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**Abstracts Booklet**

**"Technology Innovation and Transition to Cleaner Energy"**

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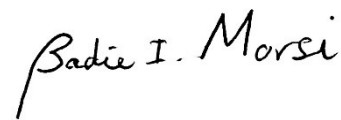
## A NOTE TO THE READER

This Abstracts Booklet is prepared solely as a convenient reference for the Conference participants. Abstracts are arranged in 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. 6.1 is the first paper to be presented in the Oral Session #6.1.

It should be cautioned that this Abstracts Booklet is prepared based on the original abstracts that were submitted unless the author noted an abstract change. The contents of the Booklet do not reflect late changes made by the authors for their presentations at the Conference. The reader should consult the Final Conference Program for any such changes. Furthermore, updated, and detailed full manuscripts, published in the Conference Proceedings, will be sent to all registered participants following the Conference.

On behalf of the Forty-First Annual International Pittsburgh Energy and Carbon Management Conference, I wish to express my sincere appreciation and gratitude to Ms. Rebecca Bauroth for her meticulous guidance of the entire conference. My profound gratefulness goes to Dr. Rui Wang for his crucial assistance and dedication in preparing this Abstracts Booklet.

Thank you,

A handwritten signature in black ink that reads "Badie I. Morsi". The signature is written in a cursive style with a large initial 'B'.

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

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**SESSION 1 (10:00 – 12:00)****Carbon Management – 1***Bingyun Li***1.1 (10:00-10:30) Photothermal reduction of CO<sub>2</sub> to formic acid over Pd/P25 composite catalyst**

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Efficient conversion of CO<sub>2</sub> into chemicals using solar energy as driving force is meaningful to alleviate the greenhouse effect and combat the energy crisis. In this work, the advantages of photocatalysis and thermal catalysis was employed to hydrogenate CO<sub>2</sub> to HCOOH on Pd/P25 catalyst. Under the condition of simulated sunlight and P(CO<sub>2</sub>):P(H<sub>2</sub>)=1:1, it is found that the catalyst obtained a HCOOH selectivity of 100%, and the 1% Pd/P25 catalyst possessed the highest HCOOH yield of 51.19 mmol·g<sup>-1</sup>·h<sup>-1</sup>, which was 4.59 times than that of P25 (11.15 mmol·g<sup>-1</sup>·h<sup>-1</sup>). Without external heating, the reaction system temperature can reach 66.7°C, CO<sub>2</sub> conversion up to 18.49%, solar-to-chemical conversion (STC) up to 14.95%, and photothermal conversion efficiency up to 50.09% for 1% Pd/P25. This can be attributed to its excellent and efficient light utilization and effective e<sup>-</sup>-h<sup>+</sup> separation. Further characterization demonstrated that the excellent performance of the Pd/P25 catalyst was mainly attributed to the loading of Pd to extend the solar absorption range of the catalyst, providing heat for the reaction and accelerating the reaction kinetically. In addition, it was also demonstrated by electrochemical characterization that the loading of Pd led to the lowest charge transport resistance, which facilitated the separation of photogenerated carriers. This study provided a promising approach for utilizing photothermal synergies to convert carbon dioxide.

**Keywords:** photothermal catalysis; photothermal effect; CO<sub>2</sub> reduction; formic acid; Pd/P25 catalyst

**1.2 (10:30-11:00) Characteristic of hydrogen production from various of feed gases in sorption enhanced water gas shift reactions**

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The sorption enhanced water gas shift reactions (SEWGS) for hydrogen production process employs sorbents to capture CO<sub>2</sub> generated during the hydrogen production process, thereby impetus the reaction equilibrium shift and enhances both the efficiency and concentration of hydrogen production. This innovative technology not only captured the greenhouse gas CO<sub>2</sub> but also held significant potential for application in the field of clean energy. However, the gases composition and content produced by classical coal gasification technology generally varied with gasification conditions, and the typical composition included CO<sub>2</sub>, H<sub>2</sub>, CO, CH<sub>4</sub> etc. The variation of gases composition could influence the floating of some reaction parameters, such as the equilibrium limit, sorbent

properties, performance evaluation parameters, and the hydrogen purity. In this work, thermodynamic analysis was employed to evaluate the influence of the feed gases component on the sorption enhanced water gas shift reaction. Calculations indicated that feed gases such as pure CO, H<sub>2</sub>/CO, and CO<sub>2</sub>/H<sub>2</sub>/CO mixtures could achieve CO conversion rates exceeding 99% and H<sub>2</sub> purities of 99% with MgO sorbent at 300°C, 0.1 MPa, and steamed to total carbon molar ratio (S/C) of 2. Further analysis of the gas composition found that a higher proportion of H<sub>2</sub> in the feedstock gas was beneficial for the production high-purity hydrogen, while a higher proportion of CO facilitated the rapid removal of the generated CO<sub>2</sub>. Regardless of the CO<sub>2</sub> content in the feedstock gas, it could be effectively removed by MgO. Furthermore, when the feed gas contained CH<sub>4</sub>, CO<sub>2</sub>, H<sub>2</sub>, CO, and other components, additional side reactions related to CH<sub>4</sub> are initiated. To achieve a dry basis H<sub>2</sub> purity of over 99%, the optimal reaction conditions were 600°C, 0.1 MPa, and an S/C ratio of 4. The yield of H<sub>2</sub> was higher when the proportion of main reactants, the combined content of CO and CH<sub>4</sub>, in the feedstock gas was greater. The conversion rates of CO and CH<sub>4</sub> were correlated with their respective input concentrations.

**Keywords:** Thermodynamics; Hydrogen production; Sorption enhanced water gas shift reactions; Sorbent; Feedstock gas

**1.3 (11:00-11:30) Adsorption and desorption kinetics of dry sorbents for CO<sub>2</sub> capture**

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In this paper, the adsorption and desorption kinetics of three commercially available activated carbons was investigated using a laboratory-scale fixed-bed reactor. The three activated carbons are CQ650 and CQ30P derived from coconut shells and coal, respectively, and activated with a combination of steam and KOH impregnation; the third activated carbon (CQ006), was derived from coal and activated using steam and an acid wash. The samples were subjected to continuous adsorption and desorption cycles at 30 – 70 °C with 10 °C increments and two CO<sub>2</sub> concentrations of 5 and 15 vol.%. The characterization of the samples showed that CQ006 exhibited the highest fixed carbon content while CQ650 had the highest N<sub>2</sub>-LPGA Brunauer-Emmett-Teller (BET) surface area of 517.14 ± 5.7 m<sup>2</sup>/g and the highest CO<sub>2</sub>-LPGA Dubinin-Radushkevich micropore surface area at 735.02 ± 27 m<sup>2</sup>/g, while SEM analysis revealed that the activated carbon samples have well-developed pore structures over the entire surface.

The three investigated sorbents performed well under cyclic operation with no significant difference in adsorption capacity between cycles. The most significant difference is the completion time, with CQ650 taking about 8600 s at 60 °C and 15 vol.% CO<sub>2</sub> feed concentration, while the quickest sorbent, CQ006, took 5900 s under the same conditions. The increased temperatures decreased the sorbents' saturation times and adsorption capacities, while the feed concentration also significantly affected the adsorbed quantity of CO<sub>2</sub> and the saturation times of the experiments. The overall desorption efficiency across the 5 temperatures (30, 40, 50, 60, and 70 °C) were 98.3% and 99.1% for the 5 and 15 vol.% CO<sub>2</sub> feed concentrations for CQ006, 96.5% and 95.1% for CQ650, and 93.4% and 92% for CQ30P at 5 and 15 vol.% CO<sub>2</sub> feed concentrations,

respectively; which will positively impact the use of these dry sorbents for carbon capture in cyclic operations.

For the kinetic modeling of the adsorption and desorption reactions, three kinetic models were examined, with Avrami model being the most suitable with a quality of fit of 99.1%, followed by the pseudo-first-order (94.7%) and the pseudo-second-order kinetic model (87.6%). The desorption activation energy was found to be generally higher than the adsorption activation energy for all the conditions, indicating that desorption (reverse adsorption reaction) requires more energy to remove the molecules from the surface of the sorbent than the energy released during binding to the surface of the sorbent. The thermodynamic results indicate that the adsorption mechanism is physical adsorption with a change in enthalpy of -10 to -20 kJ/mol. The negative change in enthalpy indicates that the reaction is exothermic, aligning with other reports from the open literature. The entropy in all the experimental conditions is also negative (-0.00198 kJ/mol to -0.00660 kJ/mol), implying that the molecules are slightly more orderly when adsorbed. A negative change in the Gibbs free energy (-18.37 kJ/mol to -22.57 kJ/mol) indicates that the reactions occur spontaneously.

**Keywords:** Carbon capture, CO<sub>2</sub>, adsorption, desorption, kinetics, activated carbon, thermodynamics.

#### 1.4 (11:30-12:00) Lessons Learned from Canadian CCUS Projects

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Canada is home to 15% of the world's carbon capture and storage capacity, including the first post-combustion capture facility fully integrated with a coal-fired power plant at Boundary Dam in Saskatchewan. Carbon captured at this facility is sent to the Weyburn-Midale enhanced oil recovery project. This project began capturing CO<sub>2</sub> in 2014 and has extended the life of the 45-year-old Boundary Dam Unit 3 (BD3). It, and other Canadian CCS projects, offer valuable lessons for the development of future projects.

While the BD3 CCS project experienced significant challenges in its first few years of operation, it demonstrated that the amine-based plant design could be scaled up at a 7000:1 ratio from a pilot project. Thermal integration with the power plant was also successful, with steam from the turbine being used to regenerate the amine used for CO<sub>2</sub> and SO<sub>2</sub> capture, and heat recovered from the steam condensate being returned to the power plant.

Particulate buildup has been a challenge for the capture plant: more fine ash particles from the power plant reach the capture plant than were anticipated. These particles foul heat exchangers and cause accelerated amine degradation, both of which reduced the plant's availability and capture capacity. The Thermal Reclaiming Unit was reconfigured to increase amine reclamation capacity and redundant heat exchangers were added to enable online cleaning.

The CO<sub>2</sub> compression and cooling system has experienced several significant outages. Coolers after the dry stages of the compressor were constructed from carbon steel, until CO<sub>2</sub> leaked into the cooling water and forced a shutdown. The tubes were replaced with stainless steel, but a manufacturing defect caused another leak in 2021. The CO<sub>2</sub> compressor motor also experienced a failure which was caused by a factory quality issue and caused an extended outage.

Since resolving these issues, the capture plant's performance has improved, with its strongest performance to date occurring between Q3 2023 and Q2 2024. Over six million tonnes of CO<sub>2</sub> have been captured since operation start-up.

The CCS Knowledge Centre undertook a feasibility study for a carbon capture facility at a cement plant in Canada. This study found that heat integration is not possible for a cement plant to the same extent as a power plant. A dedicated source of steam is required for the capture plant for amine regeneration, and it was determined that a Combined Heat and Power (CHP) plant could provide steam and electricity to both the capture plant and cement plant and improve the project's overall business case. Adding the flue gas from the CHP plant to the kiln flue gas increases the size of the capture plant, increasing the amount of steam required. An iterative process was required to correctly size both the CHP plant and capture plant.

**Keywords:** Amine Absorption, Boundary Dam, Carbon Capture and Storage, Cement Plant CCS, Combined Heat and Power.

## SESSION 2 (10:00 – 12:00)

### Value-Added Products from Coal – 1

Richard Bajura

#### 2.1 (10:00-10:30) Comparing ashes of some thermal power plants and metallurgical factory in Vietnam and their utilization

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Vietnam had an abundant amount of coal. Vietnamese coals are concentrated mainly in the Lang Son, Thai Nguyen and Quang Ninh provinces. Coals in Vietnam are used mainly for thermal power and metallurgy industries. Every year, the thermal power plant and metallurgy industries release a large amount of fly ash and bottom ash. Classifying and researching the composition of fly ash and bottom ash to come up with an optimal utilization strategy is necessary. This paper reports the results of analysis of fly ash and bottom ash of thermal power plants in Lang Son, Thai Nguyen and Quang Ninh as well as fly ash and cotton slag of Thai Nguyen metallurgy factory. From these works will be determined their utilization.

**Keywords:** fly ash, bottom ash, cotton slag, Quang Ninh, Thai Nguyen, Lang Son, Hai Duong.

#### 2.2 (10:30-11:00) Application of Composite External Donor Technology In Coal-Based Polypropylene Production

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Polypropylene (PP) is an important type of plastic, with outstanding mechanical properties, chemical corrosion resistance, and easy processability. PP is widely used in automotive, electrical appliances, daily necessities, and packaging industries. Global PP production capacity reached 108 million tons in 2023. China's annual production capacity has exceeded 40 million tons, with expected further growth. PP can be made either from oil or coal. Coal-based PP refers to propylene monomer made from coal. Since industrialized in China last decade, coal-based PP production capacity has increased dramatically, reaching 10 million tons/year, about 25% of the total capacity in China.

The coal-based PP technology, mainly from coal to methanol, then to olefin (including but not limited to propylene) is abbreviated as the MTO route. Different from conventional petroleum hydrocarbon cracking processes, the coal-to-olefin route has distinctive advantages, with olefin monomer products containing basically no sulfur, arsenic, mercury, and other impurities that are highly poisonous to polymerization catalysts, thus no need for expensive and complex purification processes to remove those impurities. Propylene with low impurity content leads to high polymerization efficiency and PP products of good quality.

Ziegler-Natta (Z-N) catalysts, discovered in the 1950s, are predominantly used in commercial PP polymerization processes. These catalysts typically consist of Ti-based catalysts containing internal electron donors on magnesium chloride support, alkyl aluminum compounds, and external electron donors. The external electron donors help control stereo-regularity and molecular weight distribution of the polypropylene product. The external electron donors are mainly silane compounds, such as dicyclopentyl dimethoxysilane (D-donor), diisopropyl dimethoxysilane (P-donor), diisobutyl dimethoxysilane (B-donor), cyclohexyl dimethoxymethylsilane (C-donor), and tetraethoxysilane (T-donor).

These donors can be categorized as strong or weak electron donors based on their electron donating ability and steric hindrance of the substituent groups on the Si atom. Generally speaking, strong donors result in high activity and high regularity but poor hydrogen response, while weak external electron donors lead to low activity and low regularity but high hydrogen sensitivity. To some extent, these two types of donors have complementary effects. High-performance polypropylene is occasionally manufactured

with composite external electron donors in oil-based polypropylene industrial production.

With substantial differences in impurities of propylene raw materials, composite external donor technologies developed for oil-based PP processes cannot be implemented as simple drop-ins for coal-based processes. Careful adjustments in composite external donors are crucial to produce superior PP products. Taking high melt flow rate, high rigidity, and high impact performance PP products as an example, our study has demonstrated the necessity of catalyst adjustment, leading to a successful commercial scale-up production of a series of PP products at 4.5 million tons/year by tailoring composite external donor catalyst systems depending on individual product performance specifications.

### 2.3 (11:00-11:30) Molecular design and performance modulation of anthracene-based solar thermal fuels

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Coal tar is one of the main by-products of the coking industry, which contains a large number of basic chemical raw materials with high value-added potential, such as anthracene, naphthalene, etc. Although effective separations have been carried out by various means, there are few studies on the preparation of fine chemicals based on the molecular structures of these compounds, which limits the development of efficient, high-value and diversified utilization technologies for these key components of coal tar. Here, we present a molecular design strategy for the preparation of solar thermal fuels using anthracene from coal tar. The prepared anthracene-based solar thermal fuel undergoes a cycloaddition reaction to form a dimer under UV irradiation ( $\geq 300$  nm) and stores the photon energy as chemical energy; and release the stored energy in the form of heat through depolymerization reaction then occurs under the stimulation of short wavelength UV light ( $\leq 300$  nm) or high temperature. Solar thermal fuels with long alkyl chains, di-anthracene and tri-anthracene were synthesized, which further enhanced the storage energy densities and prolonged the storage half-lives through increasing the molecular steric hindrance and intramolecular close-packing capability. Results showed that the photo-irradiation can be efficiently realized the depolymerization process of anthracene-based solar thermal fuels compared to the thermal excitation. The storage energy densities of anthracene-based solar thermal fuels can be enhanced from  $65 \text{ kJ mol}^{-1}$  to  $91 \text{ kJ mol}^{-1}$ , and the storage half-life is prolonged from hours to 2 months. Photo-triggered heat release from anthracene-based solar thermal fuels can increase the temperature by  $7^\circ\text{C}$ , showing enormous potential for heating applications. This molecular design strategy not only provides a unique approach to the frontier scientific problem of clean and efficient utilization of coal tar, but also enriches the existing utilization manners of solar energy.

**Keywords:** coal tar; anthracene; solar thermal fuels; solar energy storage; heat release

### 2.4 (11:30-12:00) Efficient separation of monoaromatics from direct coal liquefaction

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Separation of high-purity aromatic compounds from direct coal liquefaction (DCL) contributes to value-added utilization. The complexity of the components of DCL leads to the fact that a number of additional reactions are generally involved in the separation process for the production of aromatic monomers. A fractionation-column chromatography-extractive distillation strategy is designed for efficient separation of monoaromatics in DCL. The monocyclic aromatic hydrocarbons are enriched to 24wt% by fractionation, subsequently cycloalkanes are 100% removed by sequential gradient elution via atmospheric pressure column chromatography, and finally toluene, o-xylene, p-xylene and m-xylene are enriched to a purity of  $>99\text{wt}\%$  by distillation and extractive distillation. Quantum chemical calculations and molecular dynamics simulations are used to explore the mechanisms for the removal of cycloalkanes and the purification of monocyclic aromatic hydrocarbons at the molecular level. The results show that the difference in molecular polarity index (MPI) is responsible for the removal of cycloalkanes and low-carbon alkanes from monocyclic aromatic hydrocarbons. Vapor liquid equilibrium experiments show that the relative volatility between aromatic compounds can be improved by using Tetramethylene sulfone (Sul) and N-Methylpyrrolidone (NMP) as entrainers, and the intermolecular interaction energies and spatial distribution functions (SDFs) further proved that the interaction of Sul with m-xylene and p-xylene was stronger than that with ethylbenzene and o-xylene, and the interaction of NMP with m-xylene was stronger than that with p-xylene. The article provides a new perspective on the production of aromatic monomers from DCL.

## SESSION 3 (13:00-14:30)

### Carbon Management – 2

Omar Basha

#### 3.1 (13:00-13:30) Converting CO<sub>2</sub> into Nano-Minerals via Amino Acids

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Carbon dioxide (CO<sub>2</sub>) is believed to be a major greenhouse gas that impacts the climate change, and the management of CO<sub>2</sub> emission is critical in maintaining the environment to be human livable for millions of years to come. There are two major approaches in reducing CO<sub>2</sub> emission, one is carbon capture and storage (CCS) and the other is carbon capture and utilization (CCU). This abstract will investigate the use of amino acids to mineralize CO<sub>2</sub>, especially focusing on the potential of mineralizing CO<sub>2</sub> into nano-materials that may have biomedical applications. Solvents of KOH, K<sub>2</sub>CO<sub>3</sub>, etc. were added with amino acids, and the formation of minerals and the role of amino acids were determined. It was found that when amino acids were present in the K<sub>2</sub>CO<sub>3</sub> solvent, carbamate was formed even before reacting with CO<sub>2</sub>. Nuclear magnetic resonance (NMR) data showed that in the presence of amino acids in K<sub>2</sub>CO<sub>3</sub> solvent, bicarbonate and hydroxide were formed from carbonate hydrolysis, and amino acid reacted with bicarbonate to form carbamate before CO<sub>2</sub> bubbling and, during CO<sub>2</sub> bubbling, amino acid reacted with CO<sub>2</sub> to form carbamate which could subsequently hydrolyze into bicarbonate. Moreover, methods to apply amino acids to form unique nano-minerals were developed.

#### 3.2 (13:30-14:00) Carbon Management Driven by Wafer Scale Engines

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Engineering simulations are key to improving efficiency and effectiveness of carbon management. However, they can be computationally very expensive. Also, verifying the simulation results against real world data is critical for refining model assumptions. Advanced, explainable, and trustworthy data-driven artificial intelligence (AI) models can be both computationally and data intensive. In this work, compute acceleration of AI models was driven by the hardware acceleration using wafer scale engines. Scurry Area Canyon Reef Operators Committee (SACROC) oilfield, located in the Permian

Basin, TX, USA was selected for the geological carbon storage case study. The unit composed of bedded bioclastic limestone and thin shale beds has a potential of accepting 50 million metric tons of CO<sub>2</sub>. Available simulation data, with multiple geological realizations and injection scenarios, were used for the AI model training, validation, and testing. Performance of the wafer scale engines vs central processing units was compared using Neocortex, AI supercomputer at the Pittsburgh Supercomputing Center. Several levels of the AI model complexity were tested on permeable and fractured semi-permeable shale layers. Simple models were not able to accurately capture the patterns in CO<sub>2</sub> pressure distribution across the heterogeneous layer structure. More complex models were able to achieve high levels of precision and prediction accuracy using the loss scaling to overcome the half-precision floating-point format limitations.

### 3.3 (14:00-14:30) Direct Air Capture Deployment Assessment in Deep Mitigation Pathways Toward 2075 in the U.S.: MARKAL-NETL Modeling Results

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The study examines the MARKAL-NETL modeling results for the U.S. deep decarbonization scenarios with a specific focus on Direct Air Capture (DAC) technologies. With the emergence of DAC as a valuable Carbon Dioxide Removal (CDR) option, it is important to study the following:

- Scaling possibilities of DAC technology deployments in the U.S. under different scenario guidelines.
- Assessment of the deployment potential for different DAC technologies in the short- and long-term future.
- The impact of DAC technological advancements, delays in carbon capture and storage (CCS) technology deployments, and policies on short- and long-term DAC deployment.

MARKAL-NETL is an optimized, bottom-up, linear programming energy system model that identifies the optimal fuel and technology mixes to achieve the lowest energy system cost while meeting energy service demands and constraints. This allows the U.S. energy system to be modeled for 2010–2075 in five-year increments. MARKAL-NETL computes an inter-temporal, partial equilibrium on energy markets, meaning the quantities and prices of fuels and commodities are in equilibrium, and investments made in any given period are optimal over the time horizon as a whole. Each of the U.S. census regions in MARKAL-NETL is modeled as a distinct energy system with different regional costs, resource availability, existing capacity, and end-use demands, and regions are connected through a trade network. For this study, we examine the seven scenarios presented in Table 1.

**Table 1. Scenarios and Scenario Definitions**

Scenarios	Scenario Abbreviations	Scenario Definitions
Reference	Reference	No new climate policy after early 2022
Net-zero reference	Net Zero	U.S. energy system-wide net-zero carbon dioxide (CO <sub>2</sub> ) emissions defined as a linear CO <sub>2</sub> emissions reduction from 2020 to net-zero emissions by 2050; default assumptions for technology costs, complementary policies, and consumer preferences; CO <sub>2</sub> trade among census regions is allowed
Net-zero reference scenario with IRA	Net Zero IRA	U.S. energy system-wide net-zero CO <sub>2</sub> emissions with the Inflation Reduction Act of 2022 (IRA) provisions
Net-zero scenario with advanced DAC technologies	Net Zero DAC	U.S. energy system-wide net-zero CO <sub>2</sub> emissions with optimistic assumptions regarding the technology costs of DAC technologies
Net-zero scenario with advanced DAC technologies and IRA	Net Zero IRA DAC	U.S. energy system-wide net-zero CO <sub>2</sub> emissions with the Inflation Reduction Act of 2022 (IRA) provisions and optimistic assumptions regarding the technology costs of DAC
Net-zero reference scenario with CCS	Net Zero CCS-10	U.S. energy system-wide net-zero CO <sub>2</sub> emissions with a 10-year delay of power generation with CCS technologies

deployment delays		
Net-zero scenario with carbon capture and storage (CCS) deployment delays advanced DAC technologies	Net Zero CCS-10 DAC	U.S. energy system-wide net-zero CO <sub>2</sub> emissions with a 10-year delay of power generation with CCS technologies and optimistic assumptions regarding DAC technologies

Two groups of DAC technologies have been identified as the most promising from technical and economic perspectives—liquid solvent DAC and solid solvent DAC. Solid solvent DAC technologies are still in the earlier research stage and estimates of their costs and technical characteristics vary widely. We included the following liquid solvent DAC technologies into the model: high-temperature DAC (natural gas input), high-temperature DAC (fully electric), and high-temperature DAC (natural gas and electricity input). The results demonstrate that to achieve the Net Zero CO<sub>2</sub> emissions by 2050 with minimal mitigation actions, significant scaling of CDR in the U.S. is an enabling factor, accounting for 60 percent or more of avoided CO<sub>2</sub> emissions annually in some scenarios. The potential scale of DAC technologies and their impact on decarbonization depend on future costs and performance of the technology, potential policy actions, and the status of CCS technologies deployment.

## SESSION 4 (13:00-15:00) Value-Added Products from Coal – 2 Richard Winschel

### 4.1 (13:00-13:30) Novel PRB Coal Based Asphalt

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A novel coal-to-chemicals conversion process has recently been developed, utilizing bio-based solvents to liquefy Powder River Basin (PRB) subbituminous coal WRI and UWSER have been at the forefront in developing the utilization of coal-derived feedstock in asphalt binder formulation and as an extender for traditional paving grade asphalt. Pilot-scale preparation of PRB coal extract has been developed to produce the coal-based asphalt binder. Blending this extract with conventional asphalt binders showed how the material can act as an extender for petroleum-based asphalt by rheological characterization following Superpave standards. Coal-based asphalt binder was formulated through polymer modification using SBS, and the blends were analyzed by standard DSR techniques and the Multiple Stress Creep Recovery test (MSCR). These tests indicate substantial enhancements in rutting resistance, elastic recovery, and low-temperature relaxation properties. Furthermore, strategies were devised to improve the oxidation stability of the coal-based asphalt binder, including continued alkylation and thermal soaking, yielding promising outcomes in generating softer materials with improved aging behavior by size exclusion chromatography and SAR-AD compared to a standard petroleum-based asphalt. These findings advance our understanding of coal-derived asphalt's viability as a durable pavement material and could significantly reduce carbon emissions associated with flexible pavements, offering a promising avenue for sustainable infrastructure in the future.

### 4.2 (13:30-14:00) A Novel Approach to Manufacturing Lignite Composites with High-Filler Content

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This study pioneers the application of friction extrusion to produce high filler-content lignite composites with high mechanical performance. We describe the manufacturing of high-density polyethylene (HDPE) based lignite composite rods and bars with ~80 wt.% lignite fillers. We discuss the effect of tooling geometry on the extrudability of the high filler content composites. We also explore the effect of process conditions on the flexural and tensile properties of the extrudates. The resulting flexural strength and modulus of the as-extruded bar, ~35 MPa and 3 GPa respectively, are on par with commercial decking material properties. We attribute the enhanced mechanical performance to the high filler content in the composites as well as the increased interaction between the filler and polymer matrix owing to high extrusion forces. This breakthrough opens avenues for ShAPE technology in the development of carbon-negative construction materials, including high-quality commercial decking, flooring, and furniture.

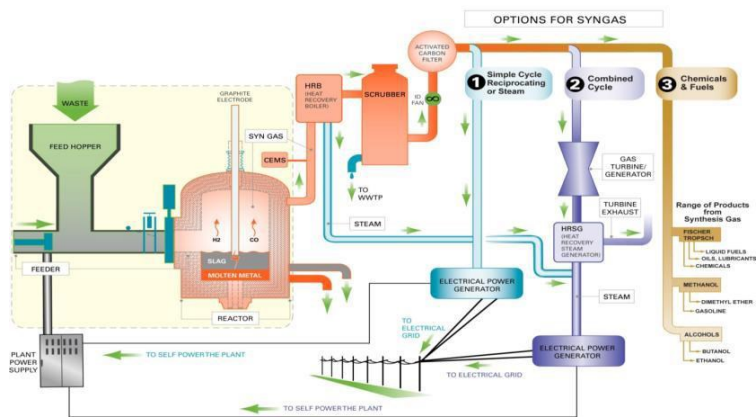
**Keywords:** Friction Extrusion, lignite composites, building materials, decking, flexural strength, and modulus.

#### 4.3 (14:00-14:30) Rock Wool Spun from Vitrified Coal Fly Ash/Slag Is Very Profitable

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An electric arc furnace (EAF) is required to attain temperatures at or around 1600° C; besides breaking the second of two carbon bonds, which means that there will be no char going to the landfill, there are three, predictably distinct reactions of coal fly ash.

If the coal fly ash has any metals (REEs and/or ferrous oxides), due to their higher density, they will collect in the bottom of the furnace, to be reclaimed and cast into metallic ingots. The inorganic fraction will float over the metals and can be recovered as a vitreous slag like material, very similar to basalt, that can easily pass the EPA's TCLP (Toxicity characteristic leaching procedure) tests. This slag fraction can be tapped on a regular basis and can be converted to fiber, for the rock wool market or can be poured while still hot into cold water where it will fracture into a sand like material that has very good physical characteristics to be used as an aggregate. Rock or mineral wool is several orders of magnitude more valuable than the aggregate one. The organic fraction is gasified and leaves the furnace as a syngas. The syngas is a very clean syngas with minimum nitrogen. By controlling the chemical reactions in the furnace, the amount of CO<sub>2</sub> can also be reduced and controlled to very low levels.



CTC's Gasification Technology

#### 4.4 (14:30-15:00) Critical Elements for the Construction of a Sustainable Closure\* for CCR Impoundment

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An alternative safe, sustainable, and cost-effective closure approach was developed to close an estimated 500 coal combustion residual (CCR) impoundments in the U.S. The traditional closure approach for these impoundments typically involves dewatering and/or establishing a suitable sloped subgrade through import and placement of fill and/or significant regrading of the CCR material. The final cover consisting of lower permeability soil and/or a geomembrane overlain by a protective soil cover is then placed to accomplish closure. This closure approach is challenging considering the low strength and high compressibility of the CCR, requiring specialized construction equipment, extended construction time, and higher capital needs compared to closure over more stable materials.

In this paper, the recent successful construction of an alternative, patented closure approach will be discussed. This alternative approach included the construction of gently sloped interim berms to form isolated cells producing ephemeral characteristics that support habitation by native plants and animals, utilizing the original grades of the impoundment.

With approval of the Permit-to-Install from the Ohio EPA, construction activities began in 2019 for the closure of a 150-acre fly ash surface impoundment. Early focus was on dewatering activities and surface preparation using low ground pressure equipment. Geomembrane installation was performed to create "cells" using the near-flat surface grades of the CCRs as the design grades of the cell floors. Berms and weirs were constructed to discharge excess stormwater runoff through a central conveyance channel, with final discharge through the existing outlet. Construction was completed in Fall 2023, and no significant construction issues (e.g., liquefaction, subgrade support loss) were encountered.

\*US Patent 10,058,904 B2

### SESSION 5 (10:00 – 12:00) Coal Science/Clean Coal and Gas to Fuels Isaac Gamwo

#### 5.1 (10:00-10:30) Evaluation of temporal variations in the chemistry of exposed coal heaps

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The study investigates the temporal variations in the chemical composition of coal heaps exposed to open environmental conditions. Coal heaps, often generated from mining operations, undergo significant changes in their chemical properties due to factors such as weathering, oxidation, and microbial activity. Three coal heaps were prepared in the premises of M/s Maithan Power Limited in Jharkhand with coals from Bharat Coking Coal Limited, Central Coalfield Limited, and Eastern Coalfield Limited; subsidiaries of Coal India Limited. A systematic analysis was conducted on coal samples at different time intervals from open storage heaps to assess changes in key parameters, including moisture content, ash content, volatile matter (VM), fixed carbon (FC), and sulphur (S) content. The degradation of coal quality was observed through proximate analysis (moisture, ash, VM, FC), ultimate analysis (C, H, N, S, O), Gross Calorific Value (GCV), and the decrease of crossing point and ignition point temperature in coal was also observed over three months.

The research findings reveal notable fluctuations in these chemical constituents over time, emphasizing the impact of seasonal variations and environmental exposure on coal quality due to the long-time exposure of coal heaps in the open environment. The results highlight the need for effective management strategies for coal storage to mitigate adverse effects on coal properties, which are crucial for downstream applications in energy production and industrial processes. This research contributes to a better understanding of the dynamic changes in coal chemistry in open environments, providing insights for optimizing coal handling and utilization practices.

## 5.2 (10:30-11:00) Preparation And Catalytic Cracking Reactivity of Zsm-5 Zeolite from Vietnamese Quang Ninh Coal Ash

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The main components of coal fly ash (CFA) generated from coal-fired power plants are SiO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub>, which are the main components of zeolite, and thus one of the effective uses of CFA attracting much attention is the synthesis of zeolite. Vietnam has abundant reserves of various types of coals which are concentrated mainly in the Quang Ninh (QN), Thai Nguyen (TN), and Lang Son (LS) provinces. QN coal is well-known worldwide for its high quality. According to the analysis data for QN coal ash of our laboratory, Al<sub>2</sub>O<sub>3</sub> and SiO<sub>2</sub> amounts are the highest among three typical coals of Vietnam. In this study the effects of preparation conditions on the synthesis of ZSM-5 using the mixture of components similar to QN CFA and the real ash components obtained from the QN coal were investigated as there are very few examples of synthesis and utilization of ZSM-5 from CFA. In order to characterize the properties of ZSM-5 zeolites prepared, XRD, nitrogen adsorption/desorption and NH<sub>3</sub>-TPD were measured. Further, catalytic cracking of low-density polyethylene (LDPE) was estimated using Curie point pyrolyzer (CPP).

QN coal was calcined at 1200°C to obtain QN real coal ash. RQNCA-C-ZSM-5-CR150 (48h) <sub>52</sub>, where R means “real”, was prepared by the similar way to QNCA-C-ZSM-5-CR150 (48h) <sub>52</sub>, which was made by model components of coal ash, by using real coal ash instead of model components of coal ash. In this study, conventional ZSM-5 (C-ZSM-5) zeolite was also prepared as a comparative reference catalyst.

0.20 mg of LDPE (Polyethylene powder, low density, 500 μm, melt flow index: 17.5–23.5 g/10 min, Thermo Fisher Scientific Inc.) and 1.00 mg of catalysts were put together in ferromagnetic pyrolysis foil. The injector of the CPP apparatus was preheated at 150°C and the needle of the injector was introduced into the injection port of GC-FID (GC-2010 plus, Shimadzu Corp.). Pyrolysis was carried out at 500°C, 5 s, under He flow (0.6 MPa). Products were directly analyzed by the GC-FID. The detail of products identification was mentioned in previous reports.

In this paper QN coal real ash was used to prepare ZSM-5 zeolite using tetrapropylammonium hydroxide (TPAOH) at 150°C for 48h. It was confirmed from the results of XRD patterns and nitrogen adsorption/desorption measurement that ZSM-5 crystals appeared at higher than SiO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> ratio of 52 and developed completely at 78. The similar results were observed for ZSM-5 synthesis not only without QN coal ash components but also with model coal ash and real QN coal ash, indicating that the effects

of components on the preparation of ZSM-5 would be rather small. When these zeolites were used for the catalytic cracking of LDPE, ZSM-5 prepared using model coal ash components exhibited the same or slightly higher conversion than conventional ZSM-5. In contrast to this, ZSM-5 prepared with real coal ash components exhibited the slightly lower conversion, suggesting that the kinds of inorganic salts might affect the reactivity in catalytic cracking of LDPE.

## 5.3 (11:00-11:30) Enhanced phenanthrene hydrogenation saturation performance over nickel-based catalyst via adjusting the interaction between Ni and support

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Polycyclic aromatic hydrocarbons (PAHs) in coal tar are teratogenic and carcinogenic, thereby posing a threat to ecological and environmental protection, as well as human life and health. Converting and saturating phenanthrene from coal tar into naphthenic hydrocarbons is important for enhancing fuel utilization efficiency, safeguarding ecological and environmental integrity. In this study, the advantages of nickel-aluminum spinel catalysts in the field of phenanthrene hydrogen saturation were systematically investigated. NiAl<sub>2</sub>O<sub>4</sub> and Ni/Al<sub>2</sub>O<sub>3</sub> catalysts with the same element composition were prepared by sol-gel method and impregnation method, respectively. The experimental results showed that under the conditions of 300 °C, 5.0 MPa, the feedstock of 1.0 wt% phenanthrene in decalin and weight hourly space velocity (WHSV) of 0.52 h<sup>-1</sup>, the phenanthrene conversion over NiAl<sub>2</sub>O<sub>4</sub> catalysts was up to 99.67 % and 93.94 % for perhydrophenanthrene yield, which is higher than that of traditional Ni/Al<sub>2</sub>O<sub>3</sub> catalysts (96.83 % and 77.25 %, respectively). Characterizations showed that the superior phenanthrene hydrogenation saturation performance was attributed to the stronger H<sub>2</sub> dissociative adsorption capacity of the active metal Ni derived from NiAl<sub>2</sub>O<sub>4</sub>. Moreover, there is a stronger metal-support interaction between the active metal Ni and the support, which puts the active metal in an electron-deficient state and facilitates the adsorption and activation of PAHs.

**Keywords:** Phenanthrene; hydrogenation saturation; nickel-aluminum spinel; metal-support interactions.

## 5.4 (11:30-12:00) Blue Ammonia and Urea Production via Coal-Gasification

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As part of a global effort to mitigate the effects of climate change, many countries have restricted their coal usage due to its extensive greenhouse gas emissions. Creative solutions are needed to make use of this cheap and abundant resource without contributing to global emissions.

Fluor envisages a coal-gasification plant that produces blue ammonia or urea, capturing over 95% of the CO<sub>2</sub> generated in the process. Large international markets and extensive infrastructure already exist for both ammonia and urea. Beyond its most common use as a fertilizer precursor, the blue ammonia can be cracked into hydrogen for power generation in fuel cells or fed directly to combustion turbines blended with nitrogen. Conversely, blue urea can be sold as a synthetic fertilizer, a vital commodity in maintaining food production, or blue Diesel Exhaust Fluid (DEF) for diesel engine NO<sub>x</sub> control.

Regardless of the facility's configuration for ammonia or urea production, coal-gasification generates an H<sub>2</sub>-rich syngas for ammonia synthesis; the ammonia and CO<sub>2</sub> recovered from the shifted syngas can then be used to produce blue urea. The remaining CO<sub>2</sub> will be sequestered underground for federal tax credit. An ammonia configuration of the coal-gasification plant will yield more CO<sub>2</sub> to be sequestered than the urea configuration since CO<sub>2</sub> is utilized in urea synthesis.

Several design aspects distinguish this facility from other coal-gasification plants. Namely, sulfur from the coal feedstock will be recovered as high-purity sulfuric acid instead of its elemental form, which can be sold as a product. Additionally, the facility will be self-sufficient, requiring no import of power. Onsite power generation will utilize the H<sub>2</sub>-rich syngas, Pressure Swing Adsorption (PSA) off-gas, and steam generated in process units and the Heat Recovery Steam Generator (HRSG) to meet the entire facility's demand.

This presentation delves into the process, overall plant performance, and indicative capital/operating and maintenance (O&M) costs for a typical coal-gasification plant with high carbon capture that produces ammonia only and urea.

## SESSION 6 (10:00 – 12:00)

### Gasification Technologies

Massood Ramezan

#### 6.1 (10:00-10:30) The formation and evolution of pores during the pyrolysis of low-rank coal and its influence on products mass transfer

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Pore is a diffusion channel in the coal reaction process, and its structure not only affects the precipitation of small molecules but also has an important impact on the tar or gasification agent entering process. However, the formation of pores in coal is due to the release of volatiles during the generation of thermal condensation, and this structure evolves with temperature and reaction time. To investigate the impact of pore development and structural changes on the diffusion or mass transfer of volatiles during pyrolysis, this study employed a bench-scale reactor. Semi-coke samples were produced at varying final pyrolysis temperatures (200–800 °C).

The surface morphologies and pore structure parameters of coal particles at different pyrolysis temperatures were qualitatively and quantitatively analyzed by scanning electron microscope and specific surface and pore size analyzer. The results show that the formation of pores includes processes such as pore generation, expansion, coalescence, self-cracking, nested secondary pores, and pore shrinkage and collapse. The pores formed by low-rank coal are mainly micropores and mesoporous, and their structures are mostly cylindrical. The specific surface area of coke and the volume of micropores have the same variation trend, and under different relative pressures ( $p/p_0 < 0.5$  and  $p/p_0 > 0.5$ ), the adsorption of N<sub>2</sub> by semi-coke shows two different adsorption characteristics.

In order to describe the dynamic process of pore formation, the fractal dimension was calculated by the FHH (Frenkel-Halsey-Hill) equation to further characterize the complexity of pore structure. The results indicate that the formation of pores undergoes a process from simplicity to complexity, with the complexity of pore structures decreasing initially and then increasing during pyrolysis. Finally, the effective diffusion coefficients and Thiele modulus of four volatile components (CO<sub>2</sub>, H<sub>2</sub>O, H<sub>2</sub>, and CO) at 300–800 °C are calculated. The results show that the effective diffusion coefficients exhibit a trend of initial increase followed by decrease, which is consistent with the trend of porosity. The Thiele modulus, on the other hand, demonstrates a gradual increase, aligning with the trend of pore complexity during this stage. This suggests that the effect of diffusion resistance on the release of volatiles is positively correlated with the complexity of pores.

**Keywords:** semi-coke; pore structure; fractal dimension; effective diffusion coefficient; Thiele modulus

#### 6.2 (10:30-11:00) Building an Energy System Based on Thar Coal

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While the world moves away from Coal, Pakistan is forced to use its indigenous Black Gold to cut down its import bill. An energy system based on imported fuel is unsustainable and insecure.

The country's import bill is around \$25.2 billion which includes imported Coal worth \$2.0 billion and LNG \$2.5 billion. The huge Coal reserve (175 billion tons) at Thar remain grossly under-utilized. Mining challenges have been overcome. Two mines are now functional, each producing 7.6 million tons per year. Power generation has started with linkage to the main transmission grid. Successful gasification has also been achieved in collaboration with experts in South Africa.

Currently efforts are underway to start large scale gasification to build a Coal based affordable energy system for the country by application of Clean Coal technologies. Multiple products are planned that include SNG, Urea, Diesel, etc.

#### 6.3 (11:00-11:30) U.S. Department of Energy/National Energy Technology Laboratory Gasification Systems Program Overview

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The U.S. Department of Energy/National Energy Technology Laboratory's Gasification Systems program is developing innovative designs and technologies for clean hydrogen production from solid feedstocks, with net-zero or net-negative carbon emissions capability. The program is focusing on clean hydrogen production by efficient high-temperature, pressurized, oxygen-blown gasification of alternative feedstock (e.g., biomass, carbonaceous waste materials such as municipal solid waste containing waste plastics, or combinations thereof) with carbon capture technologies. The emphasis on clean hydrogen is in support of the Hydrogen Shot™, helping to meet the administration's goals of complete decarbonization of power generation by 2035 and the economy by 2050. Feedstock choices enable value-added utilization of wastes (legacy waste disposal and more) to address environmental justice and job creation initiatives. Finally, clean hydrogen production from gasification can be leveraged for fuels and chemicals production, in accord with the administration's Clean Fuels & Products Shot™ as well.

Research and development are underway under technical areas including:

1. Increased efficiency, higher efficiency gasifiers at the 5–50 megawatt-electric (MWe) scale.
2. Air separation technology at a similar scale with emphasis on non-conventional membranes or sorbents, oxygen carriers, and novel methods such as solid-state cryogenics.
3. Methods to attain clean hydrogen and negative carbon dioxide (CO<sub>2</sub>) emissions, such as alternative feedstock pretreatments and more efficient CO<sub>2</sub> capture and hydrogen separations.

Both experimental investigations and sophisticated modeling and simulations of gasification processes using advanced multiphase computational fluid dynamics tools, such as NETL's MFIX, are integral to the current work.

This presentation will provide a comprehensive overview of the Gasification Systems portfolio that is spurring advances in smaller-scale, process-intensified gasifiers using alternative feedstocks, novel and/or integrated oxygen production methods, alternative feedstock pretreatment methods, and hydrogen separations/CO<sub>2</sub> capture from syngas.

1. <https://www.energy.gov/eere/fuelcells/hydrogen-shot>
2. <https://www.energy.gov/eere/clean-fuels-products-shottm-alternative-sources-carbon-based-products>

#### 6.4 (11:30-12:00) Machine Learning Enhanced LIBS to Measure and Process Biofuels and Waste Coal for Gasifier Improved Operation

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Waste coal, coupled with biomass, as feedstock in gasifiers that produce hydrogen faces some challenges, such as the large heterogenic nature of the components, the slagging operation of the gasifier due to the ash content and composition of the coal waste and biomass blend, and the need to maintain tight control of the feedstock specifications. A machine learning (ML) enhanced Laser Induced Breakdown Spectroscopy (LIBS) concept has been investigated to measure the characteristics of the feedstock going into the gasifier in situ and in near real-time, resulting in time-sensitive fuel data that gasifier operators can use in a feedback or feedforward control schemes to maximize performance and mitigate the deleterious impact of feedstock ash properties on gasifier operation. LIBS is capable of measuring the elemental spectroscopic emissions of the feedstock while it is flowing over a belt. The LIBS spectral is then processed by ML algorithms, which produce data to be used by either plant operators or by a feedback or feedforward automatic control system. LIBS-ML methods with both supervised and unsupervised neural networks, along with self-organizing maps, achieved root-mean-square errors (RMSEs) in the lab for measuring elemental concentration and higher-order parameters compatible with dedicated laboratory-grade instrumentation. Python was utilized to implement the ML algorithms in this study. By leveraging Python's robust libraries, such as scikit-learn, TensorFlow, and Keras, various methods, including Linear Regression, Decision Trees, Support Vector Machines, Random Forest, Neural Networks, and Gradient Boosting, were applied to the LIBS's measurement data set for Al, Ca, Fe, Mg, Na, Si, Ti, K, and C, to predict laboratory analysis results which included the heating value of material, ash composition, carbon composition, and sulfur composition, as well as SiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, Fe<sub>2</sub>O<sub>3</sub>, CaO, MgO, K<sub>2</sub>O, Na<sub>2</sub>O content. Different input parameters were used to predict each output; for instance, carbon content was based on the C, Ti, Al, O, and Mg elemental spectroscopic emission intensities, and ash content was based on Al, Ca, Fe, Mg, Na, Si, Ti, and K elemental spectroscopic emission intensities. Best results were achieved with an ensemble method with normalization and gradient boosting. Different hyperparameters were applied to maximize the R<sup>2</sup> value and minimize RMSE for the training and test data sets. As a result of the hyperparameter iteration, the ensemble method's main subgroups were selected as the Support Vector Regressor, Random Forest Regressor, and Multi-Layer Perceptron Regressor. With the ensemble method with normalization, the lowest R<sup>2</sup> value of the test data set is 0.896, which occurred for Al<sub>2</sub>O<sub>3</sub>. The Gradient Boosting Method is the best alternative way to maximize R<sup>2</sup> value for the dataset. With the gradient boosting regressor model, the lowest R<sup>2</sup> value of the test data set is 0.89, which occurred for MgO.

## SESSION 7 (13:00-15:00)

### Carbon Management -3

Omar Basha

#### 7.1 (13:00-13:30) Advancements in Methane-to-Methanol Conversion Technologies: A Review

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Methane conversion to methanol presents a promising pathway for reducing greenhouse gas emissions while efficiently utilizing methane as a resource. Methanol serves as a versatile platform chemical with broad applications in industries such as fuel synthesis, chemical feedstocks, and formaldehyde production. This presentation provides a literature overview of advancements in methanol production technologies, with a focus on both one-step and two-step conversion processes.

One-step direct methane-to-methanol (DMTM) processes are particularly attractive for their simplicity, as they convert methane directly into methanol without the need for intermediate steps. However, challenges remain, particularly in achieving high selectivity and catalyst stability while minimizing the formation of undesired by-products, such as carbon monoxide and carbon dioxide. Recent research efforts have introduced novel catalytic materials and reactor configurations aimed at addressing these issues and improving methanol yield.

On the other hand, two-step processes—typically involving the conversion of methane to synthesis gas (syngas) followed by methanol synthesis—are more established and offer better control over reaction parameters and product distribution. These processes, however, are more capital-intensive and operationally complex due to the additional steps of syngas generation and separation.

This presentation will discuss the technical and economic aspects of one-step versus two-step methane conversion processes, based on computational and experimental studies. Key considerations, such as catalyst design, reactor configuration, and process scalability, will be examined. Additionally, trade-offs between operational complexity and process efficiency will be discussed, offering insights into the industrial applicability of each approach.

#### 7.2 (13:30-14:00) TEA of the SMR-CCS Process for Blue Hydrogen Production Using Thirty-Six Physical Absorbents

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Hydrogen is highly recognized as a key component in the global transition to a sustainable energy future. It can be produced through water electrolysis, gasification of coal and/or biomass, methane pyrolysis, and steam methane reforming (SMR) [1]. In the US, 95% of hydrogen is currently produced via SMR [2]. To reduce CO<sub>2</sub> emissions, SMR must be integrated with carbon capture and sequestration (CCS), leading to blue hydrogen production [3]. In 2018, Lewis et al. at the US-DOE/NETL [4] simulated and conducted Techno-economic Analysis (TEA) of an SMR-CCS process for blue H<sub>2</sub> production which had the following features: (1) The entire shifted fuel gas stream from the water gas shift (WGS) reactor was sent directly to a pre-combustion CO<sub>2</sub> capture process using Methyldiethanol amine (MDEA) as a chemical solvent. From this process, the captured CO<sub>2</sub> was compressed in preparation for sequestration, whereas the clean fuel gas was sent to a Pressure Swing Adsorption (PSA) unit operating at adsorption pressure of 22.8 bar and desorption pressure of 1 bar. (2) From the PSA unit, pure H<sub>2</sub> was produced, whereas the off-gas (CH<sub>4</sub>, CO, and H<sub>2</sub>) was combined with a split stream of the natural gas used as a feed to the SMR-CCS process for combustion with an air stream to provide the heat required for the SMR. (3) The resulting post-combustion flue gas containing about 7 mol% CO<sub>2</sub> was then sent to the CANSOLV unit for CO<sub>2</sub> capture using a chemical solvent (concentrated amine).

The objective of this study was to modify the 2018 DOE/NETL's SMR-CCS process so as to improve its performance and flexibility. The key modifications were: (1) The entire shifted fuel gas stream from the WGS reactor was sent directly to a hydrogen-selective membrane (polybenzimidazole - PBI) to separate the gas into an H<sub>2</sub>-rich "permeate" and a CO<sub>2</sub>-rich "retentate". (2) The permeate was sent to a PSA unit operating at adsorption pressure of 24.5 bar and desorption pressure of 1 bar. From the PSA unit, pure H<sub>2</sub> stream was produced, whereas the off-gas (CH<sub>4</sub>, CO, and H<sub>2</sub>) was combined with a split stream of pure H<sub>2</sub> from the PSA for combustion with an air stream to provide the heat required for the SMR. The resulting post-combustion flue gas contained negligible amount of CO<sub>2</sub>, leading to the elimination of the expensive CANSOLV unit. (3) The retentate was sent to the CO<sub>2</sub> capture process, wherein with the aid of a compressor, the partial pressure of CO<sub>2</sub> was increased allowing the use of several effective physical solvents for CO<sub>2</sub> capture. The captured CO<sub>2</sub> was then compressed in preparation for sequestration, whereas the clean fuel, containing mainly methane (CH<sub>4</sub>), was recycled back to the SMR.

The modified SMR-CCS process was modeled in Aspen Plus V.12.1 with custom models for the PSA and the hydrogen-selective membrane created in Aspen Adsorption V.12.1 and Aspen Custom Modeler V.12.1, respectively to produce H<sub>2</sub> with a purity of over 99.98 mol%. The CO<sub>2</sub> capture process was carried out in a fixed-bed packed with Mellapak 250Y under the constraint of over 97 % of CO<sub>2</sub> capture from the shifted fuel gas using thirty-six (36) physical solvents, including 3 Beta-Amino Carboxylate (BAC), 11 Ionic Liquids (ILs), 5 Hydrocarbons (HCs), 7 Oxygenated Hydrocarbons (OHCs), 2 Nitrogenized Hydrocarbons (NHCs), 5 Cyclical Hydrocarbons (CycHCs), and 3 Polymers. The characteristics of the required hydrogen-selective membrane

(polybenzimidazole - PBI) membrane and PSA unit were calculated based on the shifted fuel gas rate of 437 ton/h at a pressure of 24.5 bar and a temperature of 204 °C. Also, the hydraulics and mass transfer characteristics in the CO<sub>2</sub> capture process using physical solvents were calculated, including flooding, pressure drop, liquid holdup, gas and liquid mass transfer coefficients, and normalized specific packing wetted area. Moreover, the TEA of the entire modified SMR-CCS process was conducted to obtain the Capital Expenditure (CAPEX), Operating Expenditure (OPEX), Fuel Expenditure (FEX), Levelized Cost of CO<sub>2</sub> Capture (LCOC), and Levelized Cost of H<sub>2</sub> Production (LCOH). A comparison between the modified and the original 2018 DOE/NETL's SMR-CCS process revealed that the modified process had superior performance metrics, including higher H<sub>2</sub>/CH<sub>4</sub> and H<sub>2</sub>/CO<sub>2</sub> ratios, lower CAPEX and lower LCOH. Furthermore, among the thirty-six solvents used, 1AB-DECAM with the highest CO<sub>2</sub> solubility was found to be the most economically viable solvent because it delivered the lowest LCOC at \$20.80/ton.CO<sub>2</sub> and the lowest LCOH at \$0.93/kg.H<sub>2</sub>.

In addition, an Artificial Neural Network (ANN) with 10-inputs, 2-hidden layers and 7-outputs was developed in MATLAB using the TEA results calculated for the modified SMR-CCS process using Aspen Plus V.12.1. The ANN was able to predict the CAPEX, OPEX, FEX, LCOC, and LCOH values with high statistical accuracies (The coefficients of determination (R<sup>2</sup>) was 0.9967, and the maximum Absolute Average Relative Error (AARE) was 1.16%). Also, the ANN predicted the TEA values for two solvents Icosane (C<sub>20</sub>H<sub>42</sub>) and Tetraethylene Glycol (C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>), which were not included in its training, eliminating the need for conducting Aspen Plus simulations under these conditions. Thus, the ANN model, within the ranges used in its development, is a highly effective machine learning (ML) tool, offering significant time savings in evaluating numerous physical solvents for use in the SMR-CCS process for blue hydrogen production.

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- [2] DOE. "Hydrogen Production: Natural Gas Reforming." <https://www.energy.gov/eere/fuelcells/hydrogen-production-natural-gas-reforming> (accessed).
- [3] O. Massarweh, M. Al-khuzaei, M. Al-Shafi, Y. Bicer, and A. S. Abushaikha, "Blue hydrogen production from natural gas reservoirs: A review of application and feasibility," *Journal of CO<sub>2</sub> Utilization*, vol. 70, p. 102438, 2023, doi: <https://doi.org/10.1021/ef0500538>.
- [4] E. Lewis *et al.*, "Comparison of commercial, state-of-the-art, fossil-based hydrogen production technologies," National Energy Technology Laboratory (NETL), Pittsburgh, PA, Morgantown, WV, US, 2022.

### 7.3 (14:00-14:30) Performance of Anthracite Coal-Derived Activated Carbon in Adsorbing CO<sub>2</sub> across Different Gas Concentrations

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This study investigates the CO<sub>2</sub> adsorption performance of anthracite coal-based activated carbon (ACAC) prepared via chemical activation using NaOH and K<sub>2</sub>CO<sub>3</sub> across a range of concentrations. Anthracite coal obtained from Blaschak underwent modification at temperatures spanning 500°C to 900°C with varying mass ratios of modification agents to carbon and was subsequently ground to particle sizes below 355 μm to optimize surface area and porosity. CO<sub>2</sub> adsorption experiments were conducted

at 25°C under three distinct conditions: directed air capture (0.04% CO<sub>2</sub>), lower concentration (4% CO<sub>2</sub>), and higher concentration (13% CO<sub>2</sub>) environments. The study identified the optimal ACAC formulation achieving a CO<sub>2</sub> adsorption capacity of 3.63 mmol/g at 1 bar and 0 °C following treatment with NaOH. Comparative analysis with commercial granular activated carbon (GAC) BPL showed that ACAC exhibited either comparable or superior performance, with adsorption percentages of 25.81% and 16.80% in lower and higher concentration environments, respectively, compared to BPL's 18.79% and 9.95%. Evaluation metrics such as sustained adsorption time, effective adsorption period, total adsorbed concentration, and breakthrough concentrations further supported ACAC's efficacy, highlighting its suitability for applications requiring efficient CO<sub>2</sub> capture, especially under higher concentration conditions. These findings underscore ACAC's potential as an effective and versatile sorbent for mitigating CO<sub>2</sub> emissions in diverse environmental and industrial settings.

### 7.4 (14:30-15:00) Impact of a bluff-body on pressurized oxy-combustion

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Designing an effective burner is vital for the development of pressurized oxy-fuel combustion (POC) technologies. To address this need, turbulent jet diffusion burners are adopted for POC in this research, with a bluff-body employed to create a recirculation zone to stabilize the flame. The objective of this numerical work is to perform a systematic analysis of the characteristics of such a pressurized non-premixed flame. Specifically, a 15-bar POC combustor of power 100 kW is modeled by means of Reynolds-averaged Navier-Stokes (RANS) technique via Ansys FLUENT commercial platform. The present work focuses on identifying the aerothermodynamic features of the isothermal and reacting flow with a disk-shaped bluff-body. It is shown that the fuel-oxidizer stream momentum ratio has a great impact on the temperature profile of the down-fired, co-axial, pressurized oxy-coal, diffusion flame. Moreover, a parametric study on the width of the burner tip identifies an optimal range for this pressurized burner.

## SESSION 8 (13:00-14:30)

### Clean Coal Demonstration and Commercial Projects

Thomas Sarkus

#### 8.1 (13:00-13:30) A Random Walk Through...NETL's Commercial Success Stories

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The U.S. Department of Energy's (DOE's) National Energy Technology Laboratory (NETL) has a rich history that stretches back through several predecessor organizations to 1910. This lengthy history spans three broad eras: mining safety, synthetic fuels research & development, and environmental technologies. This presentation will cover some of NETL's greatest success stories in these and other areas, including some that may surprise you. Commercialization or non-commercial application factors and approaches will be addressed, as will approximate levels of market acceptance. Hopefully, you will gain a better understanding and appreciation for the role of government-funded research, development, and technology demonstration and the contributions that NETL has made to the nation and the world over the past 114 years right up to the present day.

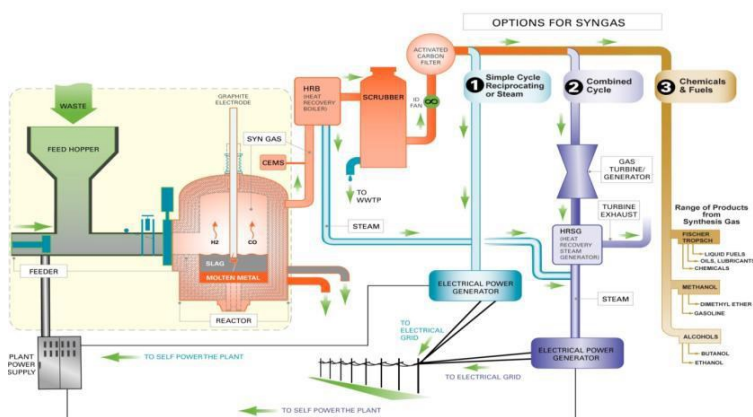
## 8.2 (13:30-14:00) Planned Unit Will Produce Ree Alloys for Permanent Magnets

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Concurrent Technologies Corporation (CTC) has received funding to design and is constructing a demonstration-sized electric arc furnace (EAF) that will achieve multiple high temperature gasification goals. The high temperature furnace is superior to those that Hitachi Metals has sold and that operate in China, because CTC's furnace achieves higher temperatures (Hitachi 1900 degrees centigrade and CTC's 3400 degrees centigrade). See our attached 2021 IPCC Paper. The NEWS is that the demonstration unit, if successful, completes the domestic supply chain: the United States would be in a position to produce alloys or metallic neodymium iron boron (NdFeB) permanent magnets. CTC has the capability to 3-D print these metallic magnets.

### Critical Smelting Temperatures for REE's

Name	Symbol	No.	Melting Temperature
Neodymium	Nd	60	2477°C
Boron	B	5	2077°C
Iron	Fe	26	1600°C



CTC's Gasification Technology

## 8.3 (14:00-14:30) Status of DOE Carbon Management Demonstration and Large Pilot Plant Projects

Thomas A. Sarkus, National Energy Technology Laboratory (NETL), U.S. Department of Energy (DOE)

A good number of large pilot plant and demonstration scale projects are being funded thanks to the Infrastructure Investment and Jobs Act (IIJA) and the Inflation Reduction Act (IRA). This presentation will summarize and list the large pilot and demonstration projects presently being funded by DOE in point-source carbon capture, direct air capture (DAC) or carbon dioxide removal (CDR), CO<sub>2</sub> transport, and CO<sub>2</sub> storage. Maps will also be shown to illustrate the nation-wide coverage of these DOE carbon management programs.

### SESSION 9 (10:00 – 12:00)

#### Clean Hydrogen

Thomas Sarkus

## 9.1 (10:00-10:30) Design of Non-Fluorinated Proton Exchange Membranes from Poly(Terphenyl Fluorenyl Isatin) with Fluorene-Linked Sulfonate Groups and Microblock Structures

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Proton exchange membranes (PEMs) are crucial components in energy storage and conversion devices, such as fuel cells and electrolyzers. Currently, perfluorosulfonic acid (PFSA)-based membranes and ionomers dominate PEM applications due to their high proton conductivity, mechanical robustness, and durability. However, their high costs, relatively high H<sub>2</sub> crossover, and environmental concerns have driven the search for PFSA alternatives. Hydrocarbon-based membranes offer potential solutions to these challenges.

In this study, we developed a series of non-fluorinated PEMs from poly(terphenyl fluorenyl isatin) with fluorene-pendent bisulfonate groups. These polymers exhibit a microblock structure, consisting of hydrophobic blocks, hydrophilic blocks, and alternating blocks, due to the varying reactivity and solubility of the hydrophobic p-terphenyl and the hydrophilic bisulfonated fluorene monomers. Consequently, the sulfonic acid groups are unevenly distributed along the polymer chains. This microstructure, along with the degree of sulfonation, significantly influences the comprehensive properties of the membranes.

The presence of microblocks and hydrogen bonding between amide groups ensures a phase-separated morphology, contributing to the membranes' excellent properties and performance. These include strong mechanical strength (47.1-63.2 MPa), high thermal stability (up to 250°C), excellent oxidative stability (<1% weight change in Fenton's reagent at 80°C for 1 hour), low swelling ratio (18-25% at 80°C), and high proton conductivity (136-169 mS/cm in pure water at 80°C). Additionally, the membranes exhibit >3x lower hydrogen crossover (0.55 mA/cm<sup>2</sup>) than Nafion 212 (1.76 mA/cm<sup>2</sup>) (tested at 80°C, 100% RH), providing the potential ability to go to thinner membranes, which will enhance energy efficiency. These metrics are approaching those of commercial Nafion membranes, highlighting their great potential for use in fuel cells and electrolyzers.

## 9.2 (10:30-11:00) Thermo-catalytic Decomposition of Natural Gas for Clean Hydrogen and Premium Carbon Using Electric Fields

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Thermo-catalytic Decomposition (TCD), an alternative energy technology, produces "turquoise" hydrogen by decarbonizing fossil fuels such as natural gas or coal-derived volatiles or heavy hydrocarbons, providing a bridge to the hydrogen economy. TCD of methane is an attractive alternative to conventional steam reforming because the process does not generate CO/CO<sub>2</sub> byproducts or consume water resources, eliminating the need for water-gas-shift and CO<sub>2</sub> removal stages. A limitation is the deactivation of the carbon catalyst, more specifically the depositing carbon exhibits lessening activity with reaction duration. Complementing TCD is regeneration. Partial oxidation by CO<sub>2</sub> creates new active sites, thereby renewing carbon catalyst activity, but only temporarily. The regeneration of deactivated carbon from TCD is analogous to coal gasification. A potential solution to maintaining carbon reactivity in both TCD and gasification (regeneration) may be to apply an external electric field. Neither TCD nor carbon oxidation have been tested under an electric field (E-field) for changes in activation energy or mechanism. For both reactions, an imposed E-field offers the possibility to maintain and potentially increase the reaction rate, occurring either by an increase in active site number or a shift in their energy level. Correspondingly, the associated activation energy for elementary reaction step(s) would also change.

Hypothesized here is that an applied E-field changes the reaction mechanism, manifested by activation energy and kinetics of deposition and regeneration. Two E-field configurations, low voltage, high current and low current, high voltage are being tested. Active site quantification and kinetic rate measurements are performed across a temperature-time matrix. Analytical techniques include XPS for quantifying active site number via chemisorbed oxygen, resolved by functional group and Raman for comparative defects. Kinetic rates are based on gravimetric measurement of deposited carbon in TCD, measurement of CO<sub>2</sub> concentration in regeneration by CO<sub>2</sub> or H<sub>2</sub> concentration in regeneration with H<sub>2</sub>O. Activation energies are extracted and evaluated for steadiness or change. Active site and kinetic dependence upon reactive gases and their concentrations are mapped parametrically as a function of applied E-field strength,

polarity, direction, and frequency. Therein changes in rates are resolved by active site number or activation energy under E-field action. Carbon catalyst metrics of activity and stability are assessed in TCD, and after regeneration to assess effectiveness. Reaction metrics include conversion and selectivity. Both metrics are quantified using on-line FTIR for gas analysis. In summary, aims to achieve process intensification utilizing the unique features of electric fields for modifying energy barriers and corresponding reaction rates.

### 9.3 (11:00-11:30) Performance Testing of a Moving-Bed Gasifier Using Coal, Biomass, and Waste Plastic Blends with Washed and Unwashed Legacy Coals and Other Waste Fuels to Generate White Hydrogen

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The objective of this effort, primarily funded by the United States Department of Energy (DOE), and led by the Electric Power Research Institute, Inc. (EPRI), with support by Hamilton Maurer International (HMI) and Sotacarbo S.p.A. (Sotacarbo), has been to qualify coal, biomass, and plastic waste blends based on performance testing of selected fuel pellet compositions in a pilot-scale updraft moving-bed (UDMB) gasifier. The testing provided 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 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 the focus. The gasifier used for testing is 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 (biomass). However, mixtures of these fuels with plastic wastes have not been prepared and gasified together. The three feedstocks were densified and pelletized by California Pellet Mill (CPM) to meet the feedstock size required by Sotacarbo's 30mm ID UDMB gasifier, under contract to HMI.

The technical tasks and results from this two-year research project included:

(1) Feed Procurement and Preparation: Nine different tri-fuel pellets were prepared from varying compositions of fresh mined PRB coal, corn stover biomass, and car fluff waste plastics. Tri-fuel pellets were produced by CPM and shipped to Sotacarbo's test facility in Carbonia, Sardinia, Italy.

(2) Test Plan Development: A test plan was created to define the test runs to be performed. The test plan detailed the different UDMB gasification tests to be performed in Sotacarbo's 12-inch ID pilot scale gasifier, the process monitoring instrumentation used, and the extractive samples recovered for analysis of the total gasification process mass and energy balance.

(3) Gasifier Testing: Nine different gasification runs were performed in the pilot-scale gasifier at Sotacarbo using nine different fuel feedstock compositions generated from varying mixtures of PRB coal, biomass, and plastic wastes. The testing generated performance data on gasification reaction efficiency and performance, yielding relevant data for models used to scale up the gasifier design. This task also included work to refurbish and reassemble the pilot gasifier at Sotacarbo and perform a baseline 100% PRB coal run.

(4) Data Analysis and Reporting: Review of the data, determination of figures of merit, and interpretation of the results are reported in the project's final report, published in March 2024. The results show that all tri-fuel pellets gasified well and maintained structural integrity throughout the gasification process. The syngas generated can be shifted to hydrogen by using commercial syngas shifting technologies.

(5) High Fidelity computational fluid dynamics (CFD) Simulation: The National Energy Technology Laboratory (NETL) team performed CFD simulations of the UDMB gasifier for two of the tri-fuel pellets gasified in Sotacarbo's pilot scale gasifier. The kinetic mechanisms for the pyrolysis of each constituent, PRB coal, corn stover biomass, and waste plastics are based on thermogravimetric analysis performed by Sotacarbo. The gasification model was validated by comparing the predicted syngas composition at the exit of the gasifier with the measured syngas composition. In addition, the reactor's measured internal temperature profile agreed well with the predicted internal reactor temperature profile. These results validate that the model can be used to predict the performance of the updraft moving bed gasifier for different feedstocks and operating conditions.

This paper summarizes the results of the completed work in which the pelletizing procedure was validated to ensure the viability of the tri-fuel pellets for the gasification runs performed at Sotacarbo's 30 mm UDMB gasifier. The gasification performance data from this series of nine runs will enable modeling of a full-scale HMI industrial scale gasifier supporting both combined heat and power, and Hydrogen production from coal (both fresh mined and legacy) combined with various biomass and waste plastics. Additionally, plans and progress on a follow-up project, being executed by the same project team, will be presented. In this project, a total of twenty (20) different feedstocks are being prepared from varying compositions of biomass (both woody biomass and corn stover) with a mixture of legacy coal waste, plastic waste, and refuse-derived fuel (RDF). The testing will provide information on gasification reaction efficiency/performance, yielding relevant data for models used to scale up the gasifier design to 50 megawatt electric (MWe) (equivalent hydrogen production). Tests will also be performed on a bench-scale fluidized-bed gasifier for comparison purposes. The results of this testing 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.

### 9.4 (11:30-12:00) HALO: Hydrogen-Recovery Using An Ai-Arc-Plasma Learning Operational System For Produced Water

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Oceanit will demonstrate field trials with the modular 10-50 kW HALO system equipped with plasma electrodes that takes minimal energy to convert produced water into valuable products, such as hydrogen. Industry partners include PIP Industries, Water Energy Services and Water Reuse Technology as wastewater solution experts that will provide supplemental equipment and site access for demonstration.

The US produces over 20 billion barrels of produced water annually. Produced water from oil and gas wells contains harmful chemicals that need to be treated before discarding/reuse. Hydrogen from produced water using electrolysis is challenging due to high levels of salt and other impurities requiring extensive pretreatments. HALO is a modular unit that when powered by renewable energy produces green hydrogen and clean water while reducing hazardous produced water waste.

By adapting Defense directed energy, Oceanit is building a unique 30-50L reactor with submerged electrodes. When powered optimal electrode configuration, arcs produce radical species nearby to split carbon and water into syngas. Hydrogen from syngas is then separated and purified. Early results point to hydrogen at under \$1/kg hydrogen. AI controls are implemented to modulate parameters dependent on solution properties to minimize energy consumed.

Transforming produced water into reusable products, such as hydrogen and value-added chemicals, provides a paradigm-changing mechanism for decarbonization in the energy industry. Oceanit proposes to enable this paradigm change by building and deploying a modular mobile resource recovery system known as HALO.

## SESSION 10 (10:00 – 12:00)

### Coal Bed Methane and Shale Gas

Richard Bajura

#### 10.1 (10:00-10:30) Analyzing Thanh Hoa, Ha Tinh and Nghe An coal samples of Vietnam

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Vietnam coals are distributed in many provinces of the country. In the previously papers, the authors studied coals in Quang Ninh, Thanh Hoa and Lang Son provinces. Studying coal samples in other provinces of Vietnam is necessary. This paper reported the analysis data of Thanh Hoa, Ha Tinh and Nghe An coal samples in Middle Zone of Vietnam. According to proximate analysis, Thanh Hoa coal sample is brown coal, Ha Tinh coal sample is lignite and Nghe An coal sample is sub-bituminous coal.

From the components of Thanh Hoa, Ha Tinh and Nghe An coal ashes and their XRD patterns, it is shown that Clinocllore 1Mla is inside Ha Tinh coal sample and Rhodochrosite is inside of Nghe An coal sample. Clinocllore 1Mla and Rhodochrosite are useful for human beings.

**Keywords:** sub-bituminous coal, brown coal, lignite, Clinocllore, Rhodochrosite, Thanh Hoa, Nghe An, Ha Tinh

## 10.2 (10:30-11:00) Research Progress and Key Scientific Issues Of Unconventional Natural Gas

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Unconventional sources of gas have recently gained much attention due to the significant contribution they are making to US gas production. Unconventional resources play an increasingly important role in the energy structure, unconventional resources in total energy take-up a small proportion. There are 5 key terms are used to distinguish different estimates of unconventional gas resources, namely: original gas in place, ultimately recoverable resources, technically recoverable resources, economically recoverable resources and reserves. China is rich in unconventional gas resources, the recoverable resources of tight gas amount to 11.3 trillion cubic meters; those of shale gas are 21.81 trillion cubic meters, and those of CBM shallower than 2000 m amount to 12.5 trillion cubic meters. Four key scientific issues including unconventional gas accumulation mechanisms, quantitative research on process of hydrocarbon generation-expulsion-migration-accumulation, law of fracture propagation and extended, and hydraulic fracturing & environmental protection have been expounded as well. Finally, typical challenges and future expectations are put forward.

## 10.3 (11:00-11:30) Understanding the Regional Variations in Pay Thickness of Unconventional Reservoirs in the Powder River Basin by Incorporating Learnings from a Site-Specific, Core-Calibrated, Geologic Model

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**Introduction:** Understanding geologic variations at the basin scale provides guidance for unconventional hydrocarbon exploration, allowing operators to efficiently strategize the development of their assets. An approach to identify and map pay zones for unconventional plays was developed for the Powder River Basin (PRB) based on knowledge learned from core data obtained as part of the US Department of Energy (DOE) field laboratory program, *Unlocking the Tight Oil Reservoirs of the PRB*. For the Turner Sandstone, pay zones were selected using specific wireline log cut-offs for gamma ray, bulk density, caliper, and water saturation curves initially found over cored intervals. For the Mowry Shale, pay zones are based on regional core analysis, Middle Member, and bentonite thicknesses, as well as thermal maturity.

**Methods/Procedures/Process:** Lithofacies in the Turner Sandstone were identified in hand samples. When compared to core-derived reservoir properties, these lithofacies identified a high-quality pay interval, with high porosity and oil saturation. The Turner Sandstone horizon was interpreted using well logs from 2,244 wells across the PRB. Petrophysical cutoffs correlating to the pay interval assessed pay thickness, and isopach maps were subsequently gridded. Cutoffs included a gamma ray value of less than 100 API, bulk density less than 2.50 g/cm<sup>3</sup>, caliper of less than 9 inches, and a calculated Simandoux water saturation of less than 70%.

Core analysis of the Mowry Shale shows the Middle Member exhibits the highest porosity, permeability, and total organic carbon values, and lowest water saturation. 1,180 wells with logs were used to measure the Middle Member thickness to generate an isopach map and calculate reservoir properties. 102 wells with Tmax thermal maturity data were gridded to cut off areas of the PRB outside the oil and gas generation window. Finally, total bentonite thickness within the Mowry Shale was calculated using

normalized gamma ray logs with values above 185 API. Bentonite beds can create fluid barriers when hydraulically fracturing the reservoir and can lead to less stimulated volumes.

**Results/Conclusions:** Increases in calculated pay thickness in the Turner Sandstone correlate with geographic locations of existing producing fields. Particularly in the Finn-Shurley field, the most productive field within the Turner Sandstone, pay thickness approaches as much as 65 feet. Pay thickness also increases over thermally mature areas of the PRB and known unconventional fields such as K-bar and Crossbow.

The Middle Member of the Mowry Shale is thickest (>180 feet) on the northwest flank of the PRB and thinnest in the southern portion of the PRB (~30 feet). However, thermal maturity trends do not coincide with thickness. The flanks of the PRB are in the early oil generation window. Generally corresponding with structural depth, the highest thermal maturation of the Mowry Shale occurs near the basin axis, where maturities reach the dry gas generation window. Bentonite thicknesses did not show a regional trend and vary on the local level from 10 to 30 feet.

**Applications/Significance:** The DOE field laboratory program contributed crucial findings for identifying novel productive zones in the Turner Sandstone and Mowry Shale. Combining modern geophysical logs and core data from this project with publicly accessible data such as well logs and thermal maturity values basin-wide makes it possible to understand favorable oil and gas productivity zones. Data from these methods can also be used to assist potential acreage acquisitions or for estimating total resources available for extraction in the basin.

## 10.4 (11:30-12:00) Road Traffic Density Analysis and Multi-Objective Optimization of Coal Hauling Trucks Selection by Considering Cost and CO<sub>2</sub> Emissions towards Cleaner Mining Production: Case Study of PT ABC

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Indonesia announced its ambitious objective to reach net zero emissions (NZE) by 2060 during the UN Climate Change Conference in 2021 (COP26). It was followed by the submission of the Enhanced Nationally Determined Contribution (NDC) document in 2022 as a document on energy transition in Indonesia, aligned with the Long-Term Low Carbon and Climate Resilience Strategy (LTS-LCCR) 2050 with a vision to achieve NZE by 2060 or sooner. One of the most impacted industries by the NZE initiative and Enhanced NDC document is the mining industry, particularly coal mining. Coal mining contributes the most to non-tax state revenue (PNBP), accounting for more than 80% in 2020–2023. Therefore, coal mining companies in Indonesia need to adjust their strategies to positively impact the NZE target.

In this research, we study the coal hauling of PT ABC, which transports coal from the coal processing plant (CPP) to the port using several types of trucks. PT ABC plans to produce approximately 25 million tons of coal in 2024 and increase production capacity to around 50 million tons the following year. The increase in production capacity will affect the number of trucks required for coal hauling, impacting traffic density and CO<sub>2</sub> emissions. According to government regulations, the maximum allowable traffic density for coal hauling should not exceed 80%.

This research aims to optimize the current truck combinations by selecting the cheapest option and the one that produces the least CO<sub>2</sub> emissions while considering traffic density limitations. Three scenarios will be considered:

1. Business as usual using gasoline trucks
2. Environmentally conscious scenario using belt conveyors
3. Environmentally conscious scenario using electric vehicles (EV) trucks.

A mixed-integer linear programming (MILP) with multi-objective optimization (MOO) will be used, employing the epsilon-constraint method. The cost and CO<sub>2</sub> emissions from all scenarios will be analyzed to determine the optimal strategy for PT ABC's coal hauling.

**Keywords:** CO<sub>2</sub> emissions, coal hauling, coal mining, epsilon-constraint method, mixed-integer linear programming, net zero emission, traffic density

**SESSION 11 (13:00-14:30)**  
**Rare Earth Elements/Energy Storage**  
*Richard Winschel*

**11.1 (13:00-13:30) Photoelectrocatalytic Hydrogen Production from Seawater Using Element-Doped TiO<sub>2</sub> Nanorods**

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As the global energy crisis intensifies, the search for clean and renewable energy sources has become imperative. Hydrogen energy is considered one of the most promising clean energy sources for the future. However, traditional methods of hydrogen production rely on freshwater resources, which are limited on Earth. In contrast, seawater is abundant, making the development of efficient photoelectrocatalytic seawater hydrogen production technology highly significant. TiO<sub>2</sub> is a commonly used photoanode catalyst, and one-dimensional nanomaterials like TiO<sub>2</sub> nanorods are particularly well-studied for their excellent photoelectrical properties and stability. This study aims to enhance the photoelectrocatalytic performance of TiO<sub>2</sub> nanorods through element doping, achieving efficient hydrogen production from seawater. In this study, TiO<sub>2</sub> nanorods were nitrogen-doped by annealing them in an NH<sub>3</sub> atmosphere. This method successfully introduced nitrogen into the TiO<sub>2</sub> lattice to improve its photoelectrocatalytic performance. Subsequently, the N-doped TiO<sub>2</sub> nanorods were characterized using techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), and photoelectrochemical testing. The results showed that N-doped TiO<sub>2</sub> nanorods exhibited significantly enhanced photoelectrocatalytic performance for seawater hydrogen production. Compared to undoped TiO<sub>2</sub>, the photoelectrocatalytic performance of N-doped TiO<sub>2</sub> improved by six times. This improvement is attributed not only to the narrowed bandgap and extended light absorption range of N-doped TiO<sub>2</sub> but also possibly to the ion-induced surface charge polarization of the catalyst in seawater, which further enhances the generation and separation efficiency of photogenerated charge carriers. This study demonstrates that element-doped TiO<sub>2</sub> is an effective method for improving photoelectrocatalytic performance. Nitrogen doping significantly enhances the photoelectrocatalytic seawater hydrogen production performance of TiO<sub>2</sub> nanorods. This provides new insights and approaches for the future development of efficient and low-cost photoelectrocatalytic seawater hydrogen production technology.

**Keywords:** Hydrogen energy; Photocatalysis; Doping; Semiconductor

**11.2 (13:30-14:00) Beyond Combustion – Coal in the 21st Century – Carbon Products from Coal**

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Coal is an important resource, both in the United States and around the world. The United States generates approximately 20 percent of its electricity through coal combustion and, at the current overall rate of consumption, has more than a 400-year supply of coal. According to the US Energy Information Administration, approximately 1 Gt of coal has been mined annually in the United States over the twenty-five-year period (1990-2014), although the 2022 total was 594 million tons. The recent decline in domestic coal production is due to the availability of inexpensive natural gas; carbon dioxide emissions; the retirement of many older coal-fired power plants; increasing electricity generation by renewable energy; and recent recessions.

In the United States, eighty percent of the coal produced is typically burned for power generation. In addition, substantial quantities of domestic coal are also used in the manufacture of steel, chemicals, and activated carbons, as well as for exports. Numerous industries, such as mining, power, rail transportation, manufacturing, chemical, steel, activated carbon, and fuels, are involved in the production, transportation, and use of coal. A second route for coal utilization is pyrolysis and gasification and they can be used to make value-added carbon products.

The United States has more than 4.4 billion tons of coal waste scattered across many sites throughout the nation. The United States Department of Energy's Carbon Ore Processing Program aims to develop value-added products from abundant supplies of domestic coal and coal waste. The program's goals include the following: cleaning up coal waste impoundments; driving down the cost of carbon product manufacturing; ensuring minimal environmental and workplace health and safety impacts; and securing domestic supplies of graphite. In addition, some other value-added products that can be made from waste coal include nanocarbons, carbon fiber, building materials, carborundum (silicon carbide), diamond films and high surface area activated carbons.

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**11.3 (14:00-14:30) Critical Mineral Supplies and Market Sector Demands for LIBs and EVs**

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From 2021 to 2026, the global permanent magnet market is projected to increase at a CAGR of 9.5%, representing an increase from 34.5 to 54.1 billion USD. Drivers for this growth include increased demand from general industrial applications and the automotive sector, with Asia Pacific representing one of the largest contributing regions. Industries that rely on permanent magnets include aerospace and defense, the automotive sector, consumer electronics, the energy and environmental sectors, general industries, medical technologies, and other applications.

Across consumer, defense, manufacturing, and power generation sectors, rare earth-based permanent magnets are valued for their superior coercivity. They are nominally referred to as neodymium iron boron (NdFeB) magnets, though the short acronym misses the praseodymium (Pr) and dysprosium (Dy) content, and the occasional inclusion of terbium (Tb). Dy and sometimes Tb are added to improve coercive stability at elevated temperatures during use.

The supply of neodymium (Nd) is limited in the US, which has little domestic production of rare earths and even smaller permanent magnet manufacturing. Increasingly, China dominates annual REE production, of which Nd, Pr, Dy, and Tb collectively account for a quarter by volume. Of the approximately 130,000 tons of NdFeB magnets produced worldwide in 2019, about 93% were sourced and produced in China.

EV (electric vehicle) demand is subject to more factors than wind energy, where investment translates into wind turbines, one of these factors being consumer acceptance. EVs merely displace the energy source; until renewables match the energy consumption represented by gasoline and diesel, they will only push fossil-based electrical production. Though the benefits of a simpler energy conversion system and local emissions are tangible economic gains, consumer acceptance may be slow, particularly until charging locations exceed the number of gas stations, at about 125,000.

**Summary:**

In this talk, clean energy demands on critical materials (Al, Co, Cu, C, Nd, Ni) due to solar, wind, power grids, and electric vehicles are outlined. Focusing on EVs, the dramatic shift to and investments for EVs by auto manufacturers are summarized as a prelude to projected near-term exponential demand.

**Acknowledgment:**

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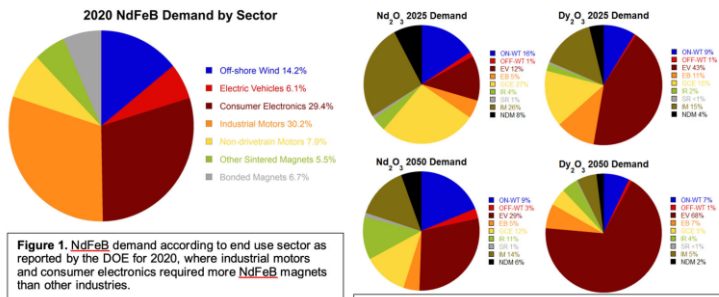


Figure 1. NdFeB demand according to end use sector as reported by the DOE for 2020, where industrial motors and consumer electronics required more NdFeB magnets than other industries.

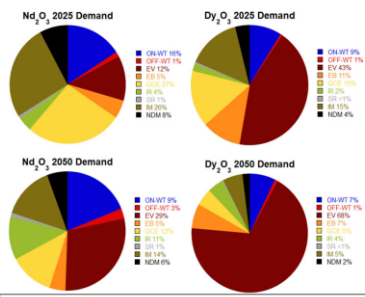


Figure 2: Share of end-use sectors for Nd (left) and Dy (right) for 2025 and 2050 based on current growth projections. Abbreviations: ON-WT – on-shore wind turbines, OFF-WT – off-shore wind turbines, EV – electric vehicles, EB – electric bicycles, GCE – global consumer electronics, IR – industrial robots, SR – service robots, IM – industrial motors, NDM – non-drive-train motors.

Reference: Heim, J. W., & Vander Wal, R. L. (2023). NdFeB Permanent Magnet Uses, Projected Growth Rates and Nd Plus Dy Demands across End-Use Sectors through 2050: A Review. *Minerals*, 13(10), 1274.

## SESSION 12 (13:00-15:00) Combustion Technologies Evan Granite

### 12.1 (13:00-13:30) Life Cycle Greenhouse Gas Emissions of Coal-Biomass Co-firing Power Plants with Carbon Capture and Storage

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The United States has set a target to achieve a net-zero economy by 2050. Bioenergy with Carbon Capture and Sequestration (BECCS) is one of the promising negative-emission routes in the mitigation portfolio to help meet this goal. Coal-biomass co-firing with carbon capture and storage (CCS) is a key BECCS technology to realize carbon mitigation at fossil-fuel power plants. The mitigation potential of co-firing is affected by numerous critical factors, such as biomass properties, co-firing level, and carbon capture rate.

The objectives of the study are to characterize and estimate the life cycle greenhouse gas (GHG) emissions and performance of coal-biomass co-firing power plants with CCS, determine the breakeven co-firing level at power plants necessary to achieve net-zero life cycle emissions, and quantify the variabilities and uncertainties in life cycle emissions. The scope of the life cycle assessment includes fuel supply, combustion-based power generation, and CO<sub>2</sub> transport and storage. A fuel-based life cycle module is developed and embedded in the Integrated Environmental Control Model (IECM), a fossil-fuel power plant modeling tool.

This study applies the enhanced IECM to conduct process-based life cycle assessments for an array of biomass co-firing scenarios. Deterministic analysis indicates that reaching net-zero life cycle emissions in a biomass co-firing plant without CCS deployment is challenging. Combining biomass co-firing and CCS deployment can significantly lower the overall life cycle emissions of power plants. Net-zero life cycle emissions can be achieved with a 20 wt.% co-firing level and 90% CCS when Powder River Basin coal is co-fired with energy crops or forestry residues. However, the breakeven co-firing level for net-zero emissions depends on the selected fuel properties. Fuel supply and plant operation are the critical stages influencing life cycle emissions of power plants with 90% CCS. Deployment of deep CCS beyond 90% CO<sub>2</sub> capture can remarkably reduce operational emissions and the breakeven co-firing level. With 99% CCS, the breakeven co-firing rate can be reduced to 12% on average. These findings highlight the trade-offs between technical performance and environmental impact of biomass co-firing at coal-fired power plants and emphasize the role of deep CCS in achieving a net-zero emissions future.

### 12.2 (13:30-14:00) Thermogravimetric Analysis Combustion Characteristics of Coal Microlithotype Particle Types

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This study examined the combustion characteristics of coal microlithotype particle type concentrates using a Thermogravimetric Analyser (TGA). Coal samples evaluated were enriched in various microlithotypes including Vitrite80, Vitrite60, VITRSF, VITSF and FUS. The TGA combustion results were post-processed to determine the sample ignition, burnout, peak temperatures and reactivity. Findings revealed that ignition temperature decrease with an increase in the concentration of Vitrite80% particles attributed to their richness in Vitritinite macerals. A similar trend was observed for Vitrite60. Conversely, FUS particles rich in inertinite macerals, exhibited the opposite trend. Additionally, burnout temperature decreased with higher concentrations of Vitrite80 and Vitrite60. Peak temperature and reactivity were influenced by the concentration of Vitrite80. This study highlights the significance of microlithotype particle type concentration in achieving lower ignition and burnout temperatures, ultimately enhancing coal reactivity.

### 12.3 (14:00-14:30) The effect of dry salt conditioning on the resistivity of South African fly ashes

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The control of particulate matter emission in coal-fired power plants is widely achieved using electrostatic precipitators (ESPs) and fabric filter plants (FFPs). The resistivity of power plant fly ash is one of the main properties impacting the collection efficiency of ESPs. Previous investigations have shown that the low amount of sodium species in South African fly ashes have resulted in higher resistivity, leading to low ESP collection efficiencies. The resistivity of these ashes can be reduced to optimum ranges by conditioning with fly ash conditioning agents.

In this paper, we report the results from the fundamental investigation of the influence of pure dry salt conditioning on the subsequent resistivity of fly ashes generated from South African coal-fired power plants. Fly ashes from two coal-fired power plants (PP-1 and PP-2) were collected and prepared for characterization using various salt concentrations of 5 wt.%, 10 wt.%, 20 wt.%, and 30 wt.% dry pure NaCl and Na<sub>2</sub>SO<sub>3</sub> conditioning agents. The preconditioned and unconditioned samples were characterized to determine several physical and chemical properties.

Results show that both unconditioned fly ashes possessed ash yields  $\geq 99.8$  wt.%, on an air-dry basis (adb), with fixed carbon contents  $\leq 0.1$  wt.%, indicating a good combustion efficiency of the coal-fired power plants' combustion units. Data from XRF analysis reveals that both unconditioned fly ashes exhibited high proportions of Al species with lesser abundances of Ca and Na species.

The conditioned and unconditioned samples were subjected to resistivity measurements, following the IEEE standard 548 of 1984, under ascending and descending temperature runs (90–330°C) as well as under 5 vol% ambient moisture conditions. The results showed that Na<sub>2</sub>SO<sub>3</sub> conditioning decreased the resistivity of the fly ashes more significantly than NaCl conditioning under both dry and moist conditions, with Na<sub>2</sub>SO<sub>3</sub> showing a greater difference between ascending and descending temperature measurements.

At temperatures below 150°C, surface resistivity has the greatest influence on the overall resistivity of the fly ashes. The influence of moisture becomes more prominent with increasing temperature, up to around 120°C, after which the resistivity decreases again. This trend can be explained by the fact that moisture is driven off from the samples leading to increased surface resistivity. At temperatures above 150°C, volume resistivity was predominant, and the chemical and bulk composition of the ash had a more dominant influence on resistivity above this temperature. Data from the resistivity measurements show that, under the surface resistivity region (90–150°C, which is within the optimal operating temperature of most power station ESPs (115–150°C)), the resistivity of both the unconditioned and conditioned fly ashes under dry (0 vol.% ambient moisture) atmosphere was high and greater than 10<sup>11</sup> Ω·cm (3.7×10<sup>11</sup>–1.2×10<sup>14</sup> Ω·cm).

Under 5 vol% ambient moisture concentration, the resistivity of the unconditioned and conditioned samples reduced by at least 1–2 orders of magnitude (1.4×10<sup>10</sup>–1.3×10<sup>13</sup> Ω·cm), which was more significant for the Na<sub>2</sub>SO<sub>3</sub>-doped samples. However, resistivity reductions that are within the optimal resistivity for efficient ESP operation (normal to moderate resistivity, 10<sup>8</sup>–10<sup>11</sup> Ω·cm) were only achieved with the Na<sub>2</sub>SO<sub>3</sub>-conditioned samples at 30 wt.% and 20–30 wt.% loading for PP-2 and PP-1 ash samples, respectively. This indicates that Na<sub>2</sub>SO<sub>3</sub> can be a more efficient fly ash conditioning approach to increase the collection efficiency of electrostatic precipitators for South African coal-fired power station ESP facilities.

In the modeling of the resistivity of the conditioned and unconditioned fly ashes, it was generally observed that the original Bickelhaupt model underestimated the resistivity of these South African fly ashes even in the presence of moisture and conditioning agents. However, the modified Bickelhaupt model based on South African fly ash properties predicted the resistivity of these ashes satisfactorily.

**Keywords:** Particulate matter emission, fly ash resistivity, dry salt conditioning, ESP, modified Bickelhaupt model

tests for evaluating the combustion characteristics of new coal sources.

#### 12.4 (14:30-15:00) Drop Tube Furnace Combustion Characteristics And Computation Fluid Dynamics Modelling of Coal Char Microlithotype Particle Types

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This study investigates the Drop Tube Furnace (DTF) and Computational Fluid Dynamics (CFD) char combustion characteristics of coal microlithotype particle concentrates. Coal samples, enriched in various microlithotypes including Vitrite80, Vitrite60, VITRSF, VITSF and FUS, were pulverised and pyrolyzed in Eskom's DTF in a nitrogen atmosphere at 1400 °C to produce the char samples. These char samples were further pulverised and sieved to produce a size fraction of +38 -75 µm and combusted at wall temperatures 1000 °C, 1200 °C and 1400 °C. Solid residue samples were collected at different probe positions (residence times) and analysed for ash yield at RT&D's Coal laboratory to determine the combustion efficiency at each probe position using the ash tracer method. A CFD Surface Reaction Discrete Phase Model (DPM) of the DTF was developed using Ansys Fluent software incorporating a User Defined Function (UDF) to set the char kinetic parameters for different microlithotype particle types. The results indicated the chars derived from the Vitrite80 rich coal samples were more reactive, ignited quicker and had a shorter burnout residence time than the other samples. This study has demonstrated the potential of using CFD modelling including microlithotype particle type features, as an alternative to costly and time-consuming DTF experimental

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