high-capacity anodes used for LiBs. The Semplastics anode material is a composite of chemically tailored inorganic silicon oxycarbide (SiOC) preceramic polymer resin and domestically sourced coal powder, designed to supplement the domestic lithium-ion battery anode supply chain and green economy.

The Department of Energy National Energy Technology Laboratory (NETL) awarded Semplastics with a three-year research grant in 2020 to develop and prove feasibility of using the PDC coal composite anode as a means to produce high-value solid products from domestic U.S. coal. To date, Semplastics has been successful in demonstrating a high-value, coal-based anode technology in full, 25 mAh single-layer pouch cells built and tested at the Battery Innovation Center in Newberry, IN. Coinciding with the project timeline, by the end of 2022, it is expected that the PDC coal anode composite technology will be demonstrated in 18650 cylindrical batteries to prove feasibility in a relative environment. During this talk, the Semplastics team will present a status update on this project including details of electrochemical performance and projected outcomes.

23.4 (13:35-13:55) Renewable Methanol Production from Carbon Dioxide and Green Hydrogen: A Techno-Economic Assessment

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This work aims to present a feasibility study of a Power-to-Fuel plant for renewable methanol production starting from green hydrogen and recycled carbon dioxide. Hydrogen is obtained by water electrolysis employing renewable electricity or absorbing the overproduction from the electrical grid. Carbon dioxide is sequestered from the flue gas of a conventional coal-fired power plant through an amine-based CO_2 capture system. The study focuses on the production of methanol at a commercial scale (500 kg/h). In this way, methanol can be considered as feasible chemical storage of renewable electricity. A size of 6.5 MW has been selected for the PEM electrolyser, for a production of 104 kg/h of green hydrogen. 723 kg/h of CO_2 are captured from coal fired plant. A comprehensive process model has been developed with the support of Aspen Plus software to simulate all the relevant sections and the overall system. After the process optimization, a detailed techno-economic analysis has been performed based on capital and operating costs assuming a 20-year lifetime and referring to the Sardinian economic scenario, since the Sardinia Island is the only Italian region that produces a surplus of electricity. A typical discounted cash flow analysis has allowed to calculate the levelized cost of methanol (LCoM): to reach the break-even point at the end of the plant lifetime a minimum selling price of 970 €/t was found, with an IRR of 8%. The analysis reveals that the LCoM is mainly affected by the electricity price and the electrolyser capital cost, as well as the capacity factor of the plant.

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SESSION 23 (14:25 – 15:45)
POWER PLANTS - 2
Ting Wang and Eric Grol

23.1 (14:25-14:45) Mitigation of Aerosol Induced Fouling from Coal Combustion

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Barr, in partnership with the University of North Dakota, Microbeam Technologies, Envergex, and MLJ Consulting, worked to develop a transformational technology that controls the formation of alkali aerosols found in coal ash. This technology mitigates ash deposition by injecting sorbents into the boiler and capturing volatile species responsible for boiler fouling, the primary cause for boiler outages. In this session, we'll explore the science behind this technology and see some real-world results of its implementation.

23.2 (14:45-15:05) Baseline Cost and Performance Assessment of Low-Rank Coal-Fueled Power Plants with Carbon Capture and Sequestration

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This presentation addresses the independent assessment of the cost and performance for select electricity generating units—pulverized coal (PC) and circulating fluidized bed (CFB) - fueled by low-rank coals (Powder River Basin (PRB) and North Dakota Lignite (NDL)). In addition, natural gas combined cycle (NGCC) plants are represented. All cases are presented both with and without 90% carbon capture and sequestration (CCS)– Shell Cansolv is used for the post-combustion capture system. All plants are at elevation, consistent with locations for economic use of the identified fuels. These analyses were carried out using an approach and methodology consistent with NETL's 2019 report titled "Cost and Performance Baseline for Fossil Energy Plants, Volume 1: Bituminous Coal and Natural Gas to Electricity (Revision 4)," facilitating comparison.

The results of this work are important inputs to assessments and determinations of technology combinations to be utilized to meet the projected demands of future power markets and provide perspective for regulators and policy makers. From a research and development perspective, these results are used to assess goals and metrics and to provide a consistent basis for comparing developing technologies.

23.3 (15:05-15:25) HIGH CO2 CAPTURE RATE COST AND PERFORMANCE BASELINE RESULTS FOR NATURAL GAS COMBINED CYCLES (NGCC)

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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 carbon management technologies for a variety of sectors including utility power. To provide a consistent and transparent design basis and methodology for technology comparisons while providing an independent representation of system cost and performance, NETL has developed a set of studies titled, "Cost and Performance Baselines for Fossil Energy Plants." The Fossil Energy Baseline study has served as a consistent baseline for NETL power system evaluations as well as a reference for many external studies in the literature and other high profile public purposes.

Recent literature has suggested that higher rates of CO2 capture on point source emissions could be achieved at relatively low incremental cost, reducing dependence upon methods to capture the residual atmospheric CO2 emissions in pursuit of net zero emissions goals. To expand upon that body of knowledge, this presentation will cover updates to the Fossil Energy Baseline study that aim to establish performance and cost references for greater than 90 % carbon capture rates on fossil-based power systems, with particular emphasis on natural gas combined cycle (NGCC) power plants. For NGCC plants, the analysis includes results for up to 97% CO2 capture based upon recent Shell Cansolv data. Also, results will be reported for H-class systems both with and without CO_2 capture – a new addition to the Fossil Energy Baseline.

23.4 (15:25-15:45) Visible Light Communications for Power Plant Applications

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Wireless communication is an integral part of modern society and is of interest to the power generation sector to reduce the installation costs for new equipment, especially sensors. However, sending data via certain parts of the electromagnetic spectrum can raise a security risk because of their transmission through barriers and typical omnidirectional characteristics. Additionally, the use of many wireless devices in a local space can cause spectrum pollution, a bad side-effect especially when dealing with machines and instrumentation that are sensitive to wireless signals. This paper documents the investigation of another form of wireless technology that uses visible light as its communication medium and helps to mitigate some of the previously mentioned problems. The criteria considered were distance of data transmission, speed of transmission, and the effects of the environment on both communication distance and speed. Aspects of optics, communications, and electronics were used to design a system that could meet the design requirements. Prototypes of the system were constructed and tested in a variety of conditions to evaluate performance in possible service conditions. These tests afforded a better understanding of visible light communication (VLC) and its benefits and shortcomings when compared to other forms of communication like Wi-Fi.

23.5 (15:45-16:05) Review of Natural Gas Liquefaction Processes and Refrigeration Cycles

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Natural gas (NG) has been widely used in recent years to replace coal, diesel, or other petroleum derived fuels to generate power because combustion of NG produces lower emissions. However, many nations have limited NG resources and transporting natural gas through land-based piping is either limited or not available. Thus, importing liquefied Natural Gas (LNG) by transporting across the oceans has become a viable method for countries historically, like Japan, China, South Korea, Taiwan and recently, European countries, like Germany, UK, due to reduction of NG provided by Russia induced by geopolitical conflicts.

In this paper, a review of various commercially available liquefaction processes for natural gas is presented. NG is refrigerated into a cryogenic state near -161 °C (-258 °F), where it is reduced to 1/600th of its original volume. The liquefaction is usually achieved in a multistage sequential refrigeration process. The liquefaction processes reviewed include Linde-Hampson Cycle, Claude Cycle, Puilips Optimized Cascade Cycle, C3MR, PRICO□, Shell DMR, Statoil/Linde Mixed Fluid, IFP/Azen LiquefinTM , etc. The pretreatment processes are also presented. In the end, a sample of the simulated 4-stage cascade LNG process is presented.

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