

In the present work, NETL researchers have studied chemical looping combustion (CLC) with an oxygen carrier NiO/bentonite (60 wt.% NiO) for the IGCC systems utilizing simulated synthesis gas. Multi cycle CLC was conducted with NiO/Bentonite in TGA at atmospheric pressure and in a high pressure reactor in a temperature range between 700- 900°C. Global reaction rates of reduction and oxidation as a function of conversion were calculated for all oxidation-reduction cycles utilizing the TGA data. The effect of particle size of the oxygen carrier on CLC was studied for the size between 20-200 mesh. The multi cycle CLC tests conducted in a high pressure packed bed flow reactor indicated constant total production of CO₂ from fuel gas at 800°C and 900°C and full consumption of hydrogen during the reaction.

43-2

Substitute Natural Gas from Coal Co-Production Project - A Status Report

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The US DOE National Energy Technology Laboratory awarded four co-production projects in December 2005. This paper presents the status and early results from the project sponsored by Arizona Public Service Company (APS). The 3-year project will research and develop a hydrogasification process to co-produce substitute natural gas (SNG) and electricity from western coals. The proposed system uses hydrogen instead of air or oxygen in the gasification process, an approach that offers higher operating efficiencies, lower water consumption, and a gas product that is richer in methane than other gasification processes. The concept has the potential to produce SNG below the projected market price for natural gas. It will separate a carbon dioxide stream ready for sequestration. In the first year the project will focus on concept design and laboratory tests; the overall objective will be to field test the hydrogasification SNG concept at one of the APS power stations.

43-3

Co-Production of Substitute Natural Gas and Electricity via Catalytic Coal Gasification

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Although coal is well known to be the most abundant fossil fuel available on this planet, its reputation as a fuel is tarnished by its inconvenient solid form, complexity for converting into useful energy and work, pollution, and a negative public image that discourages coal use. In a recently funded DOE project, RTI plans to develop key technologies to convert coal into two more desirable energy forms, namely substitute natural gas and electricity. RTI's technology platform is based on extensive research performed by Exxon in the 1970's for substitute natural gas (SNG) production via catalytic gasification. Unfortunately, this process was not economically viable because an extensive recovery process was necessary to recover the active catalyst from the ash to mix with the coal feed, the active catalyst and ash reacted at the operating conditions inhibiting effective catalyst recovery, and cryogenic separation was used to separate an SNG product and a hydrogen and carbon monoxide recycle stream. RTI has adapted a number of newer and novel technologies to overcome these problems and simultaneously achieve near zero emissions, produce a high pressure CO₂ product and co-produce electricity. In the proposed process, the active catalyst material is loaded on a support material and remains fixed in a catalytic reactor. The coal is initially preprocessed to convert the coal into a mixture of gas phase carbon species, H₂ and solid char fines prior to the catalytic reactor. In the catalytic reactor, the catalyst promotes the conversion of the gas phase carbon species and H₂ into CH₄. Because the ash is trapped in the solid char fines and the catalyst on a support, physical contact between the ash and catalyst is impossible eliminating the potential for reaction. The product gas mixture from the catalytic reactor is cleaned using the hot gas desulfurization and CO₂ capture technologies that have been developed at RTI. The product from the CO₂ capture process is a high pressure sequestration ready CO₂ byproduct. More conventional ammonia and methanation processes will be used to polish the final SNG to meet pipeline specifications. Finally, the carbon trapped in the char fines is combusted in a pressurized fluid-bed combustor to generate steam and electricity. This presentation will describe the available results from the bench-scale testing program for evaluating the technical and economic feasibility of the proposed process.

43-4

Fundamentals of an Optimized Catalyst Gasification System

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GreatPoint Energy has begun the development of a catalytic gasification process. This process is aimed at operating at lower gasification temperatures than processes previously developed. In conjunction with GreatPoint Energy, The Department of Mechanical Engineering and Energy Processes at Southern Illinois University at Carbondale has initiated fundamental studies to determine the feasibility of converting coal into methane while keeping processing temperatures below 700°C. These studies have included basic thermodynamics, laboratory scale gasification tests and laboratory

catalyst recovery tests. Three types of laboratory gasifiers have been developed. These gasifiers were used to screen catalyst systems, and process variables. Catalyst recovery screening was conducted in a Soxhlet extractor. The results demonstrate that coal can be converted to methane at temperatures as low as 500°C within reasonable reaction times of less than 1 hour and as short as 15 minutes. The optimum catalyst system utilized thus far, consists of two catalyst. One catalyst apparently activates a second catalyst to accomplish very rapid low temperature conversion of the coal. There are many advantageous to the low temperature operation. They include lower steam requirements, decrease gas separation costs, less catalyst tie-up with mineral constituents, higher catalyst recovery, smaller boiler requirements, higher methane concentration in the product gases, and less gas recycle. Basic thermodynamics will be discussed. The paper will report results from batch, high pressure mini-gasifiers, semi continuous, high pressure, mini fluid bed gasifier, and a differential bed gasifier. Future development plans will be discussed.

43-5

A Novel Catalytic Coal Gasification Process to Produce SNG

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GreatPoint Energy is commercializing a novel catalytic process for converting coal (and other carbon-based feedstocks) into high value clean substitute natural gas (SNG). Coal is available in abundance in the United States and will ensure a secure and an affordable fuel for many generations. GreatPoint converts this low cost, but dirty feedstock into the cleanest of all commercially viable fuels. GreatPoint's substitute natural gas product, called bluegas™, meets pipeline quality gas requirements, and is transported by standard natural gas pipeline. Production can be centralized in close proximity to the coal mine, where over half of the carbon (in the form of CO₂) can be sequestered. GreatPoint Energy intends to build, own, and operate bluegas™ production facilities and sell bluegas™ to regional distributors and customers in the power generation, industrial, heating and chemical sectors. The company's technology is based on the discovery that coal mixed with mixtures of alkali metal catalysts promotes coal gasification reactions including methanation at mild conditions, around 500 to 700°C. Research into this finding has led to a one-reactor system which offers an efficient and cost-effective route to produce low cost methane from coal. The objective of this paper is to describe the bluegas™ process, the status of the technology, and areas of new process development.

SESSION 44

COAL CHEMISTRY, GEOSCIENCES, AND RESOURCES: MINERAL MATTER, COAL ASH, COAL COMBUSTION

44-1

Characterization of Source Rocks Producing Respirable Quartz and Aluminosilicate Dust in Underground US Coal Mines

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A research effort has been undertaken at the Pittsburgh Research Laboratory (PRL) of the National Institute of Occupational Safety and Health (NIOSH) to characterize the source material producing respirable quartz and aluminosilicate dust in coal mines. Mine regulatory personnel suggested that problematic silicate mineral dust concentrations were known in some coal mines operating in southern West Virginia, Virginia and eastern Kentucky. Six mines were selected in this region for rock and dust sampling by PRL researchers based on elevated quartz concentrations in historical dust samples. Four of the coal mines sampled produced elevated respirable quartz dust concentrations on active production sections during sampling, the other two mines produced about 5% quartz, the regulatory reduced standard limit for quartz. Prior research has suggested that the source of respirable silicate dust in underground coal mines is typically immediate roof or floor lithology, not mineral matter bound within the mined coalbed. At some of the sites included in this research there were only potential quartz source rocks in either the floor or the roof units. At other sites sampled during the study, potential quartz sources existed in both the roof and floor lithologies. In the later cases, elemental data have suggested the enrichment of certain cations in the roof lithologies compared to floor rock may have the potential to distinguish potential quartz and aluminosilicate sources produced in respirable dust samples. Research results from Pennsylvanian-age coalbeds in western Pennsylvania surface mine sites has suggested the clastically derived mineral matter in the immediate roof rock, coal-bound mineral matter and the immediate floor lithology are derived from a common source material. Some of the enrichment of certain cation species in the roof units (i.e., Ca, Fe, Mg, Na) compared to immediate floor rock may be related to the percolation of fluids through the overburden and diminished probability for fluids to migrate effectively through the coal or coal precursor and into the floor units. Comparisons of the elemental composition of dust cassette mineral matter and possible source rocks have shown that the dust composition is not identical to any of the sampled potential source rocks. It is considered likely that the mining process, including rock breakage and the entrainment of dust particles in the ventilation air stream have modified the dust composition from the starting parent materials. However, normalizing the data has shown promise in distinguishing potential source

rocks using elemental ratios. Data from the single quartz rock sources sites have been used to assess the viability of the methodology. The elemental data suggests roof strata as the primary source of mineral-generated respirable dust produced during mining and captured by the dust samplers on the cassettes. This finding is contrast to the quartz dust sources identified in the field and by x ray diffraction analysis of roof and floor rock where at least one site showed the primary silicate dust source to be in the floor. The suite of x ray fluorescence sample data suggests a strong relationship between the overall amount of Si and the quantity of quartz in the samples. A similar relationship was not found in the parent source rocks. These findings may be significant since the potential severity of the silicosis risk to miners is strongly influenced by both the quantity of quartz and the clay minerals in the respirable dust fraction.

44-2

Studies on Abrasive Propensity of Thermal Coals of India: Effect of Ash and Quartz Contents

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A suite of 50 thermal coals from various coalfields of India, viz. Eastern Coalfield Ltd, Western Coalfield Ltd, Northern Coalfields Ltd and Talcher Coalfields Ltd, used as fuel in major thermal power stations, viz. Farakka Super Thermal Power Project (STPP), Talcher STPP, Talcher TPP, Kahalgaon TPP, Unchahar TPP, Vindhyachal STPP, Singrauli STPP, Rihand STPP, Dadri STPP, Rihand STPP, Majia TPP, Tanda TPP and NSTCL PP, in recent times has been systematically characterized for the first time for the purpose of assessing abrasive propensity in terms of their ash and quartz contents. Abrasive propensity of all the coals has been determined according to the procedure given in IS: 9949-1986, while the quartz content in each coal has been determined using Fourier Transform Infra for quantitative analysis of quartz in minerals. Thermal coal in India is of drift origin and as such, the mineral contents are high in them. Coals fed to thermal power stations have been found to contain 30-60% ash and quartz in them varies between 5 and 20% graph plotted between quartz and ash contents of the coals shows, statistically, % quartz = 0.25x % Ash, i.e., quartz makes one-fourth of the ash. There are poor correlations between abrasion index and ash content and between abrasion index and quartz content as suggested by the large scatter in respective graph with correlation coefficient of 0.56 and 0.31 respectively.

The commonly occurring minerals found in thermal coal are: kolinite, illite, montmorillonite and quartz with smaller amounts of carbonate species, pyrite and feldspar. Quartz and pyrite are the harder materials present in coal with hardness of 7.0 and 6.5 on Mohs' scale respectively, but as pyrite is present in small amounts, only about 1% of the weight of the coal, its contribution towards abrasive propensity is insignificant compared to that of quartz. Quartz is found to occur as rounded and angularly shaped particles of various sizes in coal. Although both size and shape contribute to wear, angular particles are more abrading than the rounded ones. Poor correlations between abrasion index and quartz to the factors not being given due consideration.

The correlation between abrasion index and ash content is, however, found to improve when thermal coals are bifurcated into two groups: one with quartz/ash ratio less 0.25 and the other greater than 0.25. For the two groups respectively abrasion index (AI) is given by the following empirical relations:

$$AI = 1.12 * \text{Ash} + 0.71 \quad (R^2 = 0.85)$$

$$\text{and } AI = 1.28 * \text{Ash} + 6.90 \quad (R^2 = 0.64)$$

The factor of 0.25 chosen for bifurcation has been taken from scatter diagram between the variables. This seems to be plausible as for most of thermal coals the ratio is <0.25 and the AI is given by the first relation above. For coals with the ratio >0.25, the chances for getting adventitious quartz from mining operations are higher. Quartz particles from extraneous sources are characterized by their higher angularity and as such, abrasion of coal containing these particles over and above the inherent ones is higher.

The study also shows that there is very poor correlation between AI and HGI. Although HGI is a technical design parameter and has assumed commercial importance because of its use in coal contract specification, presence of quartz in coal dictates the performance and life time of a mill. Notwithstanding the limitations, the equations proposed are instrumental in preliminary assessment of abrasive propensity of Indian coals required for maintenance schedules of power plant machinery.

44-3

Sulfur and Carbon Isotope Geochemistry of Coal and Derived Coal Combustion By-Products: An Example From an Eastern Kentucky Mine and Power Plant

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The isotopic compositions of sulfur (^{34}S) and carbon (^{13}C) were determined for the coal utilized by a power plant and for the fly ash produced as a by-product of the coal combustion in a 220-MW utility boiler. The coal samples analyzed represent different lithologies within a single mine, the coal supplied to the power plant, the pulverized feed coal, and the coal rejected by the pulverizer. The ash was collected at various stages of the ash-collection system in the plant. There is a notable enrichment in ^{34}S from the base to the top of the coal seam in the mine, with much of the variation due to an upwards enrichment in the ^{34}S values of pyrite. Variations in ^{34}S and in the amount of pyritic S in the coal delivered to the plant show that there was a change of source of coal supplied to the plant, between week one and week two of monitoring, supporting a

previous study based on metal and sulfide geochemistry for the same plant. The fly ash has a more enriched ^{34}S than the pulverized coal and, in general, the ^{34}S is more enriched in fly ashes collected at cooler points in the ash-collection system. This pattern of ^{34}S suggests an increased isotopic fractionation due to temperature, with the fly ash becoming progressively depleted in ^{34}S and the flue gas sulfur-containing components becoming progressively enriched in ^{34}S with increasing temperatures. Substantially less variation is seen in the C isotopes compared to S isotopes. There is little vertical variation in ^{13}C in the coal bed, with ^{13}C becoming slightly heavier towards the top of the coal seam. An 83 to 93% loss of solid phase carbon occurs during coal combustion in the transition from coal to ash owing to loss of CO_2 . Despite the significant difference in total carbon content only a small enrichment of 0.44 to 0.67 in ^{13}C in the ash relative to the coal is observed, demonstrating that redistribution of C isotopes in the boiler and convective passes prior to the arrival of the fly ash in the ash-collection system is minor.

44-4

A Measurement technique for Coal Ash Emissivity in High Temperature Atmospheres

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The purpose of our work is to examine the characteristics of coal ash emissivity to better understand the heat transfer mechanism through ash deposits on tubes in coal-fired boilers. This paper presents a method for determining coal ash emissivity in high temperature atmospheres and the influence of the ash surface temperature on its emissivity. Emissivity was determined by comparing theoretical radiation intensities with measurements obtained by a shield tube emissometer. An ash sample was heated in an electric furnace during the measurement and the radiation intensity from the sample was measured with a digital pyrometer. Emissivity characteristics of Powder River Basin (PRB) coal ash and bituminous coal ash were examined. The main results are as follows: (1) Emissivity of deposited ash increases with an increase in deposit surface temperature. (2) The emissivity of a sample having fused surface exceeds 0.9. (3) PRB deposits have lower emissivities compared with bituminous deposits in the range of the surface temperature from 600°C to 1100°C.

44-5

A Theoretical Study of the Kinetics of Selected Arsenic and Selenium Reactions in Coal Combustion Flue Gases

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As environmental regulations pertaining to mercury are becoming much stricter, other trace metals, particularly arsenic and selenium, are beginning to be examined as well. A noted source of compounds containing these elements is coal combustion flue gases and, as such, the mechanism(s) of their removal is a topic of much attention. Given that any removal strategy will be dependent upon the speciation, and the speciation in turn will be dependent upon the reaction kinetics of the flue gas, determination of the kinetic parameters of reactions involving these metals is key to developing effective removal techniques. Previous experimental work has been performed to determine the speciation for a variety of conditions, however the nature of many of the compounds created as a result of the combustion process makes them undetectable to current experimental techniques. To develop a more complete understanding of the overall speciation it is thus necessary to determine the importance of these compounds. To accomplish this, computational chemistry techniques are employed to determine the kinetic parameters of the elementary reactions taking place within the combustion flue gas environment. The initial phases of the overall project will be presented; namely, the theoretical computations and the development of kinetic rate expressions for a selection of arsenic and selenium reactions. Additionally, the methodology used for the calculations will also be discussed.

SESSION 45

MATERIALS, INSTRUMENTATION, AND CONTROLS - 2

45-1

Co-Coking of Hydrotreated Decant Oil/Coal Blends in a Laboratory Scale Coking Unit: Product Distribution of Distillates

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Delayed coking, used in petroleum refineries throughout the world, is a process that converts heavy petroleum residua (vacuum residua and decant oil) into light distillate fraction and coke. This is achieved by the pyrolysis and thermal degradation of the feedstock in a semi-continuous process, at temperatures between 450-500°C, in an inert atmosphere, and at pressures around 10 psig. A pilot-scale delayed coker at The Energy Institute at The Pennsylvania State University is used to provide reliable continuous delayed coking for 4-6 hours to provide acceptable quantities of liquids and cokes for the further evaluation. The unit is capable of operating under most delayed coking process conditions. The system pressure, temperature and flow rates are