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ABSTRACTS BOOKLET

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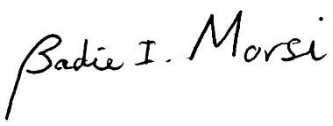
On behalf of the Thirty-Fifth Annual International Pittsburgh Coal Conference, we wish to express our sincere appreciation and gratitude to Ms. Kristen Harper for her meticulous leadership and control of the entire operation of the conference and to Mr. Rui Wang and Mr. Husain Ashkanani for their invaluable assistance in preparing this Abstracts Booklet. Special thanks go to Ms. Xinyuan ZHANG (Summer), CUMT for her great help of this year's conference.

Thank you,



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

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SESSION 1
POWER PLANTS - 1

1.1- Case Studies of Biomass Co-Firing in Full-Scale Pulverized Coal-Fired Power Plants in China

Wang Xuebin, Xi'an Jiaotong University, PR CHINA.

Biomass co-firing in pulverized coal-fired (PC) power plants is becoming more and more popular in China recently, aiming to reduce CO_2 emission, encouraged by the Chinese government. In China, four kinds of biomass co-firing modes have been tested or long-term operated in the full-scale PC power plants in the past 13 years, since the first successful case of Guodian Shiliquan Power Plant in 2005, which case imported the technologies and fuel pretreatment equipment from Denmark. The other three typical modes developed in China include (1) molding-biomass co-firing, (2) biomass powde r direct co-firing, and (3) biogas co-firing, in which, the modes (1) - (2) were designed and conducted by the authors. In this report, these four kinds of biomass co-firing modes and the corresponding tested results are introduced, the economic analysis and the existing problems of different modes are compared.

1.2- Pilot Test of Urea Hydrolysis to Ammonia with Steam Stripping

Lu Xu, Zhang Xiangyu, Zhang Bo, Xu Hongjie, Xi'an Thermal Power Research Institute Co., LTD, PR CHINA.

The process of urea hydrolysis with steam stripping was proposed in order to reduce the corrosion of ammonium carbamate on the reactor in the urea hydrolysis with higher feed concentration. In this paper the mechanism model of steam stripping process was established firstly, and then the pilot tests were conducted. The results show that, the gas-liquid equilibrium in the reactor is re-established by the stripping steam, and the ammonium carbamate in the solution is decomposed. The ammonia production rate is dominated by kinetics and the apparent kinetic parameters remain unchanged at the steam stripping conditions, thus the ammonia production rate is not influenced by the stripping steam. Because only part of the sensible heat in the stripping steam is utilized, the energy consumption of ammonia production is increased with the increasing flow of stripping steam. By selecting appropriate stripping steam flows and feed concentrations, both the hydrolysate concentration and the energy consumption can be reduced. When the feed concentration is 60% and the criteria number of stripping steam flow is increased from 0% to 29%, the steam consumption for unit ammonia production is decreased by 23%.

1.3- Impact of Flue Gas Recycle On the Efficiency of Oxy-Fuel Combustion Systems

Richard L. Axelbaum, Piyush Verma, Akshay Gopan, Zhiwei Yang, Washington University in St. Louis, USA.

Oxy-combustion typically consists of burning coal with a combination of oxygen and a large amount of recycled flue gas (60–70%). The recycled flue gas is used to manage wall heat flux and match the radiative/convective heat transfer ratios of air-fired combustion systems.
Although this approach may be justified for retrofitting air-fired power plants, for green-field applications, other methods for heat flux control and heat transfer are possible. Several new oxy-combustion process concepts have been proposed in recent years, where the level of flue gas recycle ranges from near zero to 80%. By comparing different processes with different amounts of flue gas recycle, studies have shown significant improvements in efficiency for low-recycle processes.
In this work, we employ a fundamental thermodynamic analysis to evaluate the impact of flue-gas recycle on the efficiency of oxy-combustion systems. It is shown that for 1st generation oxy-combustion systems, the inefficiency caused by flue gas recycle could lead to as much as 8–10% reduction in efficiency compared to a process with negligible recycle. Furthermore, at high flue-gas-recycle ratios, the fan power for recycle is significant, and adds an additional loss to that caused by thermodynamic inefficiencies. Analysis of the impact of recycle ratio on pressurized oxy-combustion (POC) is also presented, including a discussion on the valorization strategies of the latent heat recovery (made possible due to the higher pressure).

1.4- Preparation of Low Ash Coal by a Green Chemical Method

Lijun Zhao, National Institute of Clean-and-Low-Carbon Energy, PR CHINA.

A green chemical method has been developed for ash removal from coals. By using the sintering reaction of alkali and minerals in coals, the chemical digestion has been greatly intensified even under mild conditions, by comparison with conventional chemical methods. The green chemical method has been applied to a raw coal of 35.55% ash, and achieved a high ash removal rate of >95%, preparing a low ash coal of <2%. By comparison with the available results for high ash coals, it has been found that about half the alkali would be spared by the green chemical method with the lower temperatures of 100-150 ℃, and the resulting low ash coal can be used in many advanced fields.

1.5- Hybrid Eulerian-Lagrangian Simulation of Gas-Solid Fluidized Bed

Chen Yang, Haochuang Wu, Chongqing University.

The fluidized reactor is widely used in a number of chemical processes due to its high gas-particle contacting efficiency and excellent performance on solid mixing.
An improved numerical framework based on MP-PIC (multi-phase-particle-in-cell) method has been developed to simulate the processes of gas-solid flow and chemical reactions in a fluidized bed. In the MP-PIC method, the solid phase is treated as both continuum and discrete phase, the particle stress gradient is calculated on the Eulerian grid and the particle properties are mapped from Eulerian grid to Lagrangian coordinates by the use of interpolation functions and particle size distribution. Every particle composed of similar physical (size, temperature, density) and chemical (reactive) properties can be tracked individually, detailed microscopic properties (particle trajectory, transient forces acting on specific particle) which is extremely difficult to get by the Eulerian-Eulerian method can also be obtained at the particle level. The gas turbulent flow is solved by large eddy simulation (LES) method. Heterogeneous reactions and homogeneous reactions including char combustion, pyrolysis and volatile combustion are solved by average-cell-chemical (ACC) method.
Experiments have been carried out on a 3MW circulating fluidized bed with the height of 24.5m and cross-section of 1m2. A series of temperature and pressure metrical points have been set along with the height of furnace. The mean diameter of coke breeze used in experiments is 2.5mm, the ignition temperature is 470 oC.
Simulations and experiments were carried out under different operation conditions. Distributions of temperature, volume fraction, mean diameter, velocity and pressure were calculated. The results show that the distribution of gas-solid properties had better accuracy compared with the traditional Eulerian-Eulerian approach. The temperature of feed coal point is the highest because of fast pyrolytic reaction and volatile combustion, then the temperature decreases with the decrease of oxygen concentration. With the injection of fresh air at the secondary air inlets, the temperature increase to a new level. The distributions of temperature and gas concentration along the furnace have achieved a good accuracy compared with experimental data indicating that this numerical framework is suitable for solving complex gas-solid flow and reactions in fluidized bed reactors.

SESSION 2
COMBUSTION TECHNOLOGIES - 1

2.1- Effect of CO_2 on the Characteristics of Soot Derived from Coal Rapid Pyrolysis

Qinghua Chang, Rui Gao, Fuchen Wang, East China University of Science and Technology, PR CHINA.

Coal particles experience rapid pyrolysis in CO_2-rich atmospheres during oxy-fuel combustion, knowledge about soot formation in the CO2-rich atmosphere is required to identify the possible chemical effect of high CO2 levels on the soot characteristics. The effects of a CO_2-rich atmosphere on both the characteristics of coal-derived soot were detail investigated in present work. The rapid pyrolysis of Shenfu bituminous coal was conducted in a Drop tube furnace (DTF) in N_2 and CO_2 atmospheres with a wall temperature of 1073-1473K and residence time below 700 ms. The morphology and microstructures of N2-soot and CO2-soot were evaluated by A series of techniques (elemental analysis, HRTEM, Raman, XRD, FT-IR and thermogravimetry techniques). The soot formation was a rapid process and favored T>1273 K. CO_2 enhanced the soot formation and proceeded the dehydrogenation. The sooting tendency increased in the CO2 atmosphere compared to that in the N2 atmosphere. The increased residence time and temperature caused the continually increased C/H and C/O atomic ratios. The higher C/H atomic ratios of CO_2-soot indicate the enhanced dehydrogenation in CO2 atmosphere.

By analyzing the Raman and XRD spectrum results, some remarkable differences of the carbon microstructures for CO2-soot in comparison with N2-soot were found: CO2 improves the order of the internal carbon lattices, enhances the lateral extension of carbon nanostructures, decreases the interplanar spacing of the graphene layers and promotes the stack of polyaromatic layers. The variations of the SOLO, DUO, TRIO and QUARTO structures were also analyzed, and the contribution of CO2 was found to reduce the defects of the basic structure units (BSU).
The CO2 atmosphere can promote the polymerization of tar and enhance the graphitization of soot. The CO2-soot is more mature than the N2-soot, and the gasification reactivity of CO2-soot is relatively lower. The defects of soot are important indications of the initial gasification reactivity because there is an approximately linear correlation between r0 and the area of the FT-IR peaks in the range of 925-700 cm-1.

2.2- Flue Gas Effects on Ditomite-Based Adsorbents for Elemental Mercury Removal

Huan Liu, Zhuo Xiong, Yongchun Zhao, Junying Zhang, Huazhong University of Science & Technology, PR CHINA.

Kinds of adsorbents which are high efficiency, low-cost, and environmental-friendly for mercury removal from coal-fired flue gas are urgently needed, for that mercury pollution problem has attracted much attention in recent years. In this study, several promoted adsorbents with diatomite (D) as a carrier were attempted to remove mercury in a fixed-bed reactor system. Different reaction temperatures were designed for the optimal condition of CuBr2-Dia and KBr-Dia. Effects of flue gas components including HCl, O2, NO, and SO2 on the mercury removal performance of CuBr2-Dia were researched. To evaluate the stability of mercury adsorbed, mercury temperature-programmed desorption (Hg-TPD) experiment of the spent CuBr2-Dia was designed. Moreover, some characterization methods, such as XRF, XRD, BET, SEM, FT-IR and XPS, were applied to the adsorbents to determine their physicochemical characteristics and analyze the reaction mechanism. Characterization tests showed that diatomite had regular and porous structure caused by biogenic components, which could create conditions for Hg0 removal. CuBr2-Dia had the Hg0 removal efficiency of 93% in pure N2 and 91% in simulated flue gas (SFG) at 140℃, while KBr-Dia had that of 66%. Mercury adsorbed by CuBr2-Dia existed in stable forms. Reaction temperature had a great influence on the different active substances, based on the facts that the optimal temperature for KBr-Dia was 220℃ while that for CuBr2-Dia was 140℃. Interestingly, the average Hg0 removal efficiency of KBr-Dia increased from 40% to 80% as the temperature increased from 60℃ to 220℃. Flue gas components also had different influence on the performance of CuBr2-Dia. It showed that individual HCl had little effect but HCl played a great promoting role in the presence of O2. When different proportions of NO were added in pure N2, the Hg0 removal performance of CuBr2-Dia had an obvious promotion. Individual SO2 played a negative role in Hg0 removal. When 400, 800, and 1200ppm SO2 was added into pure N2, the average Hg0 removal efficiency declined from the initial 93% to 77%, 70%, and 59%, respectively. However, both O2 and NO could alleviate this unfavorable effect, and the latter did more. When 1200ppm SO2 and 300ppm NO simultaneously existed, the efficiency was 86%, which had an increase of 27%. Then with 4% O2 added, the efficiency could increase to 94%, suggesting that NO and O2 together could counteract the strong inhibition of 1200ppm SO2. The synergistic effect of NO and SO2 could make the functional species on the adsorbents surface changed, which had a negative impact on the active adsorption sites caused by individual NO for Hg0 removal. It is supposed that the active adsorption sites on the surfaces and in the pore wall for Hg0 removal effected by individual NO and those by NO and SO2 together were different and unrecoverable.

2.3- Experimental Analysis of Moisture Re-Adsorption of Dried Coal Using a Superheated Steam

Geunyeong Park, Korea Institute of Industrial Technology and Sungkyunkwan University; Yongwoon Lee, Tae young Chae, Won Yang, Korea Institute of Industrial Technology; Donghyun Lee, Sungkyunkwan University; Ikhwan Na, Nakkgyun Kim, Hankook Technology; SOUTH KOREA.

Recently, Korean coal-fired power plants have used sub-bituminous coals, which have higher moisture and volatile contents than bituminous coal. It causes increase in power consumption and decrease in efficiency of boilers especially. It needs to additional maintenance cost because of negative effect for coal transfer and burner. Coal is pre-dried through chemical drying, hot-air drying and superheated steam. Pre-dried coals have the characteristics of adsorbing atmospheric moisture when stored in coal yards. So its moisture readsorption characteristics need to be clarified. In this study, the moisture readsorption characteristics of dried coal were compared and analyzed through coal drying equipment using conventional coal and superheated steam. The coal used this study is the sub-bituminous coals from Indonesia, the moisture content of the coal before drying is about 37% and the moisture content of the dried coal is about 20%. To analyze the readsorption characteristics of dried coal, water was optionally soaked to coal and the drying rate was analyzed in humidity chamber. The temperature of the humidity chamber was kept 20-40oC considered Korean yards. The humidity was kept 60% and 90%, simulating spring, autumn and summer seasons. As a result, the moisture readsorption of pre-dried coal was found to lower than raw coal. Also, the higher the moisture content in the coal, the greater the drying tendency. BET surface area, Porosity and FTIR were analyzed in order to figure out effects of structural changes caused by the thermal drying process. According to the analysis, the difference in the moisture readsorption characteristics between the dried coal and raw coal was confirmed. It was confirmed that the BET surface area of the dried coal was smaller than raw coal. Functional group which enables moisture readsorption through the FTIR was found to be changed. When the dried coal through superheated steam is stored in coal yards, combustion efficiency and operation stability will be improved by lowering the characteristics of moisture readsorption of dried coal.

2.4- Study on the Migration of Chlorine in Co-Combustion Process of Medicine Dregs and Coal

Guo Yang, Sun Shaojie, Wu Jianjun, China University of Mining and Technology, PR CHINA.

The Shenmu coal and dregs (the traditional Chinese medicine slag) mixed in different proportions are co-pyrolyzed in a double-temperature zone tube furnace to obtain a semi-coke. The double-temperature zone tube furnace is also used to conduct combustion experiments on coal and dregs mixture in different proportions and semi-coke at different temperatures. The X-ray powder diffraction (XRD) and X-ray energy spectrum analysis (EDS) were performed on the burning ashes, and determination of chlorine content in combustion flue gas by ion chromatography. The results show that the ashes produced by the two different combustion processes are mainly composed of elements such as Ca, Si, Al and Fe, and the elements such as K, Na and Cl are relatively few. The presence of alkali metal is beneficial to the emission of chlorine, so the emission rate of chlorine after co-pyrolysis of the dregs and coal is higher. In addition, the emission of chlorine rate curves of the two have similarities in trend, but the values differ greatly. The physical structure and chemical properties of the dregs and coal co-pyrolysis semi-coke have undergone a series of changes, so the state of chlorine will become simpler, which leads to the increase of rate of weight loss. However, the total amount of chlorine released during the co-combustion of the dregs and coal is higher than the semi-coke combustion process. We show that the combustion of the semi-coke produced by co-pyrolysis of coal and dregs can more effectively avoid the generation of dioxins and reduce the corrosion of equipment.

2.5- Mercury Removal by Biochar Prepared Under Biomass Reburning in a Simulated Flue Gas

Ximing Hu, Jiateng Shi, Ping Lu, School of Energy and Mechanical Engineering, Nanjing Normal University, PR CHINA.

Biochar prepared under biomass reburning in a high-temperature entrained flow reactor was used as mercury sorbent. The effects of biomass species, adsorption temperature, initial mercury concentration and HCl content on elemental mercury (HgO) removal characteristics were investigated in an in-duct sorbent injection apparatus. The results showed that biochars have a certain mercury removal performance, whose efficiency is around 30%. Mercury removal efficiency of RH-biochar is little bit larger than that of WH-char, increasing reburning temperature is helpful for mercury removal. Mercury removal efficiency increases continuously to 34.2% during injecting RH1050 as adsorption temperature increase from 80 °C to 160 °C, but it shows fluctuant pattern and achieves the maximum of 36.75% at adsorption temperature of 100 °C during injecting RH1150. Mercury removal efficiency presents a pattern of increase first and decrease latter during injection of RH1050 and RH1150 as initial mercury concentration increases from 15 μg/m3 to 40 μg/m3, and the maximum average mercury removal efficiencies of 35.6% and 37.35% achieve at the initial mercury concentration of 25 μg/m3. HCl has an obvious promotion on elemental mercury removal. The average mercury removal efficiency during injecting RH1050 can be achieved more than 90% while HCl content of N2+HCl is larger than 50 μL/L.

SESSION 3
RARE EARTH ELEMENTS IN COAL AND COAL BYPRODUCTS

3.1- Rare Earth Elements in the Lignite from Mile Basin, Yunnan, China: Implication for Seawater Influence during Peat Accumulation

Jingjing Liu, Shifeng Dai, China University of Mining and Technology, PR CHINA.

The Mile Basin is one of the important lignite producing areas in Yunnan Province, southwestern China. The M1 Coal, the major minable lignite with an average thickness of 27 m, is located in the lowermost Miocene Xiaolongtan Formation in this basin. The

lignite is characterized by low-medium sulfur content (0.19-3.78%, with an average of 0.78%). The average concentrations of rare earth elements and Y vary from 4.74 to 141.35 ppm, with an average of 29.25 ppm (whole coal basis) and 219.27 ppm (ash basis). Normalized by upper continental crust (UCC), the Mile M1 lignite is characterized by the L-M-type and M-H-type enrichment in the upper and lower seam portions, respectively (Fig. 1). La and Gd show positive anomalies, with an average of LaN/LaN*=1.33 and GdN/GdN*=1.37, respectively, implying the seawater input during peat accumulation. The weak positive anomalies of Ce (CeN/CeN*= 1.05) and Y (YN/HoN =1.08) in the lignite indicate a basalt sediment source for the terrigenous mineral matter of the coal, and this is consistent with terrigenous materials as indicated by Zr/Ti-Nb/Y plot. Other indicative elements (e.g., sulfur, Sr/Ba, Ca/Mg, and Th/U) and abundance and modes of occurrence of minerals (e.g., framboidal pyrite, gypsum) of the coals also sever as strong evidence of seawater influence during peat development.

3.2- Extraction of Rare Earth Element (REE) from Coal Ash in Korea

Sungyoon Park, Yejee Lim, Nway Oo Khin, Minsoo Kim, Sangwoon Woo, Han S. Kim, Konkuk University, SOUTH KOREA.

Demand and use of coal for electric power generation are steadily increasing in South Korea. As a result, substantial amount of coal ash (about 9 million tons) is generated annually. This coal ash is being buried under the ground without a proper treatment, which contaminates the surrounding environment. Recently, recycle of coal ash for the industrial raw material has been suggested to reduce the amount of coal ash dumping. One of such attempts is to recover valuable elements from coal ash, for example, rare earth element (REE). In this study, three different types of coal ash were collected from the electric power plant and they were examined with regard to the total amount of REE present in the coal ash. REEs were extracted by aqueous regia along with hydrofluoric acid treatment and then they were quantified by inductively coupled plasma mass spectrometry. 0.1 g of the coal ash sample was acid treated with 6 ml of mixed acid (nitric acid: hydrofluoric acid: perchloric acid = 4:4:1, v/v) and the mixture was heat treated at 180°C for 4 hrs. Acids were volatilized to measure the REE content. 15 elements including Tm, Yb, Gd, Er, La, Ce, Pr, Nd, Sm, Eu, Dy, Ho, Lu, and Y were present in the fly ash as well as bottom ash. The highest level of REE was 254.6 mg/kg-coal ash (dry mass) and the average level was approximately 200 mg/kg-coal ash. In particular, Ce and La were present at the notable level, 104.0 and 60.8 mg/kg-coal ash, respectively. Overall, it was found that more REEs were extracted from fly ash than bottom ash. Currently, various coal ashes are analyzed to investigate the effects of the origin of coal ores and their physical and chemical characteristics on the REE content and extractability. Based upon these results, we are planning to develop an advanced REE recovery technology from coal ash and provide a new material recycle strategy for clean environment in the future.

3.3- Characteristics of Rare Earth Elements in Entrained Flow Gasification Residues, Ningdong, China

Xin Guo, Yuegang Tang, Yafeng Wang, Binbin Huan, Xi Pan, China University of Mining and Technology (Beijing), PR CHINA; Cortland F. Eble, Kentucky Geological Survey, USA.

In an effort to assess the abundances of economically valuable rare earth elements (REY) in coal gasification residues, samples of feed stock coal and corresponding gasification residue materials were collected from coal-to-methanol plant (GE water-slurry coal gasification, formerly Texaco) and a coal-to-olefins plant (GSP pulverized coal gasification), located at the Ningdong Energy and Chemical Industry Base, China. Concentrations of REY were analyzed using inductively coupled plasma mass spectrometry (ICP-MS), and the modes of occurrence of REY were determined by a five-step sequential chemical extraction procedure. Results indicate that the concentrations of REY in the feed coals were no higher than their average concentrations in Chinese coal, or in world coal. Both GE and GSP coal gasification residues contained relatively low concentrations of REY than world hard coal ash. However, the feed coals, and their corresponding residues, were characterized by the enrichment of LREY. The outlook coefficient (Coutl) of GE and GSP gasification residues was calculated to assess primary estimation of REY in the residues. Then a REYdef, rel–Coutl graph was employed to estimate REY potential industrial value in the gasification residues. The plots on the REYdef, rel–Coutl graph (30%≤REEdef≤51%; 0.7≤Coutl≤1.9) show that the residues produced from coal gasification in Ningdong can be regarded as promising REY raw materials for economic development. REY were primarily associated with carbonate (50-60 %) and Fe-Mn oxides (50-70 %) in both the feed coals and residues from the GE-C and GSP-C. After entrained flow coal gasification, REY associated with the carbonate and Fe-Mn oxide both increased to about 80-90%. This enrichment may provide a theoretical basis for extracting REY from the gasification residues.

3.4- Critical Elements in Changhsingian Coals of the Shugentian Coalfield, East Yunnan, China

Xue Zheng, Shifeng Dai, China University of Mining and Technology, PR CHINA.

Critical elements in coal deposits havepotential economic and strategic significancebecause oftheir high concentration in coal (or coal ashes) and clay-altered volcanic ash or other coal-bearing strata. The geochemical characteristics of these elements are also helpful to indicategeological settings of the coal-bearing basin, to reveal geological processes after coal formation, and to provide information for regional geological evolution. The aim of this study is to present the concentration and the origin of the critical elements in Changhsingian coals of the Shugentian Coalfield, eastern Yunnan Province, Southwest China.
In comparison with the average values for world hard coals, Scandium (7.40 and 27.3 ppm), V (105 and 382 ppm), Co (14.2 and 51.1 ppm), Nb (15.1 and 55.4 ppm), Ta (0.97 and 3.51 ppm), Zr (140 and 507 ppm), Hf (3.75 and 13.7 ppm), rare earth elements and yttrium (REY) (134 and 491 ppm) are enriched in the Changhsingian coals of the Shugentian Coalfield, eastern Yunnan (the former and the latter concentrations in the brackets are on whole-coal and ash basis). Vanadium (386 and 444 ppm), Nb (63.2 and 73.2 ppm), Zr (640 and 741 ppm), Hf (10.9 and 12.7 ppm) and Eu (2.90 and 3.38 ppm) are also enriched in the floors of SGT3 and SGT4 coal seams and the roofs of SGT2, SGT3 and SGT4 coal seams as compared with the average values for world clays. Normalized by upper continental crust (UCC), the Changhsingian coals exhibit positive Eu (from 1.07 to 1.28) and positive Gd anomalies (from1.13 to 1.19), due to the input of the terrigenous materials from Emeishan basalt in the sediment source region and to the injection of the hydrothermal fluids, respectively. The Emeishan basalt is the major component of the Kangdian Upland, which is the main sediment source region for the Shugentian coals and was formed by Emeishan plume ascending. Both volcanic ash and hydrothermal fluids play a significant role in the enrichment of Nb(Ta)-Zr(Hf) and REY in Shugentian coals.

3.5- Rare Earth Elements in the Coal Fly Ash of Qianxi Power Plant, Guizhou Province, Southwest of China

Lun Wu, School of Chemical & Environmental Engineering, China University of Mining & Technology (Beijing), PR CHINA; Jinhong Zhang, Associate Professor, Department of Mining and Geological Engineering, The University of Arizona, USA: Liqiang Ma, China University of Mining and Technology, PR CHINA.

Rare earth elements (REEs) play an important role in the global technology development as a critical raw material. Recently, coal and coal combustion products have been considered as a potential source of REEs. REEs in the coal fly ash of Qianxi Power Plant in the southwest of China was studied in this paper. The inductively coupled plasma mass spectrometry (ICP-MS) result shows this coal fly ash contains a relatively high concentration of around 680ppm. Independent REEs enriched particles were found in the fly ash by scanning electron microscope (SEM) and energy dispersive spectrometer (EDS). Loss on ignition (LOI) test and X ray fluorescence (XRF) demonstrated that this coal fly ash has a relatively high content of unburned coal and iron oxides. REEs content was found low in the unburned coal and magnetic materials by ICP-MS. This study also proposed a REEs enrichment process combining magnetic separation and unburned coal flotation. REEs in this coal fly ash were enriched from 680 ppm to 1100ppm， while the REEs enriched fly ash of 50% weight of the feed coal fly ash was obtained.

SESSION 4
VALUE-ADDED PRODUCTS FROM COAL - 1

4.1- Thermogravimetry Mass Spectrometry (TG-MS) Study of Pyrolytic Characteristics of Two Different-maturation Lignites

Haibo Yan, Jie Wang, East China University of Science and Technology, PR CHINA.

Lignite pyrolysis is an extremely complex process. No single analysis method can thoroughly unravel the complex compositions of products, especially liquid compounds. In this study, we use TG-MS technique to investigate the pyrolytic behaviors of Yuxi lignite and Hami lignite. Proximate and ultimate analyses showed that Yuxi lignite had a lower maturation than Hami lignite. Mass spectrometry was used to examine the evolutions of a wide range of pyrolysis compounds including gases (H2, CO, CO2, CH4, C2H6, C2H2, C2H4, C3H6 and C3H8) and condensable liquid compounds including water, methanol (m/z=32), ethanol (m/z=46), acetic acid (m/z=60), acetone or propanol (m/z=58)), furan (m/z=68), furfural (m/z=96), phenols. It was interesting to find that furan and furfural were evolved from both lignites at lower temperature. These two compounds were degraded from the preserved cellulose composition in the two lignites. Another interesting observation was that ethanol and acetone were released from both lignites with relatively high total ion signals. These compounds were rarely reported as a lignite pyrolysis product because it could not easily be collected in the condensed tar.

Compared to Hami lignite, aliphatic oxygenates showed stronger ion intensities for Yuxi lignite, consistent with a higher oxygen content in it. It was also reasonably observed that Hami lignite produced more cyclic oxygen compounds than YX lignite.

4.2- The Influence of Coal Characteristics on Coal-based Graphene

Xuan Huan, Yuegang Tang, Jingjie Xu, Miaoxin Xu, China University of Mining and Technology (Beijing), PR CHINA.

In this work, two high rank B anthracites of different ash yield and vitrinite content were used for the synthesis of coal-based graphene via modified Hummers method. Natural graphite was selected for comparison. The aim of this study is to evaluate the influence of coal characteristics on the microstructure of coal-based graphene. As-received anthracites and natural graphite were studied using optical microscopy. The as-received and demineralized anthracites, resultant graphitization and graphene products were characterized using scanning electron microscopy, transmission electron microscopy, X-ray diffraction, Fourier transform infrared spectroscopy and Raman spectroscopy. Results showed that demineralized or not, the two anthracites from different geological settings can be used for preparing coal-based graphene. The minerals inherent in anthracite was not favorable to high temperature graphitization and inhibited the ordering of graphene sheets, resulting in the existence of various inorganic elements in the prepared graphene oxides, and eventually led to multiple irregular pore defects in coal-based graphene. Inertinite, which is characterized by high carbon and low hydrogen, was beneficial to the graphitization and oxidation intercalation of coal-based graphite and ultimately improved the C/O ratio of graphene product. Based on these results, we preliminarily propose the influence mechanism of coal petrography on the preparation of coal-based graphene.

4.3- Effect of Turbostratic Carbon on Microstructure and Hydrogen Absorption Performance of Mg-C Composite from Mechanical Milling

Pei Liu, Xinyuan Li, Ruiqian Jiang, Xiaojing Liu, Yuanli Chen, Shixue Zhou, Shandong University of Science and Technology, PR CHINA.

Magnesium has attracted considerable attention as one of the most promising candidate for hydrogen storage due to its low cost, abundant resources, and high hydrogen capacity (7.6 wt.%). However, the sluggish kinetics for hydrogen sorption and the high thermal stability of MgH2 deteriorate its practical application. In order to enhance the hydrogen absorption performance, 10 wt% of carbon with different turbostratic structure and crystallinity, namely anthracite, activated carbon, needle coke, and graphite, as milling aid, is introduced to prepare nanoscale Mg-C hydrogen storage material by mechanical milling. It is demonstrated that all of them exhibit improvement on hydrogen de/absorption kinetics of Mg-anthracite (M-A), Mg-activated carbon (M-AC), Mg-needle coke (M-NC), and Mg-graphite (M-G), when comparing to that of pure MgH2. The microstructure of the composite was determined by XRD, SEM, FT-IR, and Raman. Results show that the introduction of four carbon additives can facilitate the decrease of Mg grain size, the generation of new surfaces, and shortening the diffusion path of hydrogen. Carbon with low crystallinity has more structural defects and disorders in it. The isothermal absorption tests confirmed that the hydrogen absorption kinetics of M-A, M-AC, M-NC, and M-G is much higher than that of pure MgH2. Especially, M-NC composite can release 4.3 wt.% H2 within 2 min at 340 oC with an initial hydrogen pressure of 2 MPa, superior to 0.21 wt.% H2 absorbed by pure Mg powders under the same conditions. It is proposed that the carbon with moderate defects and disorder structure have a favorable effect on the effective hydrogen absorption of Mg.

4.4- Preparation and Lithium Storage Performance of C-GQDs/α-Fe_2O_3 Nanocomposites

Yating Zhang, Kaibo Zhang, Kaili Jia, Guoyang Liu, Shaozhao Ren, Xi'an University of Science and Technology; Jieshan Qiu, Dalian University of Technology, Beijing University of Chemical Technology; PR CHINA.

An electrodeposition technique was adopted to achieve controllable preparation of nano-Fe2O3 particles on a nickel substrate by adjusting the ratio of electrolyte solvent (DMF and water). Subsequently, a solution of coal-based graphene quantum dots (C-GQDs) as the electrolyte was prepared from Taixi anthracite powder. The resulting Fe2O3 was the working electrode. This C-GQDs/α-Fe2O3 composite material was prepared via second-step electrodeposition. The lithium-ion storage performance of C-GQDs/α-Fe2O3 composites as the anode in the lithium-ion battery was studied, and the results show that the composites exhibited excellent cyclability and rate capability. When the current density was 1 A/g, the specific capacitance of C-GQDs/α-Fe2O3 composites was up to 1582.5 mAh/g, and it could maintain 1320 mAh/g after 110 cycles. The specific capacitance was 1091 mAh/g at a high current density (5 A/g).

4.5- Hollow Spherical Nano-ZnO/Coal-based Graphene Macro Porous Aerogels for Photocatalytic Conversion of Carbon Dioxide

Keke Li, Jing Zhang, Kaibo Zhang, Kaili Jia, Guoyang Liu, Yating Zhang, Xi'an University of Science and Technology; Jieshan Qiu, Dalian University of Technology, Beijing University of Chemical Technology; PR CHINA.

The development of novel coal-based carbon materials is fascinating for the value-added utilization of coal resources. In this paper, a facile, green procedure for fabrication of ultra-light and porous ZnO/coal-based graphene aerogels (ZnO/CGA) using plentiful and affordable coal as a carbon source was investigated. The photocatalytic potential of ZnO/CGA was assessed in terms of CO2 reduction into the methanol under ultraviolet light irradiation. It was found that the obtained hollow spherical ZnO/CGA composites exhibited both interconnected porous network and admirable photocatalytic activity towards CO2 conversion in comparison with that of pure ZnO. The superior photoactivity may be attributed to the highly interconnected porous network bridged numerous pathways for rapid mass transport as well as the efficient synergic effect of graphene and ZnO, which facilitated to improve the electron-hole separation rate and the transfer of photogenerated electrons. Overall, the present work not only provides a promising insight into the green utilization of coal resources, but also obtains a kind of such captivating 3D macroscopic coal-based graphene material that can be exploited in environmentally friendly applications.

SESSION 5
GASIFICATION TECHNOLOGIES - 1

5.1- Thermodynamic Analysis of Chemical Looping Gasification Coupled with Lignite Pyrolysis

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A poly-generation system integrating coal pyrolysis and chemical looping gasification (CLG) is proposed to realize the multi-generation of value-added chemicals, synthetic gas fuels and heat/electricity. In this system, the models including coal pyrolysis, coal drying, air reactor (AR) and fuel reactor (FR) are employed to simulate the coupled system using Aspen Plus software. Especially, the FR model is used to produce syngas, which is the main target product, on the basis of Gibbs free energy minimization approach. According to the thermodynamic data obtained from the simulation, chemical exergy and physical exergy are determined for process streams and thermal efficiency is discussed as well. The overall energy efficiency of the new system can achieve values of 43.12%, with the drying unit causing the highest energy destruction. The results indicate that the coupled system shows a better performance compared with its original individual processes in consideration of the thermodynamic efficiency and effects on the environment, though the additional mechanical energy consumption occurs in the new system. Moreover, being used as the gasification agent in the FR, phenol wastewater has been greatly reduced, which reduces levels of environmental pollution. Hence, this new system will be of great potential in industrial application due to its high energy utilization efficiency and low pollution.

5.2- Experimental Study on Coal Pyrolysis in a Fluidized-Bed Reactor by Using Char as Heat Carriers

Kaikun Li, Qinhui Wang, Chunjiang Yu, Mengxiang Fang, Zhongyang Luo, Zhejiang University, PR CHINA.

At present China, coal staged conversion process combined with coal pyrolysis and combustion is consider to be a promising and clean coal utilization, during which oil and gas products are co-produced under relatively mild conditions. The heat resource is an essential point for coal pyrolysis process, and solid heat carriers is proved to be of many advantages. Hot char is one of the frequently-used solid heat carriers. However, the effects of char on the distribution and characteristic of coal pyrolysis products are not quite clear, especially in fluidized bed reactor. Therefore, this study investigated the pyrolysis products properties of Runbei bituminous coal over temperature range from 550 to 800 °C in a self-designed electrically heated bubbling fluidized bed reactor by using char as solid heat carriers. For char carriers' preparation, 20g coal sample was pyrolysis at 850 oC and held for half an hour every time. For comparison, the blank experiment was carried out at the same coal feed by using quartz sand as heat carriers. And the mass ratio of char carriers to coal was set to 5:1 in each experiment. Liquids and gaseous products were collected in a tar trap and a gas bag, respectively. Char was collected in a closed metal funnel and weighed after cooling to room temperature. Water production was measured using Karl Fischer moisture meter and tar yield was calculated

by subtracting the amount of water from the total weight of liquids. Gas yields were calculated with N2 tracing method and its composition was analyzed by gas chromatography. Results showed that the existence of char carriers lower the yields of char, tar and gaseous products, and the water yields increased when temperature higher than 700 ℃. Compared with blank experiment, the volume fraction of CH4 and C2~C3 in gaseous products increased after using char as heat carriers. When temperature was lower than 600 ℃, the yield of CO2 increased while the CO yield decreased. At temperature higher than 600 ℃, the volume fraction of CO2 reduced gradually, the yield of CO increased simultaneously. This could be due to the occurrence of Boudouard reaction (CO2+C↔CO). The comparison between the results on the yield of H2 revealed that introduction the char as heat carries reduced its volume fraction in gaseous products at temperature lower than 700 oC, however promoted its yield significantly at 800 ℃. An interesting phenomenon was that the existence of char solid carriers delayed the temperature when the tar yields showed a peak value.

5.3- Influence of Temperature and Heating Rate on Product Distribution of Low-rank Coal Pyrolysis

Yu Hong, Demin He, Jun Guan, Dalian University of Technology; Xueqiang Li, Jianxuan Shang, Shanxi Coal and Chemical Industry Group Co. Ltd.; Qiumin Zhang, Dalian University of Technology; PR CHINA.

In order to investigate the evolutions of released volatiles during pyrolysis low-rank coal, the compounds in the volatile fraction were identified and semi-quantified via Py–GC/MS. In helium gas atmosphere, coal sample was pyrolyzed at every 100 °C from 300 °C to 700 °C , and under different heating rate(20, 50, 100, 300, 500 °C/min) at 600 °C. Above 200 kinds of compounds were detected, including aliphatics (alkanes, cycloalkanes, olefins, dialkenes, cycloolefins and alkynes), aromatics (alkyl-benzenes, alkyl-naphthalenes, alkyl-indenes, alkyl-fluorenes and PAHs), oxygen containing compounds (phenols, oxygen heterocycles and other oxygen containing compounds) and nitrogen containing compounds. It was found that the final temperature had highly influence on the yields and the distributions of pyrolytic products, which was slightly affected by the heating rate at the same temperature. Temperature and heating rate of pyrolysis affected the species and yields of products by both primary and secondary reactions. More species and amounts were observed with the increasing temperature. The organic structure of coal was heavily destroyed till around 400 °C as a dramatic increase of product species and yields. With increasing heating rate, the secondary reactions of volatiles were aggravated at higher ambient temperature. Moreover, it was beneficial to generate products of smaller molecules when the temperature was higher than 600 °C and the heating rate was higher than 50 °C/min. The ratio of olefins to alkanes varied with the temperature, and more unsaturated hydrocarbons were generated at higher temperature. Moreover, some structural features of the raw coal were inferred from the pyrolytic products. In all, this work can be beneficial for further understanding the process of coal pyrolysis and optimizing operating conditions during industrial applications.

5.4- Oxygen Migration and Regulation in the Process of Lignite Pyrolysis

Hai-jie Li, Xiao-hong Li, Wen-ying Li, Taiyuan University of Technology, PR CHINA.

Grading lignite pyrolysis polygeneration system is one of the key technologies to achieve clean and efficient use of lignite resources. High oxygen content is a major feature of lignite, especially organic oxygen existing in the form of oxygen-containing functional groups, such as carboxyl, hydroxyl, carbonyl and ether bonds. The form and migration of oxygen-containing functional groups directly affect the distribution of pyrolysis products, the processing technology and utilization of downstream products. Therefore, it is important to study the form and migration rule of oxygen in lignite pyrolysis process and to further control the oxygen migration path, which is significant for improving the utilization ratio of oxygen element and realizing the rational utilization of elements in coal. This paper chosen HulunBuir lignite as raw material and adopted several methods to investigate the form of oxygen-containing functional groups, including quantitative analysis of lignite industrial analysis, elemental analysis, chemical analysis and FT-IR. The result of material balance shows that the oxygen proportion of six oxygen-containing functional groups is 82.4% of the organic oxygen in HulunBuir lignite. Further analysis shows that hydroxyl not only include phenolic hydroxyl, but also alcohol hydroxyl group, which accounted for 1/3 of hydroxyl functional groups. We also conduct isothermal pyrolysis experiments using a fixed-bed reactor at 650 °C and adopt elemental analysis, chemical analysis, gas chromatography, FT-IR, GC-MS and other methods to analyze the migration of oxygen from coal to semi-coke, tar gas. Most of the organic oxygen in lignite moved to semi-coke and pyrolysis water, which occupied 27.82% and 54.31% of the total oxygen respectively, and the oxygen transferred to tar was only 3.18%. Further quantitative analysis shows that the oxygen migrated to the phenolic compound occupied 0.5% of the total amount of oxygen. In the subsequent experiment, we employ different pretreatment methods, such as heating, solvent and oxygen alkylation of HulunBuir lignite, to investigate the influence of pretreatment on oxygen transfer path in lignite pyrolysis. After comparison and analysis, the best way to regulate oxygen migration path is provide, which can make more oxygen transfer to the semi-coke and tar and improve the utilization rate of element of the whole process.

SESSION 6
COAL SCIENCE - 1

6.1- Time-Of-Flight Mass Spectrometric Study on In-Situ Pyrolysis of Coal-Based Model Compounds-Phenyl benzyl ketone (PBK)

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Pyrolysis of the coal-based aromatic model compounds, Phenyl benzyl ketone (PBK), was carried out below 50 Pa from 573 to 1373 K. Vacuum ultraviolet single-photon ionization time-of-flight mass spectrometry (VUV-SPI-TOF-MS) was used to investigate the pyrolysis process. The relative concentration of pyrolysis species were estimated by semi-quantitative analysis method. Thirteen pyrolysis species (see the form below) were observed. The initial formation temperatures (TF), the maximum relative concentration (CM) and the corresponding temperatures (TM) of pyrolysis species were listed. PBK showed no secondary pyrolysis below 973K. With temperature increases (see the Figure below, t=1023K-1373K), benzoyl decomposed to give vinyl acetylene and benzyl. and cyclopentadienyl radical was formed by benzyl dissociation via C7H6 species fulvenallene. Meanwhile, the pyrolytic fragments combined each other. Five low-content species, the peaks at m/z 182, 168, 156 and 130, were also identified. The pyrolysis of carbonyl compounds may depend solely on the dissociation of the carbon-carbonyl (-C-CO-) bond. Therefore, the decomposition of carbonyl compounds in coal pyrolysis should have activation energy similar to that of carbon-carbonyl (-C-CO-) bond in model compounds.

6.2- Effect of Inorganics in Liquid Waste from Hydrothermal Treatment on Pyrolysis Behavior of a Vitrinite-Rich Coal

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A vitrinite-rich low rank coal (BSR) from China was treated by hydrothermal treatment. The fixed bed pyrolysis was carried out to explore the effect of inorganics in liquid waste on product distribution and properties of treated coals. The results show that after hydrothermal treatment, the equilibrium moisture as well as inorganic elements (e.g. Na, Cl and Ca) was significantly reduced.

The inorganics in liquid waste from hydrothermal treatment would result in lower tar yield and higher gas yield. Calcium and sodium in treated coal is beneficial to the production of H4 and CH4 during the pyrolysis process. After separation of inorganics from treated coals, the mean pore size of chars decreased and corresponding specific surface area increased dramatically.

6.3- Investigation into the Association Characteristics of Coal Tar Derived from Low and Medium Temperature Pyrolysis of Low Rank Coal by Means of Column Chromatography

Guangsheng Li, Lei Bi, Qiang Xie, Xianglan Zhang, Haiyong Zhang, China University of Mining and Technology, PR CHINA.

Association is one of the key influencing factors on separation of coal tar. In this paper an approach to exploring the association characteristics of coal tar by means of column chromatography was presented. A coal tar sample, derived from 650 oC pyrolysis of Naomaohu long flame coal, a typical low rank coal in China, was distillated at reduced-pressure below 6.3 kPa, from which a 25~190 oC fraction was obtained. Then this coal tar fraction was successively extracted in the column chromatography by a series of solvents with different polarities, including petroleum ether, n-heptane, toluene, acetic ether, acetone, ethanol, carbinol. Finally, the 25~190 oC fraction of coal tar and all extracts from column chromatography extraction were characterized by GC-MS to determine their chemical composition. The results show that typical compounds such as naphthalene, phenol, toluene and their homologues cannot be separated thoroughly from coal tar by extraction with some weak polar solvents due to the association existing within these typical compounds and between different components in coal tar under the influence of intermolecular forces (hydrogen bonds, van der Waals forces, stacking forces, etc.). The magnitude of intermolecular forces determines the association strength

of compounds and components. Weak polar solvents can only destroy the weaker association, while strong polar solvents can destroy all the association and separate the components completely from the coal tar. Therefore, in the extraction process for separating coal tar, solvent with suitable polarity is of great significance in separation of specific component(s).

6.4- Pyrolysis Behavior of Briquette Coal from a Typical Chinese Brown Coal

Weiwei Xie, Yang Chen, Baoshi Guo, Huiya Guo, Lingmei Zhou, China University of Mining and Technology (Beijing), PR CHINA.

Brown coal, accounting for a large part of the coal resources in China, has been increasingly focused by many researches, due to the difficulties to use. In the present work, a typical Chinese brown coal was firstly made into the briquette by hot flue gas and certain pressure. The pyrolysis behavior of the briquette was investigated in a fixed bed reactor, by introducing constant N2 flow, temperature range was from room temperature to 900℃, atmospheric pressure, heating rate was 5 K/min. The results showed that the property of brown coal was upgraded by the briquette process. For pyrolysis behavior of briquette, the char yield decreased with increasing pyrolysis temperature, with the change of its property. The char produced at low temperature owned many micro-pores and poor integrity, while the surface of high temperature was smooth. The optimum value to obtain high heating value products was around 650℃.

SESSION 7
POWER PLANTS - 2

7.1- Study on the Denitration Performance of Mn-Fe Based Catalytist under Low Temperature Conditions

Wang Cuiping, Qingdao University, PR CHINA.

Mn-based catalyst is usually used to reduce the NO into N2 under lower temperature for the denitration of flue gas from coal firing. But the residual SO2 and vapor in flue gas are always inhibiting the selective catalytic reduction (SCR) activity of Mn/γ-Al2O3. So the Mn-Fe/γ-Al2O3 catalysts was investigated to improve the sulfur-resistant of the catalysts. At the same time, the influence mechanism of H2O was studied. The results show that Mn/γ-Al2O3 and the catalyst are deactivated faster in the SO2 reaction atmosphere. The deposition of ammonium sulphate and the sulfation of the active component are the most important cause for catalyst deactivation. Sulfation of the active component is effectively reduced by the addition of Fe, the stability of the ammonium sulfate salt on the surface of the catalyst is lowered, and the sul fur resistance of the catalyst is improved.

7.2- Mathematical Modeling and Controller Design for a 1000 MW Ultra-Supercritical Coal Fired Unit

He Fan, Pei-hong Wang, Zhi-gang Su, Southeast University, PR CHINA.

It is challenging to establish a dynamic mathematical model of a 1000 MW ultrasupercritical coal fired unit. This paper presents such a model in form of statespace equations, derived from mass and energy conservation laws, and it has the simplest form of model with three inputs and three outputs. In this structure, static parameters and functions were estimated by using steady data and nonlinear regression analysis, whereas dynamic parameters were identified from running data by using a discrete identification method based on immune genetic algorithm (IGA). Lastly, a simple coordinated control system based on this model was designed using PID controllers. Simulation results suggest that the model has proper steady and dynamic accuracies, and it can be used for controller design.

7.3- 1-D Analysis of a 560 MWe Power Plant Boiler Performing Under Different Coal Specifications

Hamed Jafari, Won Yang, Korea Institute of Industrial Technology; Changkook Ryu, Professor, Sungkyunkwan University, Suwon; SOUTH KOREA.

The present work takes advantage of a steady one-dimensional (1-D) combustion and heat calculation scheme in order to study the effect of coal specification on the performance of a commercial scale 560 MWe boiler. In the furnace section, the mathematical model is mainly based on Russian normative zonal method in order to deal with radiation heat absorbed by water walls and steam production. In the convective section both the impact of radiation and convection is considered in order to predict the heat exchange between flue gas and steam. Seven types of bituminous and subbituminous coals with different specifications regarding moisture content, volatile matter, fixed carbon, ash content and heating value are tested. Since the 1-D scheme is capable of considering interactions between different physical parameters and operating conditions, it will lead to study of 1- flue gas temperature distribution in the furnace and back pass, 2- The effect of flue gas temperature and flue gas fly ash content on its emissive power, 3- incident and absorbed radiation heat by the water walls as a function of height, 3- steam production (raise) rate, 4-slag deposit layer temperature, 5- heat absorbed by each of the tube banks and steam temperature in every section of the steam cycle, and 6- flue gas composition and flow rate. It is found that considering same thermal input to the boiler, the impact of noncombustible parts of coal (ash and moisture) on the thermal performance of the boiler is significant. Regarding ash, it is found that 31.3% increase in ash content of coal results in 63% increase in the emissive power of the flue gas which in turn results in 15.2% increase in steam production mass flow rate through water walls. Regarding moisture content, it is found that coals with higher moisture content usually result in higher total air required for the combustion and higher mass of flue gas production. It is also found that for coals with almost same amount of H, O, and S, the coal with higher moisture content leads to higher amount of CO2 in the flue gas.

7.4- Operation Guide System for Taean 300MW IGCC Plant

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Taean 300MW class IGCC project was launched at the end of 2006 and had begun commissioning at the end of 2015. Taean gasification plant has adopted process technology of SCGP (Shell Coal Gasification Process) and SGTT (Shell Gas Treating Technology). The plant has finished the performance test and got into commercial operation at the end of 2016. In this period, the reliability of IGCC plant was low due to frequent trip of gasification unit, in common with many other IGCC plant in early stage of commercial operation. Gasification unit is composed of gasifier producing syngas of 1550oC and syngas cooler cooling down the syngas to 250oC. Key factors to stable operate the gasification system are the gasifier operating temperature and heat duty affecting to the slagging, fouling, steam production, syngas composition and mass production. But, unfortunately, the gasifier operating temperature cannot be directly measured from instrument because of the high temperature, corrosive and slagging condition. Also, the gasifier heat duty is very sensitive to slag thickness on the wall. These factors should be properly controlled from O2/Coal ratio, Flux/Coal ratio and Steam/O2 ratio changed according to coal type and operation load. Because of lack of uniformity of constituent concentration in the same coal type, these control parameters also should be changed properly during normal operation.
So, in this study, the operation guide system was developed to improving the reliability for gasification unit in Taean IGCC plant. This system is connected with the main control system and gives real-time alarm and troubleshooting guide to the operators. This system is composed of the various simulation models predicting the performances and risks for corrosion. The simulation models provide results of the coal evaluation, optimum feedstock flow, optimum operation temperature, gasifier performances, start-up table, syngas cooling performances and thermo-fluid dynamics in a gasifier using ROM (Reduced Order Model). Also IOW (Integrity Operation Window) model guides the safe operation window using real-time operation data to protect the pipes and static equipment against corrosive condition. As a result of, the operation guide system has been contributing in raising operation reliability of Taean gasification plant.

7.5- Latest Development of International Cofiring Biomass Technology Application

Xing Zhang, IEA Clean Coal Centre, UK.

How to solve the problem of CO_2 emission reduction in thermal power units, is one of the research focuses of advanced thermal power technologies at present, while cofiring biomass technology in large coal-fired boiler is one of the options. This technology can help realize strategic adjustment of energy, improve production and living environment, and promote the efficient use of resources. Cofiring biomass in large coal-fired boilers has been applied in UK, United States, Finland, Denmark, Germany, Austria, Spain, and many countries, with installed capacity up to 850MW and good performance. In China and India, scattered burning of rural straw and other biomass has increased the haze pollution. Cofiring biomass in coal-fired power plants can solve the pollution problem while reducing the coal consumption in coal-fired units, which is a win-win both in energy saving and emission reduction. Therefore, application of cofiring biomass in coal-fired units has become a focus in relevant departments. The aim of this presentation is to provide latest data on international cofiring biomass situations in coal-fired units, the operation reliability of units, power generation efficiency, pollutant emission, and relevant preferential policies etc.

SESSION 8
COMBUSTION TECHNOLOGIES - 2

8.1- Development of Oxy-Fuel Combustion Technology in a 0.1 MWth Circulating Fluidized Bed

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In December 2015, the Conference of the Parties (COP21) agreed on an ambitious goal of keeping the increase of the global average temperature to well below 2 °C, and seeking to limit the temperature increase to 1.5 °C above pre-industrial levels. Making strict targets earlier than 2 °C will enhance the need for in-depth technology such as carbon capture and storage (CCS). Oxy combustion is considered one of the most promising carbon capture technologies. Although no significant difference was observed in the efficiency penalty for capture, the oxy-combustion technology has the least efficiency reduction. Moreover, it makes the retrofitting of existing power plants easier and can be integrated with new power plants. Although the oxy-combustion technology was first applied to pulverized coal boilers, oxy-fuel circulating fluidized bed combustion (Oxy-CFBC) has increasingly focused on a promising power generation technology for carbon capture utilization and storage which can easily diversify fuel. Oxy-CFBC has several unique advantages: 1) the amounts of flue gas recirculation are significantly less to control the boiler temperature caused by the re-circulating solids that effectively act as a heat moderator at the external heat exchanger, which allows the economics to be significantly improved through a reduction of the CFBC boiler island size; 2) Oxy-CFBC is easier to retrofit with in-situ SOx and NOx removal and reduce the load on the downstream refinery; and 3) Oxy-CFBC is flexible to the size and nature of the fuel, making it suitable for biomass co-firing, which allows for the net reduction of anthropogenic CO2 emissions. The challenge for this project is to optimize the Oxy-CFBC process to produce a small amount of flue gas with near zero-emission and high-purity CO2 using various fuels. Various element technologies were tested and validated in a 0.1 MWth Oxy-CFBC test rig to realize the process optimization. The fuels were sub-bituminous coal, lignite, and wood pellet. The proven technologies and oxy-fuel database in this test-rig are expected to be used as empirical operating parameters in a 2MWe Oxy-CFBC plant. The oxy-fuel database includes combustion characteristics, CO2 purity, pollutant removal efficiency, and ash characteristics according to various fuel and operating conditions

8.2- The Role of K_2CO_3 on Structural Changes of Coal, Biomass and Coal/Biomass Blends during Pre-Treatment Using N_2 and CO_2. Differences in the Reactivity Under Oxy-Combustion Conditions

Yuli Betancur, Taiyuan University of Technology, PR CHINA; Diana López, Universidad de Antioquia, UdeA, COLOMBIA; Zhen-yi Du, Wen-ying Li, Taiyuan University of Technology, PR CHINA.

Nowadays, coal/biomass blends are gaining importance as energy sources, since it results in the reduction of fossil fuels consumption and hence CO2 emissions, particularly if it is used under the oxy-combustion process, which is one of the most promising technologies to use in existing coal power plants due to the relatively easy adaptation with only minor modifications, as well as several advantages in terms of emissions and efficiency.
Partial replacement of coal by biomass leads to differences in the morphological and structural characteristics and behavior of obtained chars on thermochemical transformation processes such as pyrolysis, combustion and gasification, which are also involved during oxy-combustion processes, compared with the characteristics using coal individually.
Considering that the gasification process can be modified by the presence of alkali and alkaline earth metals which have catalytic effects over this process, when biomass is employed under oxy-combustion process it is possible to promote the gasification reactions due to the high CO2 concentration (balance gas) and the high mineral matter content in biomass, especially potassium.
With the aim to verify this hypothesis in the present study, corncob biomass, as well as lignite and anthracite coal were used to evaluate the potassium catalytic effect on gasification reactions. The raw materials were oven-dried at 110 °C for 24 h, grounded and sieved into particle sizes of 400–600 μm. Finally, biomass was blended with coals in a ratio of 20:80 wt % by physical mixing.
10 wt % of K in K2CO3 was added to the individual fuels and their blends, impregnated and non-impregnated chars were obtained under CO2 and N2 atmospheres at 700 °C.
The reactivity (ignition temperature and activation energy) under oxy-combustion conditions (21 % O2 -79 % CO2) was studied at 700 °C using a thermogravimetric analyzer. Differences in reactivity are discussed considering changes in physical-chemical properties characterized by Raman spectroscopy and XPS.

8.3- Performance Analysis for a Retrofitted Oxy-Fuel Boiler

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To obtain high-concentration liquid CO2 for yield improvement in an oil/gas field, the retrofit scheme of oxy-fuel boiler based on a subcritical Π-type boiler with steam output of 220 t/h in a self-supply power plant was proposed. A reasonable flue gas recirculating mode, i.e., half-dry mode is selected to apply to design oxy-fuel boiler system in view of avoid coal blocking in mill and pulverized coal piping due to water condensation. The proposed retrofit scheme is designed following minimizing retrofit work and the compatibility of air-firing and oxy-firing. The original heating surfaces of Upper air preheater, Lower economizer and Lower air preheater are split into two parts individually to heat the primary gas and the secondary gas, respectively. Besides, the other heating surfaces are kept unchanged. The performance calculations for original air-firing boiler and oxy-fuel boiler after retrofit have been performed and compared. Thermal efficiency of oxy-fuel boiler is slightly lower than that of original air-firing boiler. Heat loss of exhausted gas of oxy-fuel boiler is only about 8% of that of air-firing boiler. Meanwhile, heat loss due to flue gas treatment, which is only present in oxy-fuel boiler system, of 5.86% of oxy-fuel boiler is included. For the heating surfaces upstream of Upper economizer, oxy-fuel boiler has lower flue gas temperatures, including the adiabatic combustion temperature, compared to air-firing boiler. However, the corresponding heat transfer ability is nearly equivalent. For the heating surfaces downstream of Upper economizer, the flue gas outlet temperatures of oxy-fuel boiler are higher than those of air-firing boiler and the final heated temperatures of the primary gas and the secondary gas are also higher. The minimum flue gas outlet temperature of exhausted flue gas of boiler is higher 10℃ than the acid dew point of 154℃.

8.4- Integrated Flue Gas Purification for Staged, Pressurized Oxy-Combustion

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Pressurized oxy-combustion is a promising new technology for coal-fired power production that can deliver high combustion efficiency with a concentrated CO2 stream suitable for carbon sequestration or utilization. In this approach, the combustion takes place at elevated pressure, e.g. 15 bar, such that the dew point of the combustion flue gas is raised and the latent heat is recovered. Prior to final compression for storage or utilization, gaseous pollutants (primarily NO, NO2 and SO2) must also be removed from the combustion exhaust stream. If not carefully removed, harmful acid condensation and corrosion can occur in downstream equipment.
Pressurized oxy-combustion provides an opportunity for a different method of pollutant removal, which uses direct water contact for flue gas cooling and latent heat recovery combined with simultaneous purification via pollutant adsorption and complex liquid phase chemistry. However, several aspects require further research before large scale implementation is possible – primarily the determination of reaction kinetics and the effect of scaling. This is accomplished in two different reactors, a bench scale CSTR and a 100-kW prototype column. An ASPENTM model has also been developed in parallel to provide a numerical sub-model for integration into a full-scale process model of a Staged, Pressurized Oxy-Combustion power plant.
The CSTR experiments investigate the interaction between nitrite and sulfite in the liquid phase, quantifying parallel reaction rates for the formation of nitrous oxide (N2O) and hydroxylamine disulfonic acid (HADS). The results determine the effect of pH, molar ratio and temperature in the initial formation period, determining the liquid composition at concentrations, temperatures and reaction times applicable for commercial scrubbing columns.
The larger prototype column utilizes the liquid phase kinetics and process model to scale the liquid chemistry for gas pressures, temperatures, flowrates and pollutant concentrations equivalent to a 100-kWth oxy-combustor output. The primary objective of the column is to optimize parameters to maximize flue gas purification while controlling liquid discharge temperature and heat recovery.

8.5- Integrated Process of Coal pyrolysis with Low Alkanes Reforming of CO_2 over Modified Ni-Based Catalysts

Jiannan Lv, Yang Li, Lijun Jin, Haoquan Hu, Dalian University of Technology, PR CHINA

The studies on the integrated process of coal pyrolysis with CO2 reforming of methane indicated that radicals from methane reforming can react with coal radicals or activate other methane. Considering low activation temperature of ethane, an integrated process of coal pyrolysis with CO2 reforming of low alkanes (methane and ethane) was investigated by using Ni-based catalysts to improve tar yield. In the process, ethane was added to activate the methane at lower temperature and the effect of temperature, ratio of methane to ethane and the catalysts were examined in an atmospheric fixed-bed

reactor. The results indicated that a higher tar yield than that under N2 atmosphere could be obtained in the integrated process. The tar yield at 600 oC under methane to ethane ratio 8:1 by commercial catalyst is 1.2 times as that under N2. However, the commercial catalyst was easy to be deactivated because of coke deposition even though modified with cerium. Therefore, Ni/CeO2 catalysts with different Ni contents were prepared, which have strong resistance to carbon deposition as reported. The results showed that coke deposition over Ni/CeO2 catalysts are less than that over the commercial catalyst. Ni/CeO2 showed good catalytic activity of the reforming reaction, and more tar produced in the integrated process. The tar yield over Ni/CeO2 with 12 wt.% Ni loading is 1.2 times as that over commercial catalyst under methane to ethane ratio 8:1 at 600 oC. In addition, the catalysts prepared by co-precipitation shows a better performance in the process than that by impregnation.

SESSION 9
CLEAN COAL DEMONSTRATION AND COMMERCIAL PROJECTS - 1

9.1- Study on Process Optimization and Upgrading of Power Coal Preparation Plant in China

Zhang Zhen, China National Energy Group Ningxia Coal Group Coal Preparation Center, PR CHINA.

Combining with the characteristics of the low metamorphic degree and easy to be slimed in China, the advantages and disadvantages of traditional separation technology of power coal in China was expounded, the problems brought about by full-size coal preparation was analyzed and the idea of optimizing production technology of dry-process deep screening through relaxation screen and its successful application in Ningdong mining area were introduced. For example, it provides reforming experience for the comprehensive coal preparation and processing of power coal in China, and puts forward the basic principles of realizing the maximization of comprehensive benefit, the reliability of product quality control and the minimization of operation cost.

9.2- Numerical Investigation on Combustion and NOx Emission Characteristics in a 600 MW Tangentially Coal-fired Boiler Co-firing with Semi-coke

Zichen Tao, Chang'an Wang, Pengqian Wang, Qinqin Feng, Maobo Yuan, Defu Che, Xi'an Jiaotong University, PR CHINA.

Semi-coke is a solid product which derives from lignite or high volatile bituminous coal by low temperature retorting. Many problems limit the utilization of semi-coke, such as difficulty in the ignition and stable combustion, low burnout rate, and high NOx emission. Therefore, it is a challenge to achieve clean and efficient combustion and large-scale application for domestic power plant boilers. A numerical investigation on combustion and NOx emission characteristics in a 600 MW tangentially coal-fired boiler was performed in order to co-firing with semi-coke in the pulverized coal boilers, optimize the combustion performance of the furnace and reduce NOx emission. Through the method of blending semi-coke with bituminous coal, the problem of combustion can be solved. A series of conclusions can be obtained by the analysis of the numerical simulation results. The results show that it is preferable to inject semi-coke into burners from the second layer to upper layer, which contributes to the ignition and steady combustion of semi-coke and effectively decreases the carbon content in fly ash and NOx emission at furnace exit. On this basis, the suitable blending ratio of semi-coke is 40%, which can take both the utilization of semi-coke and contaminant emissions control. Furthermore, about 20% over-fire air rate and above 80% boiler load are conducive to the co-firing of semi-coke. From the prospect of energy conservation and pollution reduction, oxy-fuel combustion is recommended based on appropriate conditions. The present investigation will be helpful for the utilization of semi-coke and NOx emission control.

9.3- A CFD Modeling of Biomass Combustion in the Retrofit Boiler

Yu Jiang, Pusan National University; Byeong-Cheol Sim, Korea South-East Power CO.; Chung-Hwan Jeon, Pusan National University; SOUTH KOREA

In this study describes the numerical simulation of biomass combustion in a retrofit boiler, and combustion characteristics and pollutant emissions were confirmed in the analysis results. Biomass fuel is a renewable energy source that has been widely used in power generation in thermal power plants in recent years. The obsolete boiler is down shot-firing boiler, while the fuel was coal. Through the retrofit of burners and furnace type, it has the conditions for burning biomass. And we thought Computational Fluid Dynamics (CFD) tools have been increasingly used for optimizing the combustion process, and gas emission. The simulation conditions were derived from the design data and operational data of the thermal power plants in Korea. Through numerical analysis confirmed that the flow characteristics and biomass combustion in the retrofit boiler. The result shows that it was proved that the NOx emission was reduced and high burnouts when wood pellet was burnout in the boiler. The current research is beneficial to offering guidance for the operation of the biomass combustion in the retrofit boiler. And we expect this use of renewable energy combustion technology to reduce environmental pollution.

9.4- Hotspots and Technical Requirements on Coal Preparation in China

JianguoYang, You Zhou, Lixi Zhou, China University of Mining and Technology, Xuzhou, PR CHINA.

With the great increase of coal preparation capacity and the improvement of the basic research conditions in China, technics and equipment of coal preparation have been developing rapidly and great progress has been made in fundamental process research. The improvement of flotation process is a hotpot in fundamental coal preparation research. The hotspots concerned by Chinese coal processing enterprises include automation, heavy medium separation, process design and transformation, equipment development, flotation and so on. In terms of the purpose of coal preparation, realistic requirements and future development direction of coal preparation technology will be mainly focused on three aspects: the production of specific products, reduction of processing cost and intellectualization.

9.5- Improving Economics of Coal Power by Retrofitting Flameless Pressurized Oxy-Combustion with Integral CO2 Capture

Massimo Malavasi, Itea S.p.A., ITALY; Peter Reineck, Consultant to Itea S.p.A., UK; Joshua Schmitt, USA.

Future power markets are expected to require a larger quantity of load-following power plants which reduce output during the night and early morning, when the demand for electricity is the lowest, and which can respond rapidly to peak loads at any time, a consequence of the variable output of wind and solar power. A coal power plant based on Flameless Pressurized Oxy-combustion (FPO) can go from 5% to 100% of capacity rate in less than a half hour in response to fluctuating demand, while capturing over 90% of the CO2 produced for use in enhanced oil recovery (EOR) or sequestration.

FPO provides a pathway towards affordable, efficient, and clean coal power, and enables a power plant to access new revenue streams from CO2 and also from load-following. However, in an investment climate which is hostile to fossil energy, upgrading existing coal power plants to enable CO2 capture (CC) is likely to be more attractive than building new plants. This paper provides a review of the FPO technology and an update on work underway to scale-up the technology for use in commercial coal-fired power plants, and concludes with a discussion of the projected economics of new-build and retrofitted coal power plants based on FPO technology.

FPO is a proven oxy-combustion technology that was developed to recover energy from low ranking coal, as well as other brown fuels and wastes. Itea began developing FPO in 2003 on a 5-MWth pilot in Gioia del Colle, Italy, to destroy hazardous industrial waste and as such, design objectives were very high combustion efficiencies and capture of metals in the fuel in the vitreous slag.

In the FPO process, combustion takes place with oxygen; recirculated flue gas is used to moderate combustion temperatures. The resultant flue gas is primarily CO2 and water, allowing for relatively simple and cheap CO2 capture. Coal is fed as a slurry in water to the combustor which operates at c. 10 atm pressure, to improve overall efficiency. Notably, the FPO cycle recovers most of the heat of vaporisation of the contained water, enabling coals with c. 60% moisture content to be used as-mined, without drying.

FPO is a low-emission technology. Molten ash particles coalesce and drain to the outlet, substantially eliminating the particulate content in the exhaust gas and allowing the use of coals with up to 40% alkaline ash content. Zero thermal NOx minimizes overall NOx, and total organic content (TOC) at combustor exit is hundreds of times lower than for traditional combustion processes.

Work on DE-FE0027771, a 2-year DOE project led by SwRI to provide the design for a 50-MWth FPO pilot plant that can fire a wide range of high-to-low rank coals, will be completed in September 2018. The project is investigating improving the cycle for power generation with CO2 capture by incorporating a turbo-expander as a bottoming cycle, to increase overall efficiency. A cost study on the updated FPO design is part of the project. The FPO pilot plant would then be demonstrated over a 3-year test program to generate data for the design of a 500-MWth firing module commercial power plant with integral CC which could start operation in 2026. Permitting and other work on the FPO pilot plant will continue in a Phase 1 project under DE-FOA-0001788 - Fossil Fuel Large-Scale Pilots, for which SwRI's application was selected by NETL, with work expected to start in the third quarter of 2018.

A comparison of the levelised cost of electricity (LCOE) of various cases is made, including established supercritical pulverised coal (SCPC) technology with and without post-combustion CO2 capture (PCC), and FPO with integral CC firing low-ranking coals with high water and ash content. The projected economics of FPO technology will be presented for new-build plants and for a retrofit concept in which an FPO firing module replaces the sub-critical or super-critical boiler in an existing power plant.

SESSION 10
VALUE-ADDED PRODUCTS FROM COAL - 2

10.1- A Promising and Feasible Method to Enhance Oil Yield during Large-Scale Direct Liquefaction of Sodium-Rich Zhundong Coals

Xiao Li, China University of Mining and Technology, CHINA.

In the recent years, thermal treatment of coals with high-boiling point aromatic solvents has drawn much attention, as it can effectively separate coals into different value-added fractions and obtain hyper-coal with trace impurities. During the coal-slurry heating process, aromatic solvents are also prone to react with coals and it will inevitably improve reactivity of coals toward DCL. Inspired by this, whether thermal treatment of Zhundong coals (ZDC) can promote transformation of sodium species and mitigate the negative effects on oil yield has raised our great interest. Besides, the influences of solvent types on behaviors of sodium species during thermal treatment remain little known either. Therefore, effects of thermal treatment on transformation of sodium species and structural changes of ZDC were mainly investigated. After raw coal was pretreated by tetralin (THN) or 1-methylnaphthalene (1-MN) at 150 oC, 200 oC, 250 oC, or 300 oC, transformation of sodium species among different occurrence modes was examined and the structural changes of coal molecules were characterized. To further probe transformation mechanisms of sodium species during thermal treatment, X-ray photoelectron spectrometry (XPS), Fourier transform infrared spectroscopy (FTIR), and gas chromatography (GC) analyses were jointly used.

10.2- Preparation of Coal-based Conductive Carbon Membrane for Waste Water Treatment

Pan Zonglin, Yang Jiawei, Dalian University of Technology; Song Chengwen, Dalian Maritime University; Pan Yanqiu, Wang Tonghua, Dalian University of Technology; PR CHINA.

Organic contaminations in wastewater have become one of the most serious environmental problems in the world due to their toxicity, persistence and bio-refractory. As a novel technology for water treatment, electro-catalytic carbon membrane reactor (ECMR) can effectively remove the persistence organic pollutants due to the synergistic effect of electro-chemical oxidation and membrane separation. In this work, the coal-based carbon membranes (CCM) with good conductivity and thermal/chemical stability were prepared from the cheap and abundant coal. The effects of carbonization temperature (CT) on the pore structure, mechanical strength, electric conductivity, microstructure and electrochemical performance of CCM were systematically investigated. Results show that the diameter of tubular carbon membrane decreases with the increasing of CT, and the porosity and pore size distribution do not dramatically change. The conductivity of CCM increases sharply as the CT arises from 500oC to 950oC, and the electric resistivity of CCM become stable nearly 20mΩ·cm at the CT of higher than 950oC. The mechanism strength enhances with the increases of CT from 500oC to 1300oC due to the compaction of membrane structure and the order carbon microcrystalline structure of CCM. CCM exhibits higher thermal stability (air atmosphere) and chemical stability at the higher CT. Electrochemical measurements indicate that the CCM carbonized at higher CT possesses the higher OEP and phenol oxidation peak current value that means a higher electrochemical activity.

10.3- Construction of Coal-based Activated Carbons by Physical-Chemical Activation for High Performance Supercapacitor Electrodes

Xiaoming Yue, Zhaoyang An, Shengfan Xue, Jing Xu, Yajun Wu, Zijing Liu, Cuicui Xiao, Mei Ye, Shuangquan Zhang, China University of Mining and Technology, PR CHINA.

Coal-based activated carbon has been prepared with Taixi anthracite as the precursor by a facile two steps of physical-chemical activation. The columnar activated carbon is prepared from Taixi anthracite by extrusion, carbonization and physical activation with CO2. With acid pickling, part of the ash is eliminated from columnar activated carbon. Columnar activated carbon was impregnated with different concentrations of potassium hydroxide solution to optimize the amount of alkali, and then activated again to obtain activated carbons as electrode material. Activated carbons exhibit higher BET surface area and larger total pore volume than the first activated columnar activated carbon, which is beneficial for improving the electrochemical performance. The electrochemical characteristics of the as-prepared activated carbons are tested in a three-electrode cell and supercapacitors respectively. The optimized material displays a specific capacitance as high as 255.4 F/g at a current density of 0.5 A/g in 6 mol/L KOH electrolyte under a three-electrode cell. The optimized material demonstrates a superior cycle stability as an electrode material, and the capacitance decay is hardly observed after 5000 consecutive cycles.

SESSION 11
GASIFICATION TECHNOLOGIES – 2

11.1- Release of Sodium in Typical Shanxi High Ash Anthracite with Na-Flux under Fast Pyrolysis Conditions

Rui Rao, Yongchun Zhao, Gaolei Li, Hongyue Wang, Junying Zhang, Huazhong University of Science & Technology; Jin Bai, Wen Li, Chinese Academy of Sciences, PR CHINA.

It is all known that the type of sodium flux has a great influence on the sodium release ratio and the ash fusion temperatures. In this work, totally nine samples including SX coal and SX coal with 0.5%, 1%, 2% NaCl, Na2SO4, NaOH were systematically collected to study the sodium release and the mineral transformation of typical shanxi high ash anthracite (SX) with different sodium-based fluxes during pyrolysis process. Then, the sodium content was measured by Inductively Coupled Plasma Emission Spectrometer (ICP-OES) and the ash fusion temperatures (AFTs) was detected by AFTs instrument. In addition, the mineralogical composition and mineral transformation during pyrolysis were characterized by the X-ray fluorescence microprobe (XRF), X-ray diffraction (XRD) and Thermogravimetric-Analysis (TGA). Moreover, the thermodynamic simulation software HSC Chemistry 6.0 was applied to analyzed the sodium release and the mineral conversion during coal pyrolysis process.
It was proved that the addition amount of sodium has the most significant effect on the ash fusion temperatures, the lower ash fusion temperatures was detected with higher sodium content and the ash fusion temperatures can be reduced by about 150°C at most. The sodium release ratio in coal samples with NaCl and Na2SO4 flux rises while coal with NaOH flux decreases with increasing temperature. In the coal samples with NaCl flux, the Na release ratio increased with the higher flux content, but decreased with the higher addition of Na2SO4 flux and NaOH flux. The amount of NaCl and Na2SO4 have positive effect while NaOH present negative effect on sodium release ratio at the same temperature. It should be pointed that the change of sodium release ratio is not significant from 1000°C to 1100° C. The results of TGA and XRD showed that the decomposition of pyrite occurred at 460°C , the decomposition of calcite occurred at 740°C. The weight loss peak at 580°C meant the decomposition of kaolinite, and the peak at 825°C stands for the decomposition of muscovite, and there was almost no mineral decomposition weight loss after 1000 °C. According to the thermodynamic calculations, the typical Shanxi high-ash anthracite hardly releases Si and Aland Na release as NaCl before 1200°C while release as elemental-Na form with the temperature increased further under pyrolysis conditions. It was noted that the element-Cl can significantly affect the Na release process.

11.2- Investigation on Effect of Functional Groups on Volatile Evolution in Coal Pyrolysis with in situ Py-PI-TOFMS

Yang Zhou, Haoquan Hu, Lijun Jin, Yang Li, Jian Zhou, Zhiwei Shi, Dalian University of Technology, PR CHINA.

In situ pyrolysis photoionization time-of-flight mass spectrometry (py-PI-TOFMS) was implemented on eight coal samples, which were pyrolyzed in situ and soft ionized in the ion source, to enable the fragment-free detection of volatile organic compounds generated from initial pyrolytic products. The obtained mass spectra of eight coal samples revealed predominantly molecular ions with four categories: alkenes, benzenes, phenols, and dihydroxybenzenes. Temperature-evolved profiles of major products are visible via scanning of the ion current of individual compound measured during the pyrolysis processes. Furthermore, it is demonstrated by the analysis of different coal samples that both methyl and hydroxyl groups attached on the benzene rings can dramatically reduce the peak temperatures of major products' evolution, and the effect of hydroxyl group is significantly stronger than that of methyl group. The difference of peak temperatures among homologue series of alkylated benzenes and phenols were correlated to carbon content and volatile content of coal samples, which was found negatively correlated with the carbon content and positive correlated with the volatile content, respectively. In addition, the temperature difference between propylene, which was used as a benchmark, and its homologue series of alkenes first increases and then decreases with the rising carbon content. The overall results allowed to reveal the influence of the substituted groups to the volatile organic compounds during coal pyrolysis. And analogous to reported setups with online studies of coal pyrolysis, py-PI-TOFMS may be a good option for monitoring the evolution characteristics and reaction pathways of coal pyrolysis process.

11.3- The Characteristics of Tar Quality in the Process of Pyrolysis and Gasification of Naomaohu Subbituminous Coal

Huan Wang, Qian Wang, Quan Wang, Jiao Kong, Meijun Wang, Taiyuan University of Technology, PR CHINA.

In order to improve tar quality from rapid pyrolysis of low rank coal, a new integrated technique of low rank coal rapid pyrolysis and gasification in the downer-fluidized reactor with transverse tube (DFT) was designed. The influence of pyrolysis temperature on the yield of pyrolysis products and the quality of tar generated during the coupling process of coal pyrolysis and char gasification was investigated by using Naomaohu subbituminous coal due to its high tar yield. The quality of tar and syngas is improved during coupling coal pyrolysis at low- and mid-temperature with high-temperature char gasification in the DFT. Results show that the yield of obtained tar reaches 17.09 wt%(d) at 600 oC, which is about 1.69wt% higher than that of tar from the Gray-King assay. Then the yield decreases with further raising of temperature due to the second reaction and steam reforming of tar. Both the amounts of tar generated from coupling pyrolysis and single pyrolysis are reached the maximum at 600 oC, herein, the amount of hexane soluble substance (HS) in tar from coupling pyrolysis is about 20% higher than that from single pyrolysis.

11.4- Interactions between CO2 and H2O on Char Structure Evolution during Coal Char Gasification

Yajie Zhou, Shenghua Zhu, Liang Ren, Lunjing Yan, Yonghui Bai, Taiyuan University of Technology, PR CHINA.

This work focuses on the interactions between CO2 and H2O on char structure evolution during coal char gasification and alternate gasification is an effective way to reveal the interaction. The alternate process is as following: coal gasification with H2O (CO2) was first performed in a thermo gravimetric analysis (TGA) to prepare coal char residual with carbon conversion level of 25%, after Ar purged for 20 min, CO2 (H2O) was switched to prepare the final char residual with carbon conversion level of 50%. N2 adsorption and Scanning electron microscope (SEM) analysis were used to characterize the pore structure and surface morphology information. The results indicate that CO2 gasification mainly took place on char surface while H2O could diffuse into the inside of pore structure and react with char to expand the diameter of the pores. In the co-gasification, reaction could occur on both the char surface and matrix simultaneously and interactions between H2O and CO2 were observed. H2O and CO2 atmospheres seem to favor formation of mesopores and micropores, respectively. Mesopores formed by H2O gasification facilitate access of CO2 to interior of char matrix. Alternating CO2/H2O sweeping reveals synergetic interactions between the two gasifying agents.

11.5- Experimental Study of the Flat-Flame Pulverized Coal Gasification Technology

Haiquan AnLiu Zhen, Baozai Peng, Qingliang Guan, Ziyang Feng, Bing Liu, Xinhui Fang, Ya Suo, Xin Cui, Feng Huang, Wenhua Li, National Institute of Clean-and-Low-Carbon Energy, PR CHINA.

A flat-flame pulverized coal gasification technology is presented and its test results on a 3 t/d gasification test facilities are discussed. The test results show that the performance data of flat-flame gasification technology is better than the traditional top-placed single-burner technologies, and the test facility is in stable operation during the test periods. Computational fluid dynamics (CFD) tools are also employed to investigate the flow field characteristics of the flat-flame gasifier. It is revealed that, the flat-flame burner enables higher turbulent intensity and enhances the turbulent mixing between coal particles and oxidant. The overall gasification reaction rate is increased by abovementioned effects. Preliminary test results and simulation analysis validates the technical feasibility of flat-flame gasification technology and it is ready for scale-up for industrial demonstrations.

SESSION 12
COAL SCIENCE - 2

12.1- Study on the Emission and Transformation Behavior of As, Hg, Pb and Se during Coal Gangue Combustion in O_2/CO_2 Atmosphere

Fangqin Cheng, Hao Peng, Baofeng Wang, Fengling Yang, Shanxi University, PR CHINA

Transformation behavior of As, Hg, Pb and Se during coal gangue combustion in O2/CO2 atmosphere and air were studied. The results showed that As content in coal gangue which was from Pingshuo in Shanxi Province of China was as high as 4290.4ppm, Pb content was 1867.65ppm and the contents of Hg and Se were 0.961ppm and 10.22ppm relatively. The results showed that at higher temperature, more Hg and Se could transfer to the gas phase; and higher O2 concentration also made the same results. In addition, the results also showed that the As content in ash obtained from combustion of coal gangue at 1000 ℃ in O2 /CO2 atmosphere (with 40% O2) is the lowest (22.90 ppm). while the lowest Pb content was found in the ash obtained from combustion of coal gangue at 900 ℃ in air, and the value of the lowest content of Pb is 24.07pp; and the lowest Se content in ash also was got when the coal gangue is burned under this condition, and the lowest content of Se in the ash is 2.79ppm. Furthermore, the results indicated that more content of As and Pb will be volatilized when the coal gangue combusted in air than in O2/CO2 atmosphere, while O2/CO2 atmosphere is more favorable for volatilization of Hg; and when coal gangue combusted in O2 /CO2 atmosphere with 20%O2, the Se content in ash is the lowest.

12.2- The Transformation Characteristic of Sulfur Species during Thermal Extraction of Typical Low Rank Coal

Jia'nan Yin, Xiongchao Lin, Yonggang Wang, Zhen'gang Xu, China University of Mining & Technology (Beijing), PR CHINA.

Solvent extraction is an effective approach to separate and analyze the molecular structure of coal, and further classify the transformation mechanism of heteroatoms in the extraction process. The effect of temperature on the solvent extraction efficiency was studied in this paper. The molecular transformation of these heteroatom compounds during the extraction process was studied by Fourier Transform Infrared Spectroscopy (FT-IR), Atomic Emission Detector for Gas Chromatography (GC-AED) and X-ray Photoelectron Spectroscopy (XPS). The result shows that high extraction yield obtains since the solvent has polarity, the ability to impart hydrogen, and the similarity to the solubility parameter of coal. The xylene extraction yield of coal increased with the increasing temperature. The higher extraction yield will be obtained if the extraction temperature is close to the initial pyrolysis temperature of coal. Furthermore, different solvents have synergistic effect during the extraction. Analysis of the extracts reveals that the thermal extraction mainly destroyed the hydrogen and covalent bonds of the coal structure. Based on the principle of "like dissolves like", most of the extracts are alkanes, naphthenes and aromatic hydrocarbons. Pyrite and sulfate can be completely transferred into residue through extraction process. The sulfur in the extract is mainly organic sulfide which includes thiophene, sulphoxide, sulphone and their S-containing homologues. Thermal extraction not only works for deashing, dehydroxylation and desulfurization of low-rank coals but also reforms and redistributs the heteroatoms in coal.

12.3- Volatilization Characteristics of Mercury in Coal During Conventional and Microwave Drying Process

Ningning Zhang, Xi'an University of Science and Technology; Changchun Zhou, China University of Mining and Technology; PR CHINA.

During the thermal drying process of coal, the sufficient attention has been paid to the changes in the properties of coal before and after the drying process. However, the volatility characteristics of harmful trace elements in coal during the drying process are always neglected to date, whereas the volatilization of harmful trace elements not only has significant effects on the surrounding atmosphere environment but also influence the following utilization of dried coal. In this study, the volatility characteristics of both the moisture and mercury in the coal sample during conventional (electric blast oven) and microwave (microwave oven) drying processes were investigated. The results show that the moisture content of coal decreases in non-line format (decreases slowly at the first and then quickly according to the drying time) in the conventional drying process, while it decreases in line format in the microwave drying. The microwave drying process needs much shorter time required to obtain the dried coal of a certain moisture content than the conventional drying process. Under the same volatilization rate of moisture, the volatilization rate of mercury in the microwave drying process is always greater than that in the conventional drying process. Nearly half or more (49.73% and 59.26%, respectively) of the mercury in the coal slime evaporates into the atmosphere after the drying processes.

12.4- Process Development of Making High Efficiency Silicon-Calcium Fertilizer with the White Mud

Aiguo Chen, Huidong Liu, Xiaohuan Wang, Yongfeng Xiao, National Institute of Clean-and-Low-Carbon Energy, PR CHINA.

The white mud is a residue discharged by the process acid-method aluminum extraction from coal fly ash, and harmful to environment. Whether environment friendly and valuable utilization of the white mud or not has already became a key factor restricting the commercial application of acid-method fly ash aluminum extraction technology.
Through detailed and comprehensive study of mineralogical, petrological and geochemical characterization, some sole features of the white mud were revealed: 1) highly enriched in SiO2 (70-80%), while concentrations of acid soluble elements such as Na, Al, Fe and some hazardous heavy metal elements including Pb, Cr etc., were

significantly lower than its raw fly ash; 2) about 60% of SiO2 in the white mud was with relatively high reaction activity, as the Al-extracting procedure broke the Si-O-Al structure of amorphous phase of fly ash, and partly performed the activation of silica in fact.

In view of that the main production area of the white mud is also an area of environmental degradation and ecological vulnerability, based on the analysis both of technology and product market, one of the main technology project chosen for reusing the white mud was to produce Silicon-Calcium Fertilizer (SCF). It has been proved that Si is beneficial to plants, especially gramineous plants such as rice, wheat, barley, maize and sorghum etc. According to statistics, approximately 50% of the paddy rice soils in China are Si-deficient. By making High efficiency SCF from the white mud, the local soil and ecological environment would be benefited rather than being further destroyed, and the surplus SCF can be transported to the areas needed.

For making high efficiency SCF with the White mud, flotation technology was implemented firstly to remove unburned carbon, and part of heavy metal elements among the white mud simultaneously, in view of the high affinity shown by some heavy metal elements to organic matter in coal combustion fly ash. After the flotation treatment, content of SiO2 increased by about 13 wt.%, which was propitious for the preparation of SCF with a higher effective silicon.

The developed main activation process was called a one-step sodium-calcium reaction process, its reaction conditions were mild (<150℃, normal pressure environment). By this process, the white mud was entirely transformed into high-effective silicon-calcium fertilizer; its effective silicon content was as high as 35%, and containing several active nutrient elements such as Ca, Mg and K. During the process, the consumption rate of sodium was ideally controlled. Waste alkali liquor was recycled, and there was no secondary solid waste discharged.

12.5- The Behavior of the Sulfur Transformation in Semi-Coke during Catalytic Depolymerization of Zaozhuang Coal

Zeyu Peng, Taiyuan University of Technology, PR CHINA.

As a coking coal, the total sulfur content of Zaozhuang Coal is about 2.33%. Even after washed by the 1.4g/cm3 zinc chloride solution, the total sulfur is still as high as 2.07%, for which greatly limited its use for coking. Earlier study found that the adding of different amount of Co- and Ni-based catalyst had a significant effect on the yield of pyrolysis tar during the low temperature catalytic depolymerization of Zaozhuang coal. Moreover, the catalysts also showed an obvious effect on the transformation of the sulfur in the semi coke. As shown in Fig. 1, the total sulfur content of the semi-coke from pyrolysis of the Zaozhuang raw coal is 2.02%, while the total sulfur content of the semi-coke is reduced to 1.87% with the addition of 0.1% of the Co-based catalyst. With the increasing addition of Co-based catalyst, the total sulfur content of the semi-coke increases. When the Co-based catalyst added content comes to 0.6%, the total sulfur content of the semi-coke reached to 2.05%, for which exceed the semi-coke without catalyst. Then the sulfur content of the semi-coke showed an increase trend with the increase amount of the Co-based catalyst. With the addition of Co-based catalyst to the demineralized coal during catalytic depolymerization, the total sulfur content of the semi-coke first increase and then decrease with the increase of the amount of catalyst added. Similarly, when the addition amount is 0.6%, the total sulfur content reached a maximum of 2.31%. The sulfur contained in demineralized coal mainly exists in the form of organic sulfur. Thus the experiments result showed that the addition of Co-based catalyst inhibits the release of organic sulfur during pyrolysis, and the effect changes with the addition amount of Co-based catalyst. The total sulfur content of the catalytic depolymerization of Zaozhuang raw coal is significantly reduced after the addition of the Ni-based catalyst, and the total sulfur content of semi-coke changes little with the amount of the Ni-based catalyst increases. As the amount of catalyst added is increased from 0.1% to 1.0%, the total sulfur content of the semi-coke is between 1.31% and 1.38%. After the adding of Ni-based catalyst to the demineralized chars, the variation trend of total sulfur of the semi-coke is different from that of raw coal. The content of the total sulfur of semi-coke with catalyst is lower than that of the semi-coke without catalyst. However, with the increase amount of the Ni-based catalyst added, the content of the total sulfur of semi-coke first decreased and then increased. The addition of nickel-based catalyst promote the decomposition of organic sulfur in coal, but this effect does not increase with the increase of the amount of catalyst added. There is an optimal addition amount, that is, When the amount of Ni-based catalyst is 0.2% of coal, the promotion effect is most remarkable, and the semi-coke total sulfur is reduced to 1.07%.Comparing the desulfurization rate of the Co-based catalyst with the demineralized chars and the desulfurization rate of the Ni-based catalyst, it indicates that both the Co-based and Ni-based catalysts can promote the thermal decomposition of the inorganic sulfur in the coal.Conclusion:1) Co- and Ni-based catalysts promote the thermal decomposition of inorganic sulfur in Zaozhuang coal;2) Co-based catalyst inhibits the thermal interpretation of organic sulfur in Zaozhuang coal. When the addition amount of the Co-based catalyst comes to 0.6%, the inhibition effect is the most significant;3) Ni-based catalyst promotes the thermal interpretation of organic sulfur in Zaozhuang coal. The promotion is most significant when the addition amount is 0.2%.

SESSION 13
POWER PLANTS - 3

13.1- Study on the Combustion Characteristics of Blue-Coke and Its Application in Pulverized Coal-Fired Boilers

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Blue-coke was investigated for the first time as a new fuel for pulverized coal-fired boilers. The one-dimensional flame furnace combustion test bench and the pulverized coal ignition temperature test furnace were utilized to conduct experi-mental research. The experimental results showed that blue-coke has an ignition temperature of 983 K, burn-out rate of 97.41% and slagging index of 0.84. Blue-coke is a kind of fuel which is difficult to ignite, easy to burn-out and has serious slagging. The ignition and burn-out characteristics of blue-coke are between bituminous coal and lean coal, while the slagging charac-teristic is significantly stronger than that of conventional lean coal and anthracite. After careful considering the effects on the ignition, burn-out and slagging characteristics of different types of coals, the suggested blending ratio of blue-coke is around 33% when co-combusted with bituminous coal or anthracite, and it is about 67% when co-combusted with lean coal. The co-combusted experiment on a 135 MW pulverized bituminous coal boiler showed that when blending with 33% of blue-coke, various systems of the boiler operate normal, the SO2 and dust pollutants are reduced by 20% respectively, while the boiler ef-ficiency decreases by 0.4% and the capacity of the mill is affected.

13.2- NSGA-II Based Multi-objective Optimization of NOX Emission and Reheat Steam Temperature

Xian-hua Gao, Zhi-gang Su, Southeast University, PR CHINA.

It is challenging and imperative to reduce NOX emission with increasing reheat steam temperature in particular at lower load condition. To solve this problem, this paper proposes to optimize the NOX emission and reheat steam temperature simultaneously via a modified version of Non-Dominated Sorting in Genetic Algorithm (NSGA-II), in which the predictions of NOX and reheat steam temperature are achieved by a new version of multiple outputs nonlinear partial least squares model (MO-NPLS). To perform the proposed method well, some experiments are conducted on a real 1000MW ultra-supercritical unit. By comparison, the results suggest that the Pareto optimal solutions obtained by NSGA-II performs well with appropriate accuracy and outperform experimental value.

13.3- Analysis of an Integrated Mild-Partial Gasification Combined Cycle (IMPGC) Power Plant

Ting Wang, Henry A. Long, III, Energy Conversion & Conservation Center, USA.

Coal is one of the most prominent energy resources in the world today. Many countries with emerging economies, especially, are turning to coal as an economic and effective means to meet their quickly rising energy needs. Coal is also very dirty: it contains large amounts of ash, sulfur, and other pollutants that, without being adequately cleaned up, will pose serious threats to both public health and the environment. Coal plants also tend to have large carbon footprints, which many are concerned will significantly contribute to climate change. Coal gasification technologies via Integrated Gasification Combined Cycles (or IGCC) have been used to address this problem by raising the power plant efficiency with more effective pre-combustion gas cleanup process. One of the major energy losses that occurs during IGCC is during syngas cooling, as the existing commercial gas cleanup processes must occur at low temperature, wasting a lot of useful heat energy (exergy) in the meantime, even though part of the energy is recovered later. This also leads to a loss of chemical energy, as the volatile matters within the feedstock must be cracked down to the simplest and lightest carbon- and hydrogen-based compounds (mostly CO and H2 with the occasional amount of CH4 and C2H2) to avoid the condensation of larger compounds (such as tars) that would potentially damage the system. With the advent of a new "warm gas clean-up" (WGCU) process developed by Research Triangle Institute (RTI), the gases can be cleaned at much higher temperatures than they otherwise could be using traditional cleaning systems. This, in turn, means that fully cracking the volatile matters down to CO and H2 (full gasification) is not necessary. Rather, mild gasification can be used to preserve the high amounts of chemical energy in the volatile matters, and produce a syngas with around twice the heating value of conventional fully-gasified syngas. In addition, partial gasification can be used to preserve the char fines so that they can be used with existing pulverized coal power plants. Furthermore, due to the small size of the mild gasifier compared to a full-sized entrained-flow gasifier, it is possible to engineer a system that can most economically and conveniently be retrofitted onto existing pulverized coal (PC) plants to boost their

efficiency and reduce emissions without replacing the entire power plant. The resulting combined cycle system is called the Integrated Mild-Partial Gasification Combined (IMPGC) Cycle, and the benefits of such a system are analyzed and discussed in this paper.

13.4- Progress in Commissioning a Pilot-Scale Staged, Pressurized Oxy-Combustion System

Zhiwei Yang, Dishant Khatri, Adewale Adeosun, Tianxiang Li, Akshay Gopan, Benjamin M. Kumfer, Richard L. Axelbaum, Washington University in St. Louis; Ismail Celik, Department of Mechanical and Aerospace Engineering, West Virginia University; USA.

Concerns over the greenhouse gas emissions from coal-based power generation have led to several efforts towards new generations of coal combustion technologies for CO2 mitigation, including staged, pressurized oxy-combustion (SPOC), a unique process that burns coal under pressure. At higher pressure the latent heat of condensation of the moisture in the flue gas can be utilized in the Rankine cycle, increasing the plant efficiency. Also, the flue gas recycle in the SPOC process is significantly reduced, compared to first generation oxy-combustion plants, by means of fuel-staged combustion. As determined through process analyses, the SPOC process increases the net plant efficiency by more than 6 percentage points, compared to first-generation oxy-combustion plants.
This work includes two parts. In the first part, a new configuration of SPOC process which allows for modular boiler design will be proposed. With the modular boiler design, the capital cost of the plant can be reduced, since the boiler can be constructed off-site and shipped to the plant site. Also, the modular boiler design provides better plant operating flexibility, because deep turn-down can be achieved by either reducing the thermal input of each boiler or shutting down one or more boilers. In the second part, the progress of the boiler design demonstration in a 100 kWth pressurized oxy-combustion experiment facility will be presented. The boiler design features a co-axial, low mixing flow with no external recirculation. The aim of the design is to maintain an acceptable radiative wall heat flux and minimized ash deposition while burning coal under pressure. The operating pressure of the facility is 15 bar. A high-speed camera was used to capture the dynamics of the flame. Gas species and particles are sampled to characterize the combustion process inside the reactor. A large eddy simulation for the combustor was also performed. The modeling results showed flame characteristics very similar to the experiment data

SESSION 14
COMBUSTION TECHNOLOGIES - 3

14.1- Investigation on the Effect of Kaolin and Ammonium Sulfate as Additive to Melting Behavior: The Korean Rice Straw Co-Firing Case

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As the usage of coal has continuously generated carbon dioxide, the whole world has been faced climate problem such as global warming. Biomass is currently a best alternative for a part of coal as fuel, so that use of biomass is constantly increasing for power generation around the world. For promoting usage of domestic biomass in Korea the government is especially preparing to change energy policy that domestic biomass has more weight than imported biomass in terms of Renewable Energy Certificate (REC). Most herbaceous biomass are consisted of Korean biomass. So, it would be expected to apply herbaceous biomass to power plant for gaining more REC. The herbaceous however, is difference with woody biomass in terms of ash (ash content and element component). And the herbaceous biomass produced a lot of Ash in the biomass. The problem with ash is that slagging and fouling are formed in the boiler system, which reduces the efficiency of the boiler and disrupts the system, resulting in economical and efficient problems. Therefore, the purpose of this study is to investigate the effect of additive for reducing the slag of problems caused by herbaceous biomass co-firing. The Korean rice straw, one of the herbaceous was used for this study. Additive is also applied to reduce the factor that induces slag production due to chemical reaction. In this study kaolin (Al2Si2O5(OH)4) and ammonium sulfate ((NH4)2SO4) is chosen as additive and investigated the influence as compared the results. In order to determine fuel properties, there was carried out the fundamental analysis such as ultimate analysis, proximate analysis, and ICP analysis. In addition, 80kWth test facility in KITECH is used to investigate slag behavior in coal burning condition. Prior to the experiment, the selection of the additive is occurred based on FactSage, a software program for chemical equilibrium model calculations. In this experiment, the online monitoring system is used to measure the real time incremental amount and predict slagging/fouling characteristics based on this. The result from FactSage show that amount of slag in ammonium sulfate case is lower than kaolin case. The tendency of slag formed when kaolin was added to the fuel during combustion increased significantly unlike in co-firing with woody biomass. When kaolin is added, the content of slag is changed from Ca-Mg silicate with high melting point to K-Al silicate with low melting point. Due to this, the amount of slag increases. However, when (NH4)2SO4 is added, it reacts with K, which increases the formation of slag and sulfate in (NH4)2SO4, and low temperature molten silicate is converted to high temperature molten silicate. Finally, these reactions dramatically reduce the tendency of slag. This is a good agreement with 80 kWth combustion test. Experimental results show that the ash rate is 8.76 g/hr in the case of confluence and the ash rate is 0.97 g/hr in the case of adding (NH4)2SO4, and the ash reduction rate is about 88.9% when the additive is added. As a result, Kaolin (Al2Si2O5(OH)4) and (NH4)2SO4, which are additive for herbaceous biomass foliage, may have different results depending on the characteristics of the fuel. The FactSage result is consistent with the results of the experiment.

14.2- Ash Deposition and Slagging Behavior of Blended Coal with Xinjiang High-Alkali Coal in 3MWth Test Facility

Xiaojiang Wu, Xiang Zhang, Jianwen Zhang, Kai Yan, Nan Chen, Shanghai Boiler Works. Co., Ltd, PR CHINA.

The most serious ash deposition/slagging problems of Chinese high alkali coals in Xinjiang Province are the biggest troubles for power plant recently. In light of this, most of units have to be operated under a low generating capacity (70~80 % BMCR) or blend with other kind of coals which incurs the increased operating cost. This paper is aimed to clarify the ash deposition/slagging behavior of blended coal with Xinjiang High-Alkali coal (HA coal) during combustion process in boiler. One typical HA coal and another low-alkali coal (LA coal) have been mixed to study the ash melting behavior as a function of coal blending ratio, through the use of AFTs test, XRD, SEM-EDX characterization of ash samples and 3MWth pilot-scale test. The results indicate that, the trend of AFTs is not linearly related to the blending ratio of coal mixtures. Instead, it is highly linked with the changes on the liquidus temperature from the ternary phase diagram systems. The initial melting temperature of HA coal ash is approximately 275 0C lower than that of LA coal ash due to the existence of alkali and alkaline earth metals, although it has relative higher ash fusion temperature. The mixing of LA coal is not only beneficial to reduce the amount of vaporized sodium, but it also increases the initial melting temperature of blended ash due to the physical and chemical reactions between alkali and silica particles. The higher content of Na gas was formed during HA coal combustion process due to the promoted effect of the existence of Cl in HA coal. Some low melting minerals, such as Na2SO4, $Na_3Fe(SO_4)$, NaS_2O_7, were found as the dominate minerals in its deposit ash on heat transfer tubes in the temperature range 650~1000℃ when combustion HA coal. When blended with other LA coal, the amount of deposit ash was decreased and the shape of it became looser due to some high melting minerals were found in its deposit ash, such as quartz and mullite etc. The optimum blending ratio of LA coal is 20% for its safe operation for HA coal.

14.3- Influence of SO42-and Cl- on Minerals Condensation and Slagging Characteristic

henghui Yu, Cheng Zhang, Xiao-pei Zhang, Xin Li, Qing-yan Fang, Gang Chen, Huazhong University of Science and Technology, PR CHINA.

The high sodium and calcium contents in Zhundong coal and the sulfate and chlorate produced in flue gas on the surface of heat exchanger increase fouling and slagging. However, there are still many debates on the mechanism of effect of sulfate and chlorate on ash accumulation in heat exchangers. In order to study the effects of sulphate and chlorate on the condensation and accumulation of sodium and calcium on the surface of heat exchangers of coal-fired boilers, Wucaiwan coal (WCW) was selected for the study as a typical Zhundong high sodium coal. Slagging experiment of flue gas at 900oC in heat exchanger was simulated in a horizontal tube furnace. The thermocouples were used to collect the temperature of different zones, and XRD and XRF were used to analyze the composition of the slag. SEM and stereo microscope were used to analyze the morphology of the slag. The results show that slagging can be divided into three steps: the formation of sodium salt precursors, the growth of silicate loose structural layers and the adhesion of surface minerals. Temperature is selective to slag, and the content of silicon and calcium in the slag at 873 oC is high, while the content of sodium in the slag at 591oC is high. SO42-has a significant adsorption effect on sodium and calcium at high temperature, while Cl- has a significant adsorption effect on sodium at low temperature. Finally, the layered structure and the mechanism of slagging for SO42-and Cl- were proposed.

14.4- Development and Evaluation of an Innovative Wet Electrostatic Precipitator Based on Ion Jet Technology in View of Coal-Burning Pollutants on Pilot Scale

Pingyuan Liu, Liang Zhao, Qiliang Lu, Shanghai Power Equipment Research Institute Co., Ltd. PR CHINA.

According to the ion jet technology, an innovative wet electrostatic precipitator (WESP) was developed and tested in this paper to remove coal-burning pollutants in wet desulfurized flue gas. The target coal-burning pollutants include dusts, fine particles, sulfuric acid aerosols and desulfurization slurry droplets. In this innovative WESP, the target coal-burning pollutants can be collected not only by the electric field force, but also by ion jet, which will be generated in the process of electrode discharge. For the flow of charged ions, the velocity of ion jet can be as high as 1000 m/s, and thus the high speed ions can push small particles, such as dust, fine particles, sulfuric acid aerosols and desulfurization slurry droplets to the collecting wall. The removal performance of this innovative WESP for target coal-burning pollutants in typical working conditions was tested. Besides, the influences of discharge voltage, flue gas velocity and flue gas temperature on the removal efficiency were also investigated to further reveal the rule of removal performance variation. The results indicated that the higher discharge voltage is beneficial for the improvement of removal performance, while the influences of flue gas velocity and temperature are not significant. It can be also obtained from this paper that in typical working conditions, the removal efficiencies for dusts, fine particles, sulfuric acid aerosols and water droplets in wet desulfurzied flue gas by this innovative WESP base on ion jet technology can reach about 95%, 90%, 38% and 97%, respectively.

14.5- Experimental Study on Cyclone Combustion of High-Alkali Coal

Zhang Xiangyu, Zhang Bo, Lu Xu, Xu Hongjie, Xi'an Thermal Power Research Institute Co., LTD, PR CHINA.

The cyclone combustion characteristics of high-alkali coal need to be further studied. In this paper the experiments of cyclone combustion of Zhundong coal were conducted on a pilot cyclone furnace, and the characteristics of combustion and alkali metal migration were researched. The results indicate that, the pulverized coal in the cyclone furnace is attached to the wall, and is slagging in the liquid form. The staged air supply is benefit for the burnout of coal and reduction of nitrogen oxides. When the excess air ratio in the cyclone is 0.9, the NO emission is about 475 mg/m3, and the NO2 emission can be ignored, and the SO2 emission is about 1600 mg/m3. The unburned carbon content in the ash is 3.85% while it is less than 1% in the slag. The slag captured rate is nearly 58% when the R90 is equal to 19.2. As part of the alkali metals can be captured by the liquid slag layer to form aluminosilicate, the contamination and slagging on the heating surfaces of boiler tail can be relieved in the cyclone furnace.

SESSION 15
CLEAN COAL DEMONSTRATION AND COMMERCIAL PROJECTS - 2

15.1- TDS Intelligent Dry Sorting Machine's Application and Benefit

Xiaodong Ge, Tianjin Meiteng Technology Co., Ltd., PR CHINA.

Based on X-Ray or image recognition, TDS intelligent dry sorting machine uses compressed air ejection to realize coal sorting. It has the advantages of high sorting precision, wide sorting size and high intelligence. It can be applied to lump coal sort ing in thermal coal preparation plant, coking coal preparation plant pre-concentration, underground drainage and filling, especially for the selection of arid areas and lignite. TDS intelligent dry sorting machine has successively put into operation more than ten sets of projects, such as Zhaozhuang anthracite coal mine, Huozhou Ganhe and Wangjiata coal mine. Up to now, 47 units have been sold, which can achieve 1-3% coal in reject and reject in cola. All these applications show that TDS technology is mature, effective, and has wide application conditions.

15.2- TRIGTM CORE Technology of the Kemper IGCC Project

WanWang Peng, Guohai Liu, Pannalal Vimalchand. Matt Nelson, Tim Pinkston, Gasification Technology; Diane Madden, U. S. Department of Energy/National Energy Technology Laboratory; USA.

The Kemper County Project has demonstrated air-blown Transport Integrated Gasification (TRIG™) technology at a 2-on-1 combined cycle facility located in Kemper County, Mississippi. The TRIG™ technology centers around the Transport Gasifier—a pressurized, circulating fluidized bed unit that features high riser densities and high solids circulation rates. Other major features of TRIGTM technology are the Pressure Decoupled Advanced Coal feed system (PDAC) and the Continuous Fine and Coarse Ash Depressurization systems (CFAD and CCAD).

With a unique design that avoids the need for any internal moving parts, the first-of-a-kind commercial PDAC coal feed system successfully controlled the coal feed rate, while adjusting for load changes by modulating the gas motive force. At Kemper, the PDAC could operate up to 725 psig and feed lignite with moisture contents of up to 25% and at rates of up to 125,000 lb/hr per feeder. The coal is conveyed by dry air from the coal feeder to coal injection nozzles on the gasifier, reducing nitrogen consumption and dilution of the syngas.

The CCAD and CFAD systems continuously depressurized ash from the gasifier and particulate collection device (PCD) to discharge pressures required to convey ash to the ash silos. The method of the ash depressurization is through the friction created between the ash particles and the gas phase. Entrained gas is released though a pressure letdown device, creating a desirable velocity difference between the gas and solids to dissipate the pressure energy in the entrained gas. The entrained gas vented is very low, less than 0.1% of the total gas produced by the gasifier. Unlike conventional systems, the CCAD and CFAD systems do not require lock vessels, eliminating the need for nitrogen to pressurize. The systems also avoid using cycling valves in the solids stream, typical of conventional systems. At Kemper, the units featured first-of-a-kind designs and the operating results validated the design on a commercial scale.

Kemper also used a novel coarse ash cooling technology to cool the ash from a nominal gasifier operating temperature of 1800°F to less than 350°F. The innovative cooler features a special entrance region where the incoming ash at 1800°F mixes with the cooled refluxing ash to produce an ash mixture with temperatures less than 1000°F. The cooled up-flowing ash stream comes in contact with heat transfer surfaces, avoiding the use of expensive, exotic materials for the cooling surfaces. The ash cooler uses two stages of cooling to optimize the cooling surface area by maximizing the temperature differences between the solids and the coolant. The first stage cools the hot ash to about 600°F, with the second stage further cooling the ash to below 350°F. Compared to conventional screw ash coolers or rotating drum systems, the ash cooling systems at Kemper have no moving parts and, therefore, eliminate operational weaknesses such as shaft leaks.

The PCD fines, nominally 10 microns mass mean size, primarily consists of fly ash with about 10% fine char particles. They exit the PCD at temperatures of up to 600°F and are cooled in a multistage moving, fluidized bed cooler to below 350°F. In the innovatively designed fines cooler, all of the cooling surfaces are vertically oriented to minimize the accumulation of fines in any section of the cooler.

This paper discusses the innovations associated with the core TRIGTM technology featured, detailing the design and performance of these systems at the Kemper IGCC facility.

15.3- Producing Synthetic Natural Gas (Sng) From Thar Coal in Pakistan

Farid A Malik, FC College, PAKISTAN.

Ever since the discovery of huge gas reserves (12TCF) in 1952, Pakistan has developed an extensive state of the art gas transmission and distribution network spread over 20,000 km. due to mismanagement and misuse the reserves have been prematurely depleted (2TCF). The shortfall (120 MMCFD) is being met by imported Liquefied Natural Gas (LNG) which costs 35% higher than the local gas.

Now that mining has started at the largest coal deposit (175 billion tons) of the country, the possibility of producing SNG is also being considered. Dakota Gasification Company produces 175 million cubic feet of SNG per day by using 18,000 tons of Lignite whose composition is similar to Thar Coal deposit. Process development work will be carried out jointly at Centre for Coal Technology University of Punjab and Gas Technology Institute Chicago. Compared to imported LNG, SNG can be reduced at a lower cost ($9 vs. $5 per MMCFD at Dakota Gasification Company).

15.4- Novel Nanocomposite Surface Treatment for High Efficiency Low Emission Coal Power

Vinod Veedu, Matthew Nakatsuka, Erika Brown, Ganesh Arumugam, Oceanit, USA.

Fouling of heat transfer surfaces plays a significant role in the efficiency and greenhouse gas emissions of a coal-fired utility, particularly in those plants utilizing nearby bodies of unprocessed water such as rivers or oceans for cooling. Buildup of either biofilms or scale deposition can significantly increase the effective thermal resistance within the condenser unit, turbine backpressure, fuel consumption, and greenhouse gas emissions. In order to mitigate these factors, every plant must adopt some form of cleaning and mitigation strategy, all of which require significant operational expense and/or regular required offline time.

This paper details the adaptation of a novel, fouling resistant surface treatment to improve the heat transfer performance of a prototypical shell-and-tube exchanger unit. The surface treatment, unlike most conventional epoxy coatings, was applied at a thickness of less than 100µm, and was shown to have a negligible effect on thermal energy transfer in a liquid-liquid model system. Characterization of biofilm growth and attachment on the treated surface was shown to be significantly reduced, both in static and dynamically controlled testing conditions. Additionally, despite the extremely thin application, the surface treatment showed excellent abrasion and erosion resistance, even when applied to a previously worn/cleaned substrate, indicating its potential for refurbishment of existing, in-service units.

The surface treatment was applied both on a laboratory coupon scale as well as on a pilot basis, in order to demonstrate both suitability at the micro- and macro-scale. This paper will detail the changes in exchanger performance and behavior after application, along with outlining the expected improvement both in operational efficiency. Additionally, initial trials on applying the coating on the vacuum-side of a condenser unit in order to promote more efficient drop-wise condensation shall be discussed, and an estimate on the overall effect on plant operations and estimated backpressure penalty shall be determined.

15.5- Development of Coal-to-Synthetic Natural Gas (SNG) Technologies in China

Jianwei Li, Xin Xin, Jiaojiao Lei, Feng Bai, Xi'an University of Science and Technology, PR CHINA.

With the implementation of the strategy of sustainable development and environmental protection policy, the contradiction between supply and demand of natural gas in China is becoming more and more prominent. As a substitute of natural gas, Synthetic Natural Gas(“SNG”) can be used to reduce foreign dependence and ensure energy security. This article compares processes and technical characteristics of various technologies based on a comprehensive evaluation for existing technologies of coal-to-SNG at home and abroad. The methanation technology in the two-step method of coal-to-SNG was introduced, and the process flow and process characteristics of the Davy, TREMPTM, and Lurgi methanation technologies were analyzed and compared. At last, this article gives the advice on how to develop SNG industry in a healthy way.

SESSION 16
VALUE-ADDED PRODUCTS FROM COAL - 3

16.1- Reducing Alkali Species from High-Alkali Coal by Hydrothermal Pretreatment

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Despite its abundant resource, high-alkali coal (Na2O in dry ash>2%, by weight) is limited in application due to its higher ash slagging and fouling tendency during coal thermal conversion, such as coal combustion or gasification. Thereby, it is of importance to reduce the undesirable species from the high-alkali coal. In this paper, a novel method named hydrothermal pretreatment (HTP) was introduced to remove the alkali species, which was conducted within a batch-type autoclave under various temperatures. The treated coal was analyzed, along with the oxygen-containing functional groups determined by Fourier transform infrared spectrometer (FT-IR). And the alkali species and other components in the coal ash were quantified by X-ray fluorescence (XRF), then the ash slagging and fouling tendency was evaluated. Apart from this, FactSage was adopted to simulate the behavior of alkali species during coal thermal conversion.
The results show that the alkali species could be washed out, with the removal ratio up to 54.5% even under 50 °C, while the residual alkali content in treated coal exceeds 2% unless the HTP temperature reaching 300°C. HTP could remarkably reduce both the inorganic- and organic alkali from coal, and there is a positive correlation between the removal ratio and the temperature. With the temperature approaching 300°C, the alkali content could be lowered less than 2%, with a maximum removal ratio of 82.1%. The slagging and fouling tendency of the treated coal is depressed in view of the calculations based on the XRF results. Furthermore, the lowering of slagging and fouling tendency via HTP is also demonstrated by the FactSage simulations, where more high-melting-point species form rather than the low temperature eutectics for the raw coal. Besides, the coal treated via HTP is superior to the raw one in terms of certain remarkable changes, for example, the moisture, oxygen and sulfur of the treated coal decline obviously, while the calorific value rises sharply. In summary, HTP could effectively reduce the alkali species from the high-alkali coal. And the proposed mechanism may lie in that the alkali species in coal matrix became released due to the breakage of the coal functional groups and micropores during HTP.

16.2- Montan Wax Extraction from Baoqing Lignite and Its Characterization

Zhonghua Zhang, Cuiqing Zhang, Xin Cui, Shuang Lang, Congyun Liu, Wenhua Li, Future Science &Technology City, PR CHINA.

The main uses of lignite are as a fuel, but it also offers potential as a chemical feedstock. Some lignite contains waxes, also known as Montan Wax. Montan wax is a mixture of resins, asphalt and wax. It has been widely applied in daily chemical industry, precision casting, papermaking, automotive and other fields. At present, no synthetic wax or natural wax will replace lignite wax due to its excellent physicochemical properties. Montan wax is usually extracted from wax-rich lignite by using solvents (such as benzene, toluene, etc.). In view of the lack of in-depth study on the occurrence and extraction mechanism of Montan wax, the typical lignite---- Baoqing lignite which has large reserves in Heilongjiang, China, was taken as the research object, and relevant experiments and theoretical studies were carried out. The lignite was identified and analyzed for its physical and chemical structure features by FT-IR, SEM, XRD, solvent extraction-GC/MS, and TG techniques, in order to analyze the structure of the lignite and the occurrence form of Montan wax. Based on the analysis of the characteristics of wax, the extraction process was improved, and the Montan wax yield of lignite was improved effectively. It provides basis for industrial application of extraction technology of Montan wax.

16.3- Preparation of Carbon Fibers with Highspecific Surface Area by Degradative solvent Extraction product from Biomass Wastes

Chao Wu, Huazhong University of Science and Technology; Xian Lia, Huazhong University of Science and Technology, Xinjiang University; Xianqing Zhu, Kai Xu, Zhenzhong Hu, Weixiang Qian, Guangqian Luo, Huan Liu, Hongyun Hu, Hong Yao, Huazhong University of Science and Technology; PR CHINA.

A cost-effective method for preparing the mixture of thermal solvent extractionproduct from biomassand PAN based carbon fiberwith high specific surface areawas newly developed. The extraction products had many excellent properties, such as high carbon content, low ash content, high aromatic content and good thermoplastic. The extracts obtained by sawdust were the more proper extraction product mixed with PAN as the precursor of carbon fiber. Adding PAN to the extraction product was to improve the spinnability of the precursor. After stabilization and carbonization, the specific surface areaand specific volume of the fibers obviously increased. The diameter of carbon fiber prepared by the mixture of the proper extractand PAN was about 169nm~200nm.The specific surface area and specific volume of carbon fiber prepared by the mixture ofthe proper extractand PAN respectively reached to 714.24m2/g and 164.10cm3/ghigher than that of carbon fiber prepared by PAN.

16.4- Upgrading of Lignite Pyrolysis Tar by Catalytic Cracking over Different Mo-loaded HZSM-5 Catalysts

Feng Mao, Jie Wang, East China University of Science and Technology, PR CHINA.

Lignite is a low-rank coal with high content of volatile matter, which is beneficial to produce value-added chemicals by way of pyrolysis. However, lignite pyrolysis tar (LPT) often generally has very complex compositions with high fractions of heavy components and heteroatomic compounds especially oxygenates. In many cases, these compositions are undesirable because they have several negative impacts on the qualities of LPT. The catalytic cracking of LPT is perceived as an effective approach to upgrade LPT. In the present work, the experiment was carried out using a two-stage reactor. The volatile matter derived from the lignite pyrolysis in the first reactor was allowed to be subjected to the catalytic cracking in the second reactor. Four different catalysts were used to investigate their catalytic effects, including HZSM-5 without loaded metal (ori-HZSM-5), Mo-loaded HZSM-5 without sulfidation (unsulfided-Mo-HZSM-5), Mo-HZSM-5 sulfided in a stream of H2S/N2 gas (half-sulfided Mo-HZSM-5) and Mo-HZSM-5 sulfided in a stream of H2S/H2 (sulfided HZSM-5). With HZSM-5, the yields of BTXEN (benzene, toluene, xylene, ethylbenzene and naphthalene) reached a maximum of 1.26 wt.% (dry lignite) at the cracking temperature of 550 °C, in the order of fourfold the yield obtained without catalyst (only thermal cracking at the same temperature). This catalyst also distinctly showed the effect on the deoxygenation of LPT, resulting in increases in the yields of CO2, CO and H2O, accompanied by the reductions in the yields of oxygenates such as acetic acid and phenols. The yield of hydrocarbon gases C2H4 obtained with ori-HZSM-5 exhibited obvious increase compared to the yield obtained without catalyst. Unsulfided Mo-HZSM-5 and half-sulfided Mo-HZSM-5 showed a close catalytic effect. These two catalysts were somewhat better than ori-HZSM for the production of BTXEN. Sulfided Mo-HZSM-5 had excellent performance in the production of BTXEN and the yields of BTXEN achieved 1.63 wt.% (dry coal) at cracking temperature of 550 °C.

SESSION 17
GASIFICATION TECHNOLOGIES - 3

17.1- The Behavior of Volatiles' Reaction at Different Temperatures during Pyrolysis of Naomaohu Subbituminous Coal

Xiaorong Li, Xin Jin, Tianzhou Du, Jiao Kong, Meijun Wang, Weiren Bao, Taiyuan University of Technology, PR CHINA.

Naomaohu subbituminous coal (NSBC) is an oil-rich coal according to the yield of tar of 15.4% by Gray-King assay, which has been aroused great attention by medium-and-low temperature pyrolysis technology as an effective way to transform it. However, there are a series of problems in the tar obtained by pyrolysis technology, such as high in particulate and pitch contents and poor in stability. The occurrence of these problems is not only related to characteristics of coal, but also to the behavior of volatiles' reaction which leads to different composition of volatile matter under different pyrolysis conditions, especially temperature. This paper mainly studies the behavior of volatiles' reaction at temperature range from 500 to 750 oC during pyrolysis of Naomaohu subbituminous coal, which conducted in a fixed-bed reactor connected by a mass spectrometer on line to detect the composition of gas products. The liquid products contain tar and water, using comprehensive two-dimensional gas chromatography & mass spectrometer (GC × GC-MS) and a multipurpose water titrator to analyze, respectively. With the increase of pyrolysis temperature from 500 oC to 750 oC, the yield of volatile matter consisting of liquid and gas products increases all the time. Above 600 oC, the yield of gas products increases continuously, while tar yield attains the maximum of 12.1 wt% at 600 oC, then that of tar gradually decreases to 11.7 wt% at 750 oC because of the existing of temperature gradient of reactor possibly. When the temperature is above 600 oC, it leads to volatiles generated from coal pyrolysis as the heat carrier to promote part of tar cooled down at the end of the reactor at 600 oC to volatilize and react again, which more disproportionation reactions of large-molecular-weight tar components cracking to form light gas and condensing into heavy products occur. The heavy products contain heavy tar and coke including black solid on the wall of the reactor and matter insoluble in tetrahydrofuran in tar. It is found the yield of coke increases obviously above 600 oC and accounts for 0.6% and 0.3% of total volatile and coal at 750 oC, respectively. It is also observed that both BTX and PCX yield increase firstly and then decrease at different temperatures. Meanwhile, the yield of water is approximately 10–13 wt% at different pyrolysis temperatures.

17.2- Hydrogenation of Pinewood Hydropyrolysis Volatile Matter over Iron-Loaded Charcoal for Producing Light Hydrocarbons

Nan Zheng, Jie Wang, East China University of Science and Technology, PR CHINA.

Biomass, as the most abundant carbon-based renewable resource, is widely considered an alternative of fossil fuels. However, biomass generally has low carbon content and high oxygen content, leading to a low utilization efficiency as a fuel. Hydropyrolysis is perceived as a technical approach to enhance the carbon utilization efficiency and the product values. This work aims to produce gaseous hydrocarbons and light liquid hydrocarbons by catalytic hydropyrolysis of lignocellulose biomass using iron-loaded charcoal as a catalyst. Hydropyrolysis experiment was carried out in a two-stage fixed-bed reactor under a stream of pressurized hydrogen. A sample of pinewood was hydropyrolyzed in the first reactor with a gradual heat up to 700 °C. The volatile matter was allowed to pass through a bed of Fe-loaded charcoal for catalytic hydrocracking at a predetermined temperature. Two iron precursors (FeSO4 • 7H2O and Fe (NO3)3 • 9H2O) were used to prepare the Fe-loaded charcoal catalysts, designated as Fe (s)-loaded charcoal and Fe (n)-loaded charcoal, respectively. The effects of cracking temperature, hydrogen pressure and Fe loadings on the charcoal were investigated. Result showed that via only thermal cracking under 5.0 MPa (namely without catalyst), the yield of CH4 plus C2H6 and the yield of BTX (benzene, toluene, m-xylene) were gradually increased from 7.2 to 19.8wt% and from 1.7 to 3.5wt%, respectively, with the increase of cracking temperature from 500 to 650 °C. The hydrocracking with the charcoal only (no Fe loaded) led to slight changes in the yields of products. In contrast, when using 3 wt.% Fe (s)-loaded charcoal as a catalyst, the yield of BTX reached a maximum of 4.1wt% at 600 °C, with yield of CH4 plus C2H6 of 21.8wt%. The result clearly demonstrated the catalytic effect of Fe (s)-loaded charcoal on the hydrogenation of the pinewood volatile matter. It was interesting to find that the Fe (n)-loaded charcoal showed a distinctly different catalytic effect from the Fe (s)-loaded charcoal. With the former catalyst, the yield of CH4 plus C2H6 reached as high as 30.5wt% at 600 °C, while the yield of BTX was lower than that obtained with the latter catalyst. This result implied that the Fe (n)-loaded charcoal had a stronger effect on the hydrogenation reaction. Considering that BTX are a high-value product and the iron sulfate is a cheaper compound, Fe (s)-loaded charcoal appears to be a better catalyst between the two choices. In this presentation, we will further report how these two catalysts behaved differently in the catalytic activity.

17.3- Pyrolysis of Peat in the Presence of Phosphoric Acid

Feng Deng, China University of Mining and Technology (Beijing), Guizhou University of Engineering Science; Qiang Xie, Dingcheng Liang, Deqian Liu, China University of Mining and Technology (Beijing); PR CHINA.

Peat-H3PO4 mixtures were obtained by mixing peat sample and phosphoric acid at different concentrations. and corresponding char samples were derived by pyrolysis of these mixtures. Then proximate analysis and ultimate analysis of chars were conducted, and XRF, XRD, TG-DTG, FTIR and SEM were exploited to characterize the peat and the derived chars. The results indicate that the presence of phosphoric acid in peat during pyrolysis results in the increases of both ash content and carbon content in chars. More ash comes from that the aluminum ions of KAl(NH2)4 in the raw material react with phosphoric acid to produce insoluble aluminum phosphate, while the higher carbon content is caused by the effect that phosphoric acid promotes peat pyrolysis, which shifts the temperature range in which main pyrolysis reactions take place to low temperature, thereby the formation of tar is blocked in & low temperature range, as a result less volatile matters evolve from pyrolysis. Besides, phosphoric acid in raw materials also has cross-linking effect that can change the reaction pathway, in which the hydroxyl groups in the peat hydrolyze and form double bonds, and the loss of the hydroxyl-containing groups is controlled by phosphate ester bond. Thus, the derived char from the co-pyrolysis of phosphoric acid and peat has porous nature, which suggests that phosphoric acid presented in peat has the effect of promoting the development of the pore structure during pyrolysis, and the derived char is a promising precursor of activated carbon.

17.4- Effects of Inherent Alkali and Alkaline Earth Metals and Externally Loaded Na on Production of NH3 and HCN during the Pyrolysis / Steam Gasification of Shengli Lignite

Panpan Zheng, Yonggang Wang, China University of Mining and Technology (Beijing), PR CHINA; Lei Bai, West Virginia University, USA; Chen Liu, Weijie Guo, Xiongchao Lin, China University of Mining and Technology (Beijing), PR CHINA.

This work is to investigate the effects of inherent alkali and alkaline earth metals (AAEMs) and externally loaded Na on the production of NH3 and HCN during the pyrolysis and steam gasification of Shengli lignite at temperature of 1073K in a fluidized-bed/fixed-bed quartz reactor. The result indicated that the inherent AAEMs promoted the generation of NH3, while inhibited the formation of HCN during the pyrolysis and steam gasification of Shengli lignite. The effects of externally loaded Na on the formation of NH3 in the pyrolysis and steam gasification process were different. Specifically, the externally loaded Na inhibited the generation of NH3 in the coal pyrolysis process, while the generation of NH3 was promoted by the externally loaded Na in the coal steam gasification. Additionally, inhibitory effect of externally loaded Na on the generation of HCN was observed both in the pyrolysis and steam gasification of Shengli lignite.

17.5- Experimental Study on Electrostatic Precipitation under Coal Pyrolysis Gas at High Temperatures

Quanlin Chen, Jianmeng Cen, Mengxiang Fang, Qinhui Wang, Zhejiang University, PR CHINA.

High temperature dust removal is crucial to the development of clean coal utilization technology. Electrostatic precipitator has the advantages of high dust removal efficiency and low pressure drop, thus, it is a promising technology in the field of high temperature dust removal. In this paper, a lab scale electrostatic precipitator has been set up to study the characteristics of electrostatic precipitation under coal pyrolysis gas at the temperature of 400 – 600 oC. When the temperature increased from 400 oC to 600 oC, the maximum dust removal efficiency dropped from 91% to 71%, while the energy consumption index increased from 56 W/(g/Nm3) to 95 W/(g/Nm3). In order to explore the reasons of low efficiency and high energy consumption of electrostatic precipitator under coal pyrolysis gas at high temperatures, discharge experiments were carried out under the gas media of coal pyrolysis gas, N2 and air at high temperatures. Discharge characteristics of coal pyrolysis gas and N2 are similar and no corona exists during discharge process. Compared with air, discharge currents under coal pyrolysis gas are much higher. According to the above results, a method of improving the discharge and precipitation characteristics of coal pyrolysis gas by adjusting the polarity of the power supply is proposed. The characteristics of positive and negative electrostatic precipitation under N2 gas media are compared. The results show that, at 400 oC, the maximum removal efficiency of negative electrostatic precipitator is 82%, and the maximum removal efficiency of positive electrostatic precipitator can reach 98%. When the dust removal efficiency is 70%, the energy consumption of negative electrostatic precipitator is about 200 times higher than that of positive electrostatic precipitator.

SESSION 18
COAL SCIENCE - 3

18.1- Differentiation of Enriched Organically-Associated Trace Elements in the Macerals of High-Ge Coals from China

Qiang Wei, Shifeng Dai, China University of Mining and Technology, China

It is widely acknowledged that the abnormally enriched trace elements including Ge, W, As, Sb, Be, U, and Nb in the high-Ge coals from the Wulantuga (Inner Mongolia) and/or Lincang (Yunnan Province) germanium ore deposits are presumed to be associated with organic matter to varying degrees. However, the associations between these elements and various organic (and possibly inorganic) components in coal were not well recognized.

In order to characterize the relationship between organically-bound elements and macerals, two high-Ge coals from Wulantuga (WLTG C6-2: 58.4% huminite, 40.7% inertinite) and Lincang (LC S3-6: 98.7% huminite) were first micronized to average ~3 μm using a fluid energy mill to ensure effective isolation of coal components, and density-gradient centrifugation (DGC) was then applied to separate each coal into a series of density fractions (maceral concentrates), followed by determining the trace element concentrations using ICP-MS and conducting petrographic analysis for each fraction. In the Wulantuga coal, huminite fractions contain more Ge relative to inertinite, possibly due to differences in sites capable of holding Ge; the preferential enrichments of Be and As in inertinite probably result from association with minerals in the heavier fractions; a mixed organic-inorganic affinity for W is supported by its variable content versus density and the positive Ge-W correlation; niobium displays a similar distribution to W, and Sb is slightly more enriched in huminite-rich fractions. In the Lincang coal, Ge shows a clear increase with fraction density, perhaps due to more bonding sites in denser huminites; beryllium, Sb, and U present preferential enrichments in heavier fractions, which result from more bonding sites in denser huminite macerals and/or their inorganic associations; tungsten, Nb, and Th share comparable variations vs. fraction density, suggesting similar occurrences; and As content changes gently across DGC profile.

As an indirect method, DGC has inevitable defects for element affinity characterization. For example, even a tiny amount of inorganic matter can make the fraction density less accurate and the interpretation for element affinity less reliable. Therefore, in-situ electron probe micro-analysis (EPMA) was also employed in the present study to further clarify the element associations with coal components. WDS element mapping and point analysis show that, compared to inertinite, preferential enrichments of Ge, W, and As can be observed in the huminite of the Wulantuga coal. The concentrations of Ge, W, As, and U in both the Wulantuga and Lincang coals are higher in ulminite and gelinite relative to less compact huminite macerals. Germanium, W, and U have a major organic affinity, and the positive correlation between the in-situ Ge and W concentrations approves their co-existence in the organic matter. EPMA and EDS analyses demonstrate that As has a mixed organic and iron sulfide/sulfate affinity.

As the differentiation of enriched organically-bound elements across various macerals in the high-Ge coals has been confirmed through both the indirect (DGC) and direct (EPMA) techniques, the probable cause for this observation can be inferred as the structure distinctions of macerals, which warrants further studies to verify.

18.2- Interpretation of Element Release under Process Gas Atmosphere by Means of ETV-ICP OES

Caroline Hommel, D. Vogt, S. Guhl, B. Meyer, TU Bergakademie Freiberg, GERMANY.

Fouling and slagging in coal-fired power plants could causes loss of efficiency or downtime, therefore estimating the process-behavior of energy resources is necessary. Knowing the coating potential, process parameters for combustion or the feed and its mixture is adaptable. Owing to changing coal quality and new used co-fired material, established solution strategies are not immediately applicable any more. Developing new ones, analysis of real process samples takes the center stage. The results obtained will further the understanding of coal specific mechanisms of fouling and slagging. This will be paramount in forecasting models and giving recommendations for boiler operation.

A fundamental aspect thereby is the temperature dependent release of pollutants and disturbing components in the boiler atmosphere. This results in several requirements for the analysis method employed. In addition to direct solids analysis qualitative as well as quantitative results must be obtained. Furthermore, the temperature dependent release of disturbing elements must be detectable, preferably in simulated flue gas atmosphere at temperatures up to 1600 °C. Basicity constitutes the ratio between the basic and acidic components of the input material and can be viewed as a possible index for deposit formation. Besides alkalis, aluminum and silicon, sulfur in various chemical binding forms contributes to fouling and must therefore consistently be considered in analysis.

The method of electrothermal evaporation with inductively coupled plasma and optical emission spectroscopy (ETV-ICP OES) enables the simultaneous analysis of a large number of elements quantitatively as well as qualitatively in a wide range of concentration (ppb - %). Owing the freely adjustable temperature program the temperature/time dependent release of elements can be observed, which partly allows for conclusions regarding the binding characteristics and association of some elements. The suitability of ETV-ICP OES for coal characterization has been shown in various papers.

With a modified graphite furnace in the ETV oven it is possible to simulate different flue gas atmospheres and analyze the release characteristics of relevant elements up to a temperature of 1600 °C. This provides also an opportunity to recreate other processes like gasification.

With the help of the modified ETV-ICP OES the release characteristics of disturbing components in brown coal from the Rhineland will be analyzed and the results will be presented.

18.3- Migration and Removal of Minerals and Hazardous Trace Elements in Coal during Coal Washing

Chengwei Yang, Yuegang Tang, Chengwei Yang, Kangnan Feng, Xingyuan Li, Wenqiang Ma, China University of Mining and Technology (Beijing), PR CHINA.

A number of washing products from three coal washeries and some raw coal samples were selected to study the removal rate of ash, sulfur and 16 hazardous trace elements during coal washing, and to explore the clean potential of hazardous elements systematically. The petrology, mineralogy, and chemistry of the samples were investigated using optical microscope, scanning electron microscopy with energy dispersive X-ray spectroscopy (SEM-EDX), inductively coupled plasma mass spectrometry (ICP-MS). The results showed that the minerals of the raw coal and clean coal of FH-15, HL-2 and GY-10 mainly consist of clay minerals and pyrite. The five main occurrence forms of pyrite and clay minerals have been summarized, and four types of pyrite inlays (I, II, III, IV) have been classified. The removal difficulty of pyrite decreases from the type I to the type IV. Considering the occurrence form, embedding type and relative content of pyrite, The removal rate of pyrite was classified into four types: the worst removal rate (particle size 2-6 μm), a poor removal rate (<2 μm), a moderate removal rate (6-20 μm), and the best removal rate (>20 μm). The removal rate of hazardous trace element in Fenghuang (FH) clean coal and Huangling (HL) clean coal are above 70%, and the removal rate of the hazardous trace elements increase with the coal particle decreasing. The removal rate of the hazardous trace elements in Gaoyang (GY) clean coal is low, and the average removal rate of Hg is -150.44% indicating the enrichment of Hg.

The relationship between the sedimentary environment of the three mining areas and the degree of coal selectivity was briefly analyzed. The FH-15 coal seam is a lagoon-tidal flat-tidal-marsh facies deposition system, and the washability of the coal is poor The HL-2 coal seam belongs to the lakeside-marsh facies deposition system and the local part is a foliate sedimentary system, and the washability of the coal is worse. The GY-10 coal seam is mainly a coastal-lagoon facies deposition system, and the coal washability is the worst.

18.4- Partitioning and Migration of Pb and Cr in an Ultra-Low Emission Pulverized Coal Boiler

Lin Chang, Huan Liu, Shibo Zhang, Yongchun Zhao, Junying Zhang, Huazhong University of Science & Technology, PR CHINA.

Trace elements (TEs) cause damage to humans which have attracted worldwide concern. In this work, TEs (Pb, Cr) partitioning and migration were investigated in an ultra-low emission pulverized coal boiler equipped with selective catalytic reduction (SCR), low temperature (LTE), electrostatic precipitator (ESP), wet flue gas desulfurization (WFGD) system, and wet electrostatic precipitator (WESP). Simultaneous samples were conducted at both inlet and outlet of the equipment above. Meanwhile, feed coal, bottom ash, fly ash (collected from 5-level electric fields), gypsum, desulfurization slurry, WFGD effluent, WFGD treated water, and WESP effluent were systematically collected and analyzed. Results show that total removal efficiency of air pollution control devices reaches 96.83% and 94.11% for Pb and Cr, respectively, leading to stack emission concentration of Pb and Cr are 0.101 μg/m3 and 0.481 μg/m3, respectively. Pb and Cr have stronger affinity for fly ash rather than bottom ash. Furthermore, the adsorption ability of Pb and Cr is in inverse proportion to the particle diameter of fly ash. With the average particle diameter decreases from 96.66 μm to 19.65 μm, the concentration of Pb and Cr increases about 60% and 650%, respectively. TEs partitioning results indicate that limestone contributes most Pb in the WFGD system. Moreover, the effluent treatment device removes over 95% of Pb and Cr in the WFGD waste slurry. The application of WESP not only promotes fine particles removal but also be conducive to Pb and Cr control. The alkaline environment water in the WESP inhibits equipment corrosion as well as the leaching of Pb and Cr from solid phase to liquid phase.

18.5- Arsenic Distribution and Speciation of High-Arsenic Ashes from a Lignite Fired Power Plant in Inner Mongolia, China

Bengen Gong, Qirun Yong, Zhuo Xiong, Yongchun Zhao, Junying Zhang, Huazhong University of Science & Technology, PR CHINA.

The distribution and speciation of high-arsenic lignites from four coalmines and high-arsenic ashes from the pithead power plant in Inner Mongolia, China were investigated. Totally thirteen samples were systematically collected, including four high-arsenic coal samples, four high-arsenic fly ash samples (FA), three slag samples (SL), two flue gas desulfurization gypsum samples (FGDG), and four soil samples (SO) nearby the coal ash dump. The chemical and mineralogical composition, and microstructure of samples were characterized by the X-ray fluorescence microprobe (XRF), X-ray diffraction (XRD), and environment scanning electron microscopy equipped with energy dispersive X-ray spectrometry (ESEM-EDX), respectively. The arsenic contents were determined by the atomic fluorescence spectroscopy (AFS), and the arsenic speciation were determined by the high performance liquid chromatography-hydride generation-atomic fluorescence spectrometry (HPLC-HG-AFS).

The results show that arsenic content in the high-arsenic lignite is up to 40 μg/g, and that in the high-arsenic fly ash can reach 110 μg/g. Arsenic is enriched in the finer size fraction of fly ash, and the As migration occurs from the fly ash to environment after long-term stacked. Arsenic content of ferrosphere in fly ash is much lower than that in the original fly ash, and it can also migrate out after FA long-term stacked. By analyzing the As contents in a large number of microscopic particles of the fly ash and the slag, it was found that the As contents in the particles of fly ash are in the range of 0 ~ 1.9% with an average value of 0.44%, and that of slag particles are 0 ~ 0.94% with an average content of 0.43%. There are relative high positive correlations between As with Fe, Ca and Mg, which indicates arsenic is mainly combined with Ca, Mg, Fe - bearing materials during the formation of coal-fired products. The fresh fly ash mainly contains pentavalent arsenic (As(V)), with a small proportion of trivalent arsenic (As(III)) being only 1.22%. The proportion of As(III) in the fly ash increases with the decrease of the particle size. After the fly ash was stacked in the atmospheric environment for some times, the As species in fly ash became basically As(V), the As(III) in fresh fly ash will be oxidized to As(V). As(III) is enriched in the ferrospheres of fly ash, and may decrease due to the increase of stacking time in the environment. The As(III) in the fresh slag is higher than in the fresh fly ash. and the As(III) in slag will be converted into As(V) due to the slag stacking in the environment. Arsenic species in the flue gas desulfurization gypsum is just As(V). The proportion of As(III) in soil is higher than that in fly ash. The influence mechanism of arsenic to the soil was established, and the As(III) and As(V) can transform to each other in the environment

SESSION 19
CARBON MANAGEMENT - 1

19.1- Analysis of the Application Potential of CCUS in Four Majoir Industries in China

Xiaochun Li, Chinese Academy of Sciences, PR CHINA.

CCUS is an important option for mitigating CO2 emissions. Countries all over the world paid great attention to it andhas increased research and development. This report will analyze the Chinese CCUS potential of the major industries from the perspective of technology and economy.

19.2- Commissioning and Completion of the Wyoming Integrated Test Center

Jason Begger, Wyoming Infrastructure Authority; William J. Morris, Wyoming Integrated Test Center; USA.

The state of Wyoming completed construction of a world class integrated test center (ITC) for evaluating post combustion CO2 capture technologies in 2018. An asset of the Wyoming Infrastructure Authority, (WIA) with additional funding and support from Tri-State Generation and Transmission, Basin Electric Power Cooperative, and the National Rural Electrical Cooperative Association, the center features over 20 MW equivalent (MWe) of coal derived flue gas from the adjacent Dry Fork Power Station in Gillette, WY, USA.

In 2014, with the support and encouragement of Governor Matthew H. Mead, the Wyoming State Legislature allocated $15 million in funding for the design, construction and operation of an integrated test center to study the capture, utilization and storage of CO2 emissions from a Wyoming coal fired power plant. An additional $5 million commitment from private industry was required and was secured from Tri-State Generation and Transmission Association in addition to $1 million pledged from the National Rural Electric Cooperative Association. Basin Electric Cooperative is providing the host site and additional in-kind contributions.

The Dry Fork Station, operated by Basin Electric Cooperative, is a state of the art plant with best available NOX and SO2 control technology providing reliable low emissions flue gas to the test center. The plant utilizes coal from the adjacent Dry Fork mine in the Powder River Basin. Approximately 2 MWe is provided to 5 small test bays of 0.4 MWe each which may be operated concurrently or independently. The test bays utilize a flue gas system with recirculation fans allowing any one of the test bays to come online or shut down without disrupting the flue gas supply or operations of any of the other test bays. The large test center and small test center bays are also able to operate independently of one another. Each test bay is provided with its own flue gas, power, and water supply. The test bays are located in a secure area adjacent to the plant to allow researchers to operate independently of plant operations.

The small-scale test bays are hosting the international NRG COSIA Carbon XPRIZE CO2 capture and conversion competition (coal track) from 2018-2020. The large pilot test bay can provide 18 to 20 MWe of flue gas for a single technology test or be further subdivided to host multiple technologies at greater than 1 MWe scale. It is expected to host at least one international technology developer in 2018-2019. The ITC is open to those in private industry, government agencies, government laboratories, university faculty and staff, and individuals who have the capability to conduct self-sustained CO2 capture testing from an operating coal fired power station. Wyoming's ITC will serve as a catalyst for aligning Wyoming's efforts for research, testing, pre-commercialization, and commercialization of CCUS technologies. This paper will cover commissioning and initial testing activities in 2018 as well as summarizing the capabilities of the center for future technology development and CO2 utilization within the state of Wyoming.

19.3- Research Status of Carbon Dioxide Utilization Technology

Jianwei Li, Jiaojiao Lei, Xing Xin, Feng Bai, Xi'an University of Science and Technology, PR CHINA.

In recent years, the industrial chain upsteps unceasingly with the development of coal chemical industry. At the same time, substantial carbon dioxide emissions are worth serious consideration. In this paper, the latest progress of carbon dioxide utilization technology is reviewed. Three technologies, including hydrogenation conversion, synthetic polymer and CO2-methane co-transformation, are mainly introduced. By comparison, the best way to achieve the large-scale use of carbon dioxide is CO2-CH4 co-transformation technology. When this technology is coupled with coal pyrolysis, it can not only achieve the effective utilization of energy but also reduce the emission of CO_2, which has practical significance for the development of coal chemical industry. Consequently, we should keep an eye on the correlational research and exploit the technology.

19.4- CO2 Capture from Flue Gas Using Membranes: Current Status and the Next Steps

Richard Baker, Ivy Huang, Tim Merkel, Membrane Technology and Research, Inc., USA.

Global climate change due to CO2 emissions is a growing worldwide problem. One proposed solution to the problem is CO2 capture and sequestration (CCS) at coal power plants and various industrial processes, where almost 40% of CO2 emissions are generated.

The only current demonstrated CCS technology is amine absorption. Two-full-scale amine CO2 capture plants have been built and are in operation, but there is little enthusiasm to build more. The principle problem is the processes' high cost. The use of membranes has emerged as the most promising second generation CCS technology. Membrane technology is at the development stage. Pilot plants have been built and the process is expected to have a lower cost than amine absorption, as well as offering significant operational advantages such as simple flow scheme, much smaller footprint, no new emission issues and no hazardous chemicals to handle and dispose; also the process is powered by electricity so that no changes to the power plant steam cycle are needed.

In this paper, the current status of membrane technology applied to CO2 capture will be reviewed and recent new development will be highlighted. The key factors that make this technology lower cost and lower energy consumption will be discussed, and the next steps required to take the technology to full scale will be addressed.

SESSION 20
COMBUSTION TECHNOLOGIES - 4

20.1- Synergistic Mercury Removal with a Medium and Low Temperature SCR Catalyst of Fe-Modified Mnox/Tio2 from Coal Combustion Flue Gas

Shibo Zhang, Yongchun Zhao, Junying Zhang, Huazhong University of Science & Technology, PR CHINA.

Fe-modified MnOx/TiO2 (Fe-MnOx/TiO2) was synthesized by a sol-gel method and employed as the catalyst of selective catalytic reduction (SCR) for synergistic mercury removal from coal combustion flue gas. The experimental results demonstrated that the introduction of Fe improved the Hg0 removal activity of the catalyst. And the Hg0 removal efficiency over Fe-MnOx/TiO_2 was more excellent in the low temperature range. For the effects of the individual flue gas components, the Fe doping enhanced the promotion of HCl and impaired the inhibitions of SO2 and NH3 on the Hg0 removal efficiency. As a result, the catalytic activity in simulated coal-fired flue gas showed an obvious modification with the introduction of Fe into the catalyst, and the considerable and stable efficiencies were obtained when performing simultaneous NO and Hg0 removal over the Fe-MnOx/TiO2 catalyst. The characterization analyses were then carried out and the results showed that the introduction of Fe improved the BET surface area, the dispersity of the metal oxides, the redox behavior and surface concentrations of chemisorbed oxygen and Mn4+ of the catalyst, which were all in favor of the catalytic activity. Meanwhile, the existence of Fe in the catalyst could form certain protection on the Mn4+ from SO2 so that the sulfur resistance was strengthened as well.

20.2- Numerical Investigation on Co-Firing Ammonia with Pulverized Coal in Boiler

Juwei Zhang, Takamasa Ito, Sakiko Ishihara, Toshiro Fujimori, IHI Corporation, Ltd., JAPAN.

Ammonia (NH3) is a kind of carbon-free sustainable alternative fuel. Recently, using NH3 as an energy carrier of hydrogen has attracted great attention. It is because that NH3 has high hydrogen capacity, high boiling point, existing infrastructure for production, and much safer transportation, compared with hydrogen. In this study, a combustion facility (10 MWth) was simulated with computational fluid dynamics (CFD) to evaluate the effects of NH3 co-firing on characteristics of combustion, heat transfer and NOx emission. The experimental data were used to validated the CFD approach According to this study, NH3 co-firing leads to a low flame temperature, less heat absorbed by walls, high unburn carbon and lower NOx emission. In addition, NOx emission is monotonously decreased as increasing the air staging ratio in the conditions of coal-firing, however, this effect can be only found at low air staging ratios in the condition of NH3 co-firing.

20.3- Evolution of Organically Bound Metals during Zhundong Sub-Bituminous Coal Combustion

Xianpeng Zeng, Dunxi Yu, Huazhong University of Science and Technology, PR CHINA.

Zhundong sub-bituminous coal is a Chinese low rank coal of huge reserves, and will play an important role in the national energy supply. However, currently, severe fouling, slagging and erosion problems have occurred during Zhundong coal combustion, which significantly limited its utilization. To solve these problems, the ash formation and deposition mechanism of Zhundong coal should be well understood. There have been some literatures dealing with the ash formation and deposition after combustion. However, little work has been done on the evolution of inorganic elements during Zhundong coal combustion, which can clearly elucidate the transformation process from the inorganics to ash.

In this paper, a Zhundong coal rich of organically bound elements was burned in a well-controlled drop tube furnace, and the char particles were collected and quenched at various residence time by a water-cooled sampling probe. The evolution of organically bound metals on the surface of char particles during combustion of Zhundong coal was studied in detail by scanning electron microscopy (SEM). Besides, the low temperature ash of Zhundong coal was prepared to gain insight into the dispersion state of inorganic elements in the raw coal. Char samples were also analyzed by X-ray powder diffraction (XRD) to investigate the mineral transformation process during Zhundong coal combustion. Based on these methods, the evolution of organically bound metals during Zhundong coal combustion was well understood.

20.4- Migration and Transformation of Mercury in Coal Gangue Fired Power Plant with FF and WFGD

Yuming Zhou, Binbin Zhu, Bengen Gong, Yongchun Zhao, Junying Zhang, Huazhong University of Science & Technology, PR CHINA.

The migration and transformation characteristics of Hg from a coal gangue fired power plant with fluidized boiler was investigated. All the solid and liquid fire products were sampled including feed coal gangue, bottom ash, fly ash, lime, gypsum, process water and FGD effluent. The flue gas was sampled simultaneously at the inlet and outlet of fiber filter (FF) and wet flue gas desulfurization (WFGD) by EPA 30B method under 100% load (50MW) and 60% load (30MW). Under 100% load, the Hg concentration in flue gas at the inlet of FF and outlet of WFGD was 7.965μg/m³ and 0.232μg/m³ respectively, and Hg concentration in flue gas at the inlet of FF and outlet of WFGD was 4.693μg/m³ and 0.148μg/m³ under 60% load. The co-beneficial Hg removal efficiencies of FF+WFGD was 96.99% and 96.85% respectively. Relative enrichment index (REI) calculation showed that, the Hg absorbed in fly ash was much more than bottom ash, more than 99% Hg present in solid fire products especially fly ash, which attributed to high ash content of coal gangue caused dense fly ash in flue gas. As the FF has remarkable removal ability of submicron fly ash, both Hg0, Hg2+ and Hgp were removed as the fly ash could absorb Hg0 and Hg2+ on it. Fluidized boiler caused relative temperature flu gas also in favor of Hg absorption at the surface of fly ash. However, the concentration at the outlet of WFGD is higher than it at outlet of FF, the results showed that, a part of Hg2+ reduced and released as Hg0, especially under lower load. Comparison of Hg concentration in flue gas under 100% and 60% load, the ratio is approximately 5:3, which ascribed to less feed coal gangue under lower boiler load. The atmospheric emission factor of the power station is 0.592g/TJ and 0.378g/TJ under 100% and 60% load, respectively. Thus, relative high fly ash concentration in flue gas and effective FF is beneficial for the reduction of Hg emission to atmosphere.

SESSION 21
COAL BED AND SHALE GAS - 1

21.1- Impact of Tectonic Deformation on Coal Methane Adsorption Capacity

Wu LI, China University of Mining & Technology, PR CHINA.

Tectonic deformation can cause significant changes in the physical and chemical structures of coal by damaging the macrostructure and macromolecular. For the thorough research on coal tectonic deformation impact on gas adsorption capacity, this paper collected and summarized parameters of experimental adsorption isotherms, coal maceral, proximate analysis and ultimate analysis, systematically discussed the adsorption properties of different structure coals and the influences of temperature and pressure on coal adsorption. Furthermore, the Semi-quantitative relationship between structure parameters of coal and methane adsorption capacity. Results show that (1) Due to different tectonic stresses, the molecular and porous structures of different types of te ctonic coal exhibit significant differences. Sample N25 which is in fault zone has highest methane adsorption capacity. (2) Coal methane adsorption capacity decreases along with increasing temperature. At a pressure of 12 MPa, primary coal (N32) showed Langmuir volume (VL) of 15.38, 9.58, and 7.86 cm3/g and Langmuir pressure (PL) values of 3. 82, 2.07, and 1.81 MPa at temperatures of 30, 50, and 70 °C. (3) The Langmuir volume appears to have a linear relationshipwith parameters ID1/IG, fa, Al/OX, and A factor.

21.2- The Feasible Discussion of Gas Recovery about Coal bed methane, Tight gas and Shale gas -"Three gases" Commingling

Haiquan Zhong, Mengqi Hu, Pengbo He, Southwest Petroleum University at Chengdu, PR CHINA.

There are abundant resources and great potential of unconventional gas-coal bed methane、tight gas、shale gas. But it also faces the fact that the unconventional gas is under the low production of single well and bad economic performance overall in our country. According to the exploration of coal bed methane, tight gas and shale gas are parts of longitudinally overlap and the characteristics of each layer of reserves are quite rich. At the same time the production of any kind of resources is low production and high mining costs and easy to cause the actual gas waste of resources in some areas. This article is mainly analyzed and discussed from the reservoir characteristics, the development ways and the gas recovery sections to find that selecting favorable areas. Through the reasonable gas reservoir engineering design, optimizing of production pipe string design, and introducing the new gas recovery methods, etc. To carry out the mining of "three gases"-coal bed methane, tight gas and shale gas or "two gases" is feasible and of very important practical significance.

We believe that in the current downturn of oil and gas industry, the new unconventional gas mining process will be very good use of different kinds of natural gas, improving

the production of a single well, but also provide a new direction for the development of unconventional gas.

21.3- Experimental Study on Adsorption and Permeability of Coal Rock under the Action of Artificial Electric Field

Shao Xianjie, Li Feng, Oyaka Dickens, Peng Yingming, Li Mingfeng, Liu Zeheng, Yanshan University, PR CHINA.

With the reasonable design of the experimental instrument, the change of adsorption capacity and seepage capacity of coal under artificial electric field was tested by N2 respectively. The permeability of 4 coal samples was tested. The experimental results show that the gas permeability of coal increases by an average of 4.0% respectively under the artificial electric field. According to the adsorption experiments of 4 coal samples, the adsorption amount was reduced by 15.3%. Theoretically, the adsorption amount of coal matrix on CBM was affected by both Joule heat effect and adsorption potential trough depth. According to the experimental results, under the function of the additional artificial electric field, as the temperature of joule heating effect increases and the depth of adsorption potential trough becomes shallower, the adsorption capacity of coal matrix decreases.With the decrease of gas adsorption, the effective pore diameter in coal matrix increases, leading to the increase of permeability and diffusion rate.Therefore, artificial electric field technology can be applied to increase the production of coalbed methane wells.

21.4- Study on Adsorption Capacity and Influencing Factors of Middle-High-Order Coal-Rocks in China

Ma Pinghua, Wang Xixi, Yan Yi, Li Feng, Shao Xianjie, Yanshan University, PR CHINA.

In China, there are abundant CBM resources. However, due to the complex coal-forming environment and high degree of metamorphism, there are many factors that affect the adsorption capacity of coal, resulting in large changes in production. Through the study on the influencing factors, the theoretical basis and technical support for efficient development of coalbed methane in China has been provided. Based on a large number of experimental data, the influencing factors such as micro-components, industrial components, metamorphism, and pore structure on the adsorption capacity of coal rock was analyzed. The results indicate that: (1) with the increase of the content of the vitrinite, the adsorption capacity increased, but it's not sensitive to the change of the content of inertinite. (2) With the increase of fixed carbon content, the adsorption capacity increased. ash and moisture are not conducive to the adsorption of coal. (3) The adsorption capacity of coal changes parabolically with the deepening of the degree of metamorphism. When Rmax is in the range of 2.3% to 2.5%, the adsorption capacity is strongest. (4) The influence of the pore structure characteristics of coal on the adsorption capacity of coal is manifold. The adsorption capacity of coal with micropore development is strong, and the general adsorption capacity of coal with macropore development is poor. Finally, 11 coal parameters were optimized, and a hierarchical structure model was constructed. A set of evaluation system of coal rock adsorption capacity was established by using fuzzy analytic hierarchy process. As long as there are relevant parameters of coal-rock, its adsorption capacity can be easily obtained, which provides a basic index for the development of coalbed methane.

SESSION 22
VALUE-ADDED PRODUCTS FROM COAL – 4

22.1- Experimental Research of the effect of Properties of coal charge on Ferro-coke Properties

Shi-Zhuang Shi, Zhen Xu, Jin-Hui Zhou, Yong-Hui Luo, Gong-Er Wang, Yan-Gao Mao, Qi Zheng, Qing-Wen Dong, Shuai Lu, Wuhan University of Science and Technology, PR CHINA.

Atblendingratio of iron ore powder of 10%, the influence of properties of coal charge (ash content, sulfur content, volatile content, caking index) on ferro-coke properties (ash content, sulfur content, porosity, mechanical strength, thermal properties and reduction degree of iron ores) was studied systematically. The results show that the influence of cokemaking coal blend properties on ferro-coke properties are remarkable, the change of ash and sulfur contents in ferro-coke depends on coal charges; porosities of ferro-coke and reduction degree of iron ore in ferro-coke increase monotonously along with increasing of volatile content of coal charges; near Vdaf=28%, G=81, mechanical strength of ferro-coke is the best; when Vdaf=27.64~29.84%, G=70.00~81.19, thermal property of ferro-coke is the better. By means of adjusting the properties of coal charge ferro-coke with different properties can be produced.

22.2- Study on Properties of Indonesian Coal and its Compatibility with Domestic Coal for Coking

Shi-Zhuang Shi, Zhen Xu, Jin-Hui Zhou, Yan-Gao Mao, Qi Zheng, Yong-Hui Luo, Gong-Er Wang, Qing-Wen Dong, Zhi-Long Lin, University of Science and Technology, PR CHINA.

In this paper, a coking company compared Indonesian coal with the same sort of domestic coking coal and did coal blending coking experiment to find out the characteristics of the Indonesian coal and the cooperation with domestic coking coal. Studies have shown that the Indonesian coal are low ash, low sulfur, strong bonding, high expansibility, low liquidity and single, they also have high active, and the live idle index reach as high as more than 24, but domestic coking coal have a little of mixture, and the live idle index is for 1 ~ 2, more balanced; the Indonesian single coal coke is poorer, its breaking strength and coke strength after reaction (CSR) are low. however, the abrasion strength and coke reactivity index (CRI) increased; When replaced the domestic brands of coal with Indonesia coal, the coke quality decreased obviously, and the breaking strength and coke strength after reaction also reduced, coke reactivity index and the abrasion strength increased a little. the more replacement, the greater of the amount of down, therefore, it cannot simply replace the domestic coal with Indonesia coal and also should be optimized coal blending coal to make full use of the characteristics of the Indonesian coal, and to improve the quality of coke.

22.3- The Relationship between the Improvements of Tamping Coke Quality and Quality of Coal Charge

Shi-Zhuang Shi, Zhen Xu, Jin-Hui Zhou, Qi Zheng, Yan-Gao Mao, Yong-Hui Luo, Gong-Er Wang, Zhi-Long Lin, Shuai Lu, Wuhan University of Science and Technology, PR CHINA.

Coke quality can be improved by stamping coking process, but the improvement effect depends on the property of coal charge. Through the cokemaking experiment with blended coal, the relationship between the property of coal charge and the improvement of stamping coke quality compared to conventional coke quality was studied. The mathematical relationship between the improvement effect of stamping coke quality and property of coal charge was established. On the basis of the mathematical relationship, the range of property of coal charge was determined.

22.4- Contribution to the Briquetting and Coking Behaviour of Non-Baking Coals of Different Rank

Franz Fehse, Hans-Werner Schröder, TU Bergakademie Freiberg; Ronald Kim, ThyssenKrupp Industrial Solutions AG; GERMANY.

By using brown coal as a feed stock for lump creation the raw material base for metallurgical industry could be considerably enlarged. An important process step for the lump coke creation of brown coal is the previous briquetting of the coal since the brown coal does not offer any baking capacity.

The most important process steps for the creation of lump coke from brown coal are the processing of the coal (comminution, drying and screening), the briquetting and the gentle pyrolysis of the briquettes. By using new processing approaches and coking additives the coke quality increases significantly.

In systematic experimental investigations the coke quality from i. a. Australian, German and Indonesian brown coal, Chinese lignite and South African high volatile coal was determined by variation of different processing approaches. For example the brown coal was highly comminuted and disintegrated in a twin-screw extruder, a swing mill and a modified flat die press. Since higher ranked coals do not offer a high binding potential the addition of briquetting and coking additives, e. g. molasses, spent sulphite liquor, draff or mashed potatoes, was investigated.

Whereas the Australian brown coal offered high quality briquettes and coke even under conventional processing conditions, high quality briquettes and cokes could only be produced for the other coals with a higher technological expense. By stressing the coals e. g. in the modifiend flat die press or in the twin-screw extruder the compressive strength of the coke could be more than doubled (e. g. for the Indonesian coal from 25 MPa to 65 MPa). And the abrasion resistance may exceed 90 % after 300 revolutions in an IfB drum.

By using coking additives like spent sulphite liquor, molasses and draff melted bridges between the coke particles were partially created and lead to a higher coke strength as well, due to the transformation of ingredients like cellulose, lignin (spent sulphite liquor), sugar (molasses) and proteins (draff).

At the end of the investigations for each coal a heating regime for reaching the maximum coke quality was adapted. And for one of the coal samples the scale-up behaviour in semi-industrial scale was investigated

22.5- Understanding the Contribution of Component Coals in Coke Oven Blend

Philip Bennett, CoalTech Pty. Ltd.; Adrian Reifenstein, ALS Coal; AUSTRALIA.

All steelworks blend several coals to make a coke oven feed to minimise coal costs while ensuring resultant coke quality meets their BF requirements. The blending strategies used by steelworks vary and are normally not made known to coal producers. In coke making, the generation of swelling pressure is an important consideration as excessive pressure will result in high pushing forces whereas insufficient pressure may lead to poor coke quality. Previous research by Australian Coal Research Program (ACARP) and published in the literature has demonstrated that the properties of the plastic layer influence both oven wall pressure (OWP) and the structure of the final coke. The structure of the coke controls coke strength. The plastic layer is formed during the transition of coal to semi-coke and is influenced by fluidity, size distribution and swelling of the coal, and the coking conditions such as bulk density and heating rate. Due to the complex interaction of these parameters, it is very difficult to model the plastic layer formation just based on laboratory tests. ALS designed a modified Sole Heated Oven (SHO) to measure the properties of the plastic layer. In ACARP projects C21058 and C24056 tests were conducted that accurately measured the changes in force acting on the plastic layer due to small changes in the compression of the plastic layer. After the release of this compression of the plastic layer, the plastic layer undergoes relaxation where the force decreases back to its starting value. The data from these tests allowed the determination of the Relaxation Modulus and the Relaxation time of the plastic layer for single coals and blends of these coals. Relaxation Modulus and the Relaxation time are properties of a viscoelastic solid. For a viscoelastic solid under a fixed load the porous structure is controlled by the applied load. The applied load compresses the plastic layer resulting in lower porosity at higher loads. The strain at a given load is defined as the amount of measured compression divided by the calculated thickness of the plastic layer at zero load. The coke strength, as measured by the I600 drum test, and the apparent porosity of the coke showed that the coke breakage of a semi-hard coking coal (A) was adhesion control and the strength increased with the addition of soft coking coal (C) or hard coking coal (B). Both coals B and C had coke strength controlled by the porosity of the coke. For blends of A and C and of A and B porosity is linearly dependent on the strain at the test load. The highly non-linear influence of blend composition of coals C and B on coke strength reflects the non-linearity of porosity with strain due to the soft coking coal (C) filling the voids of coal B. The amount of coal C filling the voids of coal B is dependent of the applied load. It is speculated that the coal particles of coal B swell during coking leading to an increase in the volume of the interparticle voids. The amount of swell is dependent on the applied load. Coal A has little swell during coking and, at higher proportions of coal A, the collapse of the softened coal particles leads to a low volume of the interparticle voids that cannot be filled by either coal B nor coal C. Japanese research has shown the importance of permeability, penetration of the interparticle voids, by soft coking coal on coke strength. The SHO data can be fitted to a form of the Maxwell model for a viscoelastic foam. This model links the stress required for a given strain in the plastic layer.the SHO was further developed leading to a coking pressure test which simulates the physical processes that occur in a coke oven where expansion is limited. ALS has conducted SHO coking pressure tests on a range of single coals. These results have shown that there is a strong correlation between the measured coking pressure in the ALS SHO and predicted OWP using relationships developed by CPM in France and BHP Billiton in Australia. This paper details the development of the modified SHO and interpretation of experimental results.

SESSION 23
GASIFICATION TECHNOLOGIES - 4

23.1- Establishment and Application of Two-Step Reaction Equilibrium Calculation Model for UCG (Underground Coal Gasification)

Tianhong Duan, China University of Mining and Technology (CUMT), PR CHINA.

Traditional coal gasification parameters calculation methods are based on data of surface coal gasification can't be used directly in the underground coal gasification parameters calculation. This resulted in the differences between calculation results by the existing theories and actual results are great. The aim of this study is to calculate gasification parameters that influence design and operation of UCG exactly. A Two-Step Reaction Equilibrium Calculation Model, which calculates UCG parameters over two stages and then merges the resulting data, has been established. In addition, a suitable method for establishing optimal gasification agent parameters is proposed. Corresponding MATLAB routines were compiled and applied to the field tests of UCG. And it is proven that simulation results coincide with the actual field test data to a great extent.

23.2- Applying Spontaneous Adiabatic Test Procedure to Determine CO_2 Gasification Reactivity and Kinetics of Coal for UCG Applications

JC van Dyk, North-West University; J Brand, African Carbon Energy; FB Waanders, North-West University; SOUTH AFRICA.

UCG is a gasification process used to produce synthesis gas from coal in situ (underground in the coal seam) by injecting air or oxygen, with or without steam, into coal seams and extracting the product gas via the production well and may also be thought of as a thermo-chemical mining process. The coal face becomes a gasification front and results in high temperatures (>1000 oC) that cause the hydrocarbons contained in the coal to effectively re-form into gas. This resulting synthetic gas ("syngas") can be used to produce electricity, as well as chemicals, liquid fuels, hydrogen and synthetic natural gas.

The effectiveness and carbon efficiency of UCG can further be improved by applying CO2 gasification / recycling of waste captured CO2 as gasification agent (replacing part of the oxygen and steam as gasification agent). With CO2 based gasification, the most important reaction is the reduction process, (also known as the Boudouard Reaction, where CO2+C→2CO above 850°C.

CO2 gasification, and specifically applied to an Underground Coal Gasification process, is a practical solution to improve both carbon efficiency and lower the CO2 footprint. The main aim of this study is to determine the minimum O2 addition and mininmun CO_2 temperature (350 °C). During a previous experimental study (Part 1 of this study), it was observed that at a higher mass flux of both CO2 and O2, an increase of 6% more CO was present in the reactor effluent stream. However, during both of the practical tests, the O2 concentration in the reactor agent stream remained approximately the same. This indicates that the CO2 gasification process is favoured at higher temperatures. At higher mass fluxes, the bed obtained an overall greater conversion, resulting in a lower residual bed height and increased ash bed height.

Understanding the properties of a coal is critical to effectively and efficiently operating a UCG process under CO2 saturated environments andthe Spontaneous Combustion and Reactivity behaviour– may supply technical detail and scientific insight into gasification behaviour and carbon conversion of the coal.

Adiabatic oven testing using R70 and SponComSIM™ tests is usually applied as a precautionary measurement of the self-heating properties of coal, e.g. to manage coal on stockpiles or during transport. In this study, we aim to show how the novel approach of using R70 and SponComSIM™ tests to quantify the optimal conditions (temperature, duration, self-heating, carbon conversion) at which a coal can be successfully gasified with CO2 as agent.

23.3- Role of Solids in Viscosity of Brown Coal Slags: How It Affects TCV and Transition to Non-Newtonian Flow

Alexander Ilyushechkin, San Shwe Hla, Daniel Roberts, CSIRO Energy, AUSTRALIA; Alex Kondratiev, National University of Science & Technology MISIS, RUSSIA.

Slag flow characteristics, such as viscosity, play a critical role in stable operation of entrained flow gasifiers. For continuous and trouble-free slag taping, a slag viscosity range of 5–25 Pa s at temperatures 1200–1500ºC is usually considered suitable, and the viscosity behaviour of fully liquid slags has been investigated by a large amount of experimental and modelling work over the last few decades.

It is common, however, for slags to form with significant amounts of solids. This formation of solids is an important consideration in studies of coal suitability for gasification: as well as needing to form a slag of suitable viscosity, the setting of suitable operating conditions is also affected by the temperature at which the slags become heterogeneous (i.e. liquidus temperatures, Tliq), that at which viscosity increases dramatically and unpredictably (temperature of critical viscosity, TCV), and how the slag flow behaviour becomes non-Newtonian (temperature of non-Newtonian transition, Tnon-Newtonian). All of these characteristics strongly depend on slag bulk composition and the primary phase field, and how they impact the formation of solids in the melt.

This work is part of a wider study of the use of Australian lignites in slagging gasifiers, and describes how solids affect slag flow behaviour and their characteristics for compositions of brown coal ashes from different primary phase fields, especially those which have liquidus temperatures within the typical operating temperature range. Three types of transition from Newtonian to non-Newtonian behaviour are are demonstrated. The relationships between TCV, Tliq and temperatures of transition to non-Newtonian flow are shown for slags from spinel and olivine primary phase fields, and experimental data are used to evaluate existing viscosity models.

23.4- Experimental Study on Liquid Hydrocarbon Formation during Pressurized Underground Coal Gasification Conditions

JC van Dyk, JF Brand, FB Waanders, North-West University, SOUTH AFRICA; M Nguyen, D Scheithauer, TU Bergakademie Freiberg; B Meyer, DBI-Virtuhcon GmbH & TU Bergakademie Freiberg, GERMANY.

UCG is a gasification process used to produce synthesis gas from coal in situ (underground in the coal seam) by injecting air or oxygen, with or without steam, into coal seams and extracting the product gas via surface wells. The resulting synthetic gas ("syngas") can be used to produce electricity, as well as chemicals, liquid fuels, hydrogen and synthetic natural gas. Together with the resulting syngas, some of the coal components, especially condensable water, oils, tars, inorganic trace elements and a small fraction fly ash as particulate matter make its way to the surface via the production well and can cause negative impacts on downstream processes. Tar and oil formation during pressurised Underground Coal Gasification condition will be discussed in this paper.

The project aims at generating and characterizing tar/oil (condensable hydrocarbon fraction) from a South African Highveld coal sample under conditions that imitate the pyrolysis stage of Underground Coal Gasification (UCG). For the generation of the tar/oil fraction, a pressurized pyrolysis plant of the Institute of Energy Process Engineering and Chemical Engineering at TU Bergakademie Freiberg is used.

The experimental equipment is a counter-current fixed bed reactor, in which the preheated purge gas Argon and if necessary the previously generated steam is introduced at the bottom of the reactor. The fixed bed is gradually building up during the experiment as the feedstock is introduced from a storage tank via a screw feeding system into the reactor. The system is electrically heated and can be operated at pressures up to 30 bars. The tar/oil fraction is collected within a condensation system, whereby a solvent is used to remove the tar/oil from the condensers. Permanent gases are analysed after pressure reduction.

To generated tar/oil under UCG conditions, the following conditions will be used:
Pressure: 30 bars
Superficial flow velocity: 0.05 m/s
Particle size: 2.0 - 6.3 mm
Temperature(s): 650 °C; 800 °C
Steam addition: 0 - 0. 15 kg/kg coal

The results from this study, both on quality and quantity, on the liquid hydrocarbon formation during a UCG process will be discussed.

23.5- Investigation the Shape of Cavity and Pollutants Migration Behavior after Underground Coal Gasification

Maofei Niu, Shuqin Liu, China University of Mining and Technology (Beijing), PR CHINA.

The investigation of the gasification cavity and the gasification face expansion from underground coal gasification is of great importance to understand the real combustion status and to guide the layout of the gasifier. It is of great scientific significance and practical value to understand its contamination risk and make a control through the whole process.

In this study, based on drilling exploration of a field test of underground coal gasification, samples of coal, char, ash, slag and rock along the drilling boreholes were obtained, and then proximate analysis, XRD and SEM-EDS analysis were performed to investigate the changes of their properties. then the leaching experiment of samples were performed. Moreover, the migration behavior of the typical pollution indicators, volatile phenols, ammonia nitrogen and COD were analyzed, and the migration path of pollutants was also discussed.

The results show that high activity lignite underground gasification through blowing air, the expanded width of gasification surface is less than 17m. About 4m away from the directional drilling channel, perpendicular to the direction of the airflow, high temperature gasification reaction occurs in the coal seam and accompanied by the formation of the typical minerals such as anorthite. In this area carbon residue in the ash is about 10%, and coal seam gasification causes the loose and collapse of overburden. The migration of typical pollutants mainly occurs in the center of gasification zone and their vertical migration along the roof are found. The caving zone and fractured zone in the roof provide the main channel for contaminant migration. The tendency of pollutants migration toward the floor rock through permeation is very low. The position 17m away from the directional drilling channel is close to the boundary of heat transfer, where only the upper coal seam is affected by heat, and the the deformation of roof rock is not observed. Near the gasification boundary, no migration path is formed in the roof of the coal seam, and the pollutant migration is not detected. In addition, the comprehensive profile of the combustion cavity is plotted. The scientific site selection of the gasification coal field is the most important step for UCG pollution control.

SESSION 24
COAL SCIENCE - 4

24.1- Theoretical Investigation on the Distribution of Hydroxyl Group in Coal Structure

Hongjun Fan, Lu Li, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, PR CHINA.

Coal structure is very complicated and highly depends on the origin, history, and age or rank of the particular coal. The ratio of various functional groups in coal may be studied by existing analysis technology, but the connections of these functional groups are still mostly unknown because of lack of very effective way to get this information yet. In this work we assume that the most stable position for a certain group could be the most plausible position for that group in the coal structure. Considering the oxygen is the most predominant heteroatom in coal, and the phenolic hydroxyl appears to be the most abundant oxygen functional group, we have studied the most plausible position for hydroxyl group in coal with the help of Density Functional Theory (DFT) calculations. We found the order of preferential position for hydroxyl group is: (1) pyridine rings; (2) polycyclic aromatic hydrocarbons; (3) monocyclic aromatic molecules; (4) alicyclic rings. Besides, double substituted hydroxyl groups on pyridine and aromatic ring are possible. Hydroxyl groups tend to be in the positions where they can form hydrogen bond each other. Electron donating and withdrawing groups do not obviously change the preference of hydroxyl group unless there is hydrogen bond formed.

24.2- Sulfur Transformation during Pyrolysis of Maceral Concentrates Derived from Density Classification of High Organic Sulfur Coking Coal

Shaolin Liu, Yangfeng Shen, Jiao Kong, Xiaobao Duan, Meijun Wang, Taiyuan University of Technology, PR CHINA.

The partial substitution of high quality coking coal by coking and fat coal with high sulfur content during coal blending coking process offers a relatively economical means for coal utilization, however, due to its natural characteristic, the proportion of high sulfur coal in blended coal is limited vastly. The distribution and occurrence of sulfur in the macerals have an important influence on the residual sulfur in coke, therefore, it is of great significance to study the sulfur transformation during pyrolysis of different macerals. In this study, a typical high organic sulfur coking coal was systematically investigated, and the raw coal sample was primarily separated into six fractions based on different densities by float-sink experiments. Experimental results show that the lower density fractions have more content of vitrinite and exinite but less inertinite, which leads to higher organic sulfur contents. This shows that there is a good correlation between the content of organic sulfur and types of marceal in coal, since organic sulfur usually exists as part of the coal matrix. Based on the characteristic peaks of each sulfur forms appeared in the XPS (X-ray photoelectron spectroscopy) spectra of different fractions, the classification process of coal could not only change sulfur forms, but the relative content of sulfur in density fractions. During pyrolysis of different fractions in a fixed-bed reactor, the maximum release peak temperature of H2S and SO2 from the lower density vitrinite-rich fraction is decreased, and the cumulative amount is higher than that of the inertinite-rich ones. The different evolution behaviors of sulfur-containing gases suggested that lower density fraction had higher content of aliphatic and aromatic sulfur, and lower pyritic-sulfur compared to higher density fraction.

24.3- Study on FTIR of High-Organic-Sulfur Coal and the Structure of Sulfur-Containing Compounds of its Extracts

Yuegang Tang, Cong Chen, Xiaolong Li, Yewei Sun, China University of Mining and Technology (Beijing), PR CHINA.

Based on coal structure chemistry and organic geochemistry of coal, typical high-organic-sulfur coals with different metamorphic degrees in China and their extracts were studied using Fourier Transform Infrared Spectroscopy (FTIR) and Gas Chromatography-mass Spectrometer (GC-MS) to explore the evolution characteristics of coal structure and the evolution characteristics of the organic sulfur structure following the degree of metamorphism. The FTIR analysis of coal samples showed that the proportions of substituted aromatics in the low metamorphic coal varied diminutively while varied greatly in high metamorphic coal. The proportions of ortho-disubstituted aromatic hydrocarbons and ortho-trisubstituted aromatic hydrocarbons was similar and had a good positive correlation. The proportion of ortho-penta-substituted aromatic hydrocarbons was low and was in inverse proportional relationship with proportions of ortho-disubstituted aromatic hydrocarbons and ortho-trisubstituted aromatic hydrocarbons. Content of carbonyl and methyl decreased while content of methylene increased as the coal metamorphism increases. GC-MS analysis of sulfur-containing compounds in the aromatic component of the extracted product showed that with coal metamorphism increasing, the relative content of dibenzothiophene and methyldibenzothiophene increased, the relative content of trimethyldibenzothiophene

decreased and the relative content of dimethyldibenzothiophene primarily increased and then decreased. The above results reflected that as the coal rank increases, the active functional groups in the coal transfer to stable functional groups, the side chains decrease, and the degree of condensation increases. The coal structure generally showed a tendency of the methyl groups and side chains decrease, resulting in the increase of aromatic structures.

SESSION 25
CARBON MANAGEMENT - 2

25.1- Progress and Outlook of Yanchang Full-Chain CCUS Project

Ruiming Gao, Research Institute of Yanchang Petroleum（Group) Co. LTD, PR CHINA.

As a Fortune Global 500 companies, Yanchang Petroleum will conscientiously implement the development concept of innovation, 'coordination, green, openness, and sharin'. As early as 2009, Yanchang Petroleum Group started a demonstration project for carbon dioxide capture, storage and enhanced oil recovery technology. implemented a full-chain project to capture carbon dioxide from coal chemical industry and use CO2 flooding to enhance oil recovery. This report will introduce the progress and outlook of the project.

25.2- Preparation and CO_2 Adsorption of Amine Modified Titanate Nanotubes

Xiaohua WangYao Zhou, Xi 'An University of Science & Technology, PR CHINA.

A new synthesis of low-cost and efficient carbon dioxide adsorbent-titanate nanotube was proposed. Porous titanate nanotubes were synthesized at different temperatures by microwave hydrothermal method andfurther modified by different amines such as diethylenetriamine (DETA), triethylenetetramine (TETA) and tetraethylenepentamine (TEPA). The synthetic adsorbents were characterized by scanning electron microscopy (SEM), low-temperature nitrogen adsorption (BET), Fourier transform infrared spectroscopy (FTIR). The CO_2 adsorption capacities of synthetic adsorbents were characterized by carbon dioxide high temperature and high pressure gas adsorption instrument. The results showed that the CO2 adsorption capacities of modified titanium-based adsorbent were strongly affected by pore volume and specific surface area of the support. The TETA impregnated adsorbent has the best CO2 adsorption capacity. When the CO2 partial pressure was 3MPa and the reaction temperature is 75℃, the adsorption capacity reaches 3.35mmol/g. This tubular structures and stable amine impregnated Titanium-based adsorbent with good stability and high CO2 adsorption capacity exhibit great potential application in CO2 removal from coalbed methane (CBM).

25.3- Energy Efficiency Improvement and Debottlenecking for IGCC-CCS

Presenting Author: Omar M. Basha, North Carolina A&T State University; Co-Authors: Nicholas Siefert, Isaac Gamwo, National Energy Technology Laboratory, U.S. Department of Energy; Badie I. Morsi, University of Pittsburgh; USA

Over the past decade, the US and Europe have seen a wave of retirements of coal fired power plants, and this trend is expected to continue in the future as coal's bottom line continues to erode. The only way forward for coal lies in the development, optimization or retrofitting of clean coal power plants, with minimal emissions, in order to meet growing regulations. This work will focus on the Integrated Gasification Combined Cycle process, with pre-combustion capture (IGCC-CCS), by identifying energy pinch points throughout the process, and highlighting and ranking debottlenecking strategies and outlooks, and their feasibility for future widescale implementation.

SESSION 26
COMBUSTION TECHNOLOGIES - 5

26.1- Effect of Natural and Forced Convection on Ignition and Soot Yields for Single Coal Particle Combustion

Lele Feng, Yuxin Wu, Tsinghua University; Kailong Xu, CAEP Software Center for High Performance Numerical Simulation; Hai Zhang, Tsinghua University; PR CHINA.

Understanding coal ignition behavior is of great importance for combustor design and operation. Meanwhile, particular matter emission has drawn increasing attention in coal utilization industries. It is necessary to study the effect of convection on ignition behavior and soot yields, especially for coal combustion under high Re number condition, such as MILD combustion. In previous work, a model based on one dimensional equations has been validated for prediction of coal ignition, flame temperature and soot yields. In present work, the effects of natural and forced convection on mass and heat transfer are analyzed by classical similarity rules. Based on that, a so-called superficial mass diffusivity and a superficial thermal diffusivity are calculated according to the local Re, Sc and Pt number, as well as the real mass and thermal diffusivity. Further, the superficial mass and thermal diffusivity are applied to the modeling of single coal combustion to represent the effect of convection. This method is validated by comparing predicted ignition time and temperature with previous experimental results for a typical Datong bituminous Coal from China. It is shown that both natural and forced convection decrease ignition time compared to microgravity condition. The effect of convection intensity, particle diameter and oxygen mole fraction on the ignition behavior and soot volume fraction are numerically studied for a Pittsburgh bituminous coal. As the convection intensity increases, the ignition time decreases, which is due to a larger thermal diffusivity. For same reason, the flame temperature decreases with increasing convection intensity. At same time, the maximum soot volume fraction decreases, due to a slower formation rate at lower flame temperature and a larger mass diffusivity. At a given Re number, as particle diameter increases, the ignition time, flame temperature and maximum soot volume fraction all increases. This indicates that a small size of coal particle may be a better choice for MILD coal combustion. What is more, the ignition behavior and soot yields of small particles are more sensitive to a changing Re than those of large particles. At a given Re number, as oxygen mole fraction increases, ignition time decreases, while maximum soot volume fraction increases first and then decreases. The ignition behavior and soot yields with low oxygen concentration are more sensitive to a changing Re than those with high oxygen concentration.

26.2- Kinetic Study of the Pore Development for Solid Fuel Reactivity Using FERPM

Kyung-won Park, Gyeong-Min Kim, Chung-Hwan Jeon, Pusan National University, SOUTH KOREA.

In order to have a better understanding of the pore development for carbonaceous solid fuel char reaction model, thermal gravimetric experiment was proceeded about Semi-anthracite coal (Carbo one), Sub-bituminous coal(Adaro)and Biomass (Kenaf, WP). Fuel sample was pulverized the size of 75-90 μm and biomass was 400-600 μm, respectively. TGA (Thermogravimetric Analysis) was derived and three reaction models HM (Homogeneous Model), RPM (Random Pore Model) and FERPM (Flexibility-Enhanced Random Pore Model) were applied in isothermal (650°C) and different heating rate(5,10,20°C/min) conditions. The obtained results show that the high degree of carbonization fuel was well corresponded to the RPM and FERPM. As the carbon composition in the solid fuel was decreased, the results indicated that FERPM is well-matched to experiment data in overall combustion process. In the early range of char reaction for carbonaceous fuel, combustion of high carbon fuel reacts mainly. On the other hand, in the latter period of reaction, low carbon samples have a dominant reaction of char combustion. In this comparison between experiment and reaction model, FERPM was the best fitted for carbonaceous solid fuel.

26.3- A Transient Process Simulation on Thermal Explosion of Propylene Recovery Reactor Linked with Calorimetric Techniques

Chi-Min Shu, Yi-Hong Chung, Zhao-Min Jiang, Yunlin University of Science and Technology, TAIWAN, ROC

On 30 July, 2011 a serious explosion in a Taiwanese local plant associated with propylene recovery process shook the public's faith in chemical process safety. The recovery process was implemented to remove the H2S, COS, and also humidity reducing. It mainly proceeded by two adsorbents, BASF selexsorb CD and UOP SG series, respectively. However, gas phase propylene greatly alleviated the heat removal ability. Then, the adsorption heat triggered a chain reaction that finally caused the explosion and fire disaster. To prevent such the situation, we explored the characteristics between propylene and adsorbent comprehensively in this study. Vent sizing package 2 (VSP2), which can create pseudo-adiabatic conditions for acquiring precise process thermal parameters, was accompanied with the gas chromatography-mass spectrometry (GC-MS), specific surface area and porosity analyzer. Complicated situations, such as heat transfer and fluid status related to disaster, were properly handled by computational fluid dynamics (CFD) software.

A severe oligomerization reaction was revealed in our micro-scale experiments when the temperature exceeded 150 °C. On the other hand, through CFD transient simulations, the phenomena of heat accumulation in the middle of reactor can be demonstrated obviously.

In summary, to understand the potential hazard of the propylene purification process, we used restore experiment and transient simulations, which had great effects. Based on these, methods and fault system analysis can correct this process and lessen the risk effectively.

26.4- Method for Improving Power Efficiency of Coal Fired Power Plants Fitted with CCUS

Geoffrey D Bongers, Gamma Energy Technology P/L; Nikolai K Kinaev, Strategic Energy Consulting P/L; Zvonko Pregelj, Altaprom International P/L; AUSTRALIA.

A novel patented method for improving power efficiency of carbon capture from coal fired power plants was examined at the concept level using a combination of Excel based thermodynamic and parametric models. The results showed that enhanced cleaning of the flue gas from the coal fired power plant, mixing it with air, feeding the mixture into a combined cycle natural gas fired F class turbo-generator and capturing the carbon dioxide using an amine-based absorbent increased the overall efficiency of the system by around 8% compared to the case of decarbonizing the flue gas streams separately or in combination, mainly due to increase of CO2 concentration in the flue gas.
The method was seen to be particularly suitable for retrofitting CCUS to existing coal fired power plants, especially as it also increased the net power output by the about 130% for the modelled case. The modelling used an amine-based capture process, although it was noted that any gas separation technique could be used in theory, albeit with perhaps different relative impacts. In addition, whilst not confirmed by detailed modelling, it is expected that the increase in overall efficiency will be dependent upon the relative efficiencies of the coal plant and the combined cycle plant such that increasing the efficiency of the combined cycle plant and / or decreasing the efficiency of the coal fired power would lead to further improvement in the relative efficiency gain, making this technology even more attractive for upgrading older coal fired power plants. Consequently, development of the technology, including the study of other cases and optimization opportunities already identified, is expected to further improve the results.

SESSION 27
COAL BED AND SHALE GAS - 2

27.1- Paleotectonic Stress Field Reconstruction and Prediction of Natural Fractures in the Longmaxi Shale Reservoir

Nanchuan Region, South China, Wei JU, China University of Mining & Technology, PR CHINA.

Natural fractures serve as significant storage spaces for hydrocarbons and are favorable for fluid flow in shale gas reservoirs; therefore, predicting the intensity and distribution of natural fractures within reservoirs are of extreme significance for shale gas exploration and development. In the Nanchuan region, most natural fractures within the Longmaxi Formation were formed in the Late Yanshanian period. They are generally in high dip angles, and the dominant fracture strikes are distributed in the ~NE-SW and ~NW-SE directions. Therefore, in this study, the Late Yanshanian paleotectonic stress field was numerically investigated. The comprehensive rupture rate (CRR) was defined and calculated as an indicator to quantitatively predict the intensity and distribution of natural fractures within the Longmaxi Formation. The results indicated that the intensity and distribution of natural fractures in the Longmaxi Formation of Nanchuan region were resulted from many factors including tectonic activities and brittle minerals. Regions with well-developed fractures were located in/around fault zones and fold zones, among fault/fold orientations change, and at fault tips. The present study provides preliminary insights into natural fractures within the Longmaxi Formation, which can guide and support shale gas exploration and development in the Nanchuan region, South China.

27.2- CSIRO Ventilation Air Methane Abatement Research

Shi Su, Xin Yu, Jon Yin, Jun-Seok Bae, Yonggang Jin, Michael Cunnington, Ramesh Thiruvenkatachari, CSIRO, AUSTRALIA.

Ventilation air methane (VAM) is a significant greenhouse gas source with a Global Warming Potential more than 28 times that of carbon dioxide. VAM abatement has been challenging to the coal mining industry because (1) VAM represents the largest proportion of coal mine methane emissions and (2) its air volume flow rate is large and the methane concentration is dilute and variable. CSIRO commenced the VAM abatement research in 2000, ranging from fundamental studies including theoretical analysis and lab-scale experiments, through to mine site sampling, techno-economic assessment, and pilot scale prototype unit development and site trials. To date, an exhaustive range of VAM mitigation and utilization ideas and concepts, taking into account mine site VAM characteristics, have been evaluated and developed. This presentation will introduce a suite of CSIRO-developed technologies for VAM abatement and associated safety management, which have been proven feasible and practical for mine site deployment through lab-scale studies, pilot-scale prototype unit development and site trials using real VAM. These technologies are able to abate VAM via thermal destruction, utilization for power generation, and enrichment. In comparison with their competitors, they possess significant advantages, such as lower capital cost, lower operational and maintenance cost because of lower power consumption, no dust deposition issues. In addition, CSIRO has been developing emerging technologies for the ultra-low concentration VAM abatement, e.g. photocatalytic oxidation destruction under ambient temperature and pressure conditions. The photocatalytic oxidation is very promising in destructing VAM at a very low concentration (e.g. less than 0.3 vol % and even at hundreds ppm levels), which cannot be effectively treated by existing VAM abatement technologies. This technology can be potentially applied in open cut or offset areas for methane abatement.

27.3- Optimization of Technology for Development of Thin Interbedded Coalbed Methane in Western Guizhou Province of China

Shao Xianjie, Liu Zeheng, Li Feng, Oyaka Dickens, Yanshan University; Jin Liuqing, Guizhou Shale Gas Co., Ltd; Li Mingfeng, Yanshan University; PR CHINA.

Western Guizhou Province is one of the areas with relatively rich coalbed methane in China. However, the coal seams are thin, contain many layers, and are interbedded in the longitudinal direction. Therefore, it is difficult to develop, resulting in a large amount of unexploited coalbed methane resources. At present, there is an urgent need to build a set of development technologies for thin interbedded CBM to improve the development effect and accelerate the pace of development. Based on data of drilling, logging, fracturing, drainage and single well production dynamics, this paper analyzes the development effects of a single well, ascertains the factors that affect the development effect, and points out the problems existing in the development. The influence of different combined thicknesses and lengths of layer series of development on the development effect is studied. Using the CBM production forecasting software as a way of determining the bottom hole flow pressure to predict the production under different conditions, it is believed that the lower limit of the thickness of the development layer is 5m, the upper limit of the length of layer series of development is 841.28m, and the number of combined layers should not exceed 8. According to the distribution of in-situ stress, the natural fractures and the extension direction of fractures in the fracturing wells, it is proposed that the best effect can been acquired in the arrangement of rhombic well patterns which long diagonal line along the direction of 53° or 327°. The well pattern density is 11holes/km2 and the well spacing is 440m×200m. The relationship between gas production and drainage intensity, bottom-hole flow pressure, and casing pressure during the drainage process was studied by reservoir engineering theory and production statistics. It is believed that if the downhole flow pressure is controlled within the range of 0.5 to 1.7 MPa and the mantle pressure is controlled within the range of 0.3 to 1.2MPa, it can guarantee a stable production condition of the gas well and the effect is optimal.

27.4- Experiment on Improving Gas Diffusion rate of Coal Petrography by Vibration Waves

Shao Xianjie, Oyaka Dickens, Li Feng, Li Mingfeng, Liu Zeheng, Peng Yingming, Yanshan University, PR CHINA.

The adsorption-diffusion method was adopted to measure the diffusion coefficient of coal through optimal designing of the experimental instruments. Coal-rock was cut and ground into slices of several millimeters thick samples. The coal sample was dried, evacuated and then placed in a closed container. The entire experimental system was passed into the gas after evacuation, and the relationship between the gas adsorption amount of the coal sample and time change was recorded. During this process, firstly, the gas is adsorbed on the surface of the coal samples, then spread into the interior until the whole sample reaches the adsorption saturation. According to the relationship of pressure and time change, several parameters can be calculated including: the adsorption amount of coal sample surface, balance adsorption of coal sample and diffusion coefficient. After studying the effects of vibration and non-vibration conditions on diffusion, it was found out that the vibration wave makes diffusion coefficient of coal sample increase from 6.7%~77.4% with the average increase of 51.4%；And also the vibration wave weakens the adsorption ability of coal sample, the average adsorption quantity decreases by 23.2%. As vibration wave propagates in the coal medium, the propagation direction of longitudinal wave is the same as that of the particles in the coal medium, and the coal medium will be subjected to cyclic stretching and compression, which makes the coal body elastically deformed; and the propagation direction of the transverse wave is perpendicular to the vibration direction of the coal medium particle, so that the coal body has a certain shearing effect which causes longitudinal elastic deformation. when this cyclic elastic deformation exceeds the fatigue strength of coal, the coal body will produce new micro-cracks and pores, thus the diffusion of coalbed methane is promoted. In addition, in the process of vibration wave propagation, the local thermal effect is generated in the coal body, the kinetic energy of the gas molecule increases, the adsorption capacity of the gas reduces and the diffusion ability is improved. The results show that the vibration technology can make the methane molecule desorb, increase the diffusion coefficient, hence increasing the production of coalbed methane. Physical simulation experiments are being carried out on this technology in the laboratory. Technology is being refined and field experiments are expected to be carried out in the future.

SESSION 28
VALUE-ADDED PRODUCTS FROM COAL - 5

28.1- Effect of Straw Addition to Coal on Coal-Based Activated Carbon for Methane Decomposition

YaJie Wang, Lijun Jin, Yang Li, He Yang, Haoquan Hu, Dalian University of Technology, PR CHINA.

Activated carbon (AC) is a promising catalyst for methane decomposition due to low cost, easy modification of its properties and high temperature resistance. The carbon source will affect the properties of the resultant AC and its catalytic performance in methane decomposition. In this paper, Buliangou (BLG) coal combined with biomass straw was used as the carbon precursor to prepare AC at 850 oC by KOH activation. The effect of straw addition amount to coal on the pore structure, surface chemistry of the prepared AC and its catalytic performance on methane decomposition was investigated. The result of thermo-gravimetric analysis showed that the addition of straw promoted coal pyrolysis, but the promotion was weakened as the amount of biomass straw increases. The addition of straw obviously benefits the mesoporous development of AC. the total specific surface area and pore volume of AC first increase and then decrease with the increase of straw amount. When the mass ratio of BLG coal and straw is 1:1, the resultant AC has the largest specific surface area and pore volume, and higher activity and better stability in the methane decomposition. Higher mesoporosity is the main reason for the better catalytic performance of AC in methane decomposition to hydrogen.

28.2- Effect of Carbon from Anthracite Coal on the Hydrogen Absorption and Desorption Performance of Magnesium Based Hydrogen Storage Materials

Xiaojing Liu, Co-Authors: Xiaojing Liu, Shixue Zhou, Shandong University of Science and Technology, PR CHINA.

Magnesium-nickel hydrogen storage material was prepared by adding carbon with ball milling and static hydrogen storage. The morphology, crystalline structure of the magnesium-nickel-carbon composite was determined by TEM, HRTEM, SEM analysis. The carbon plays a role of dispersant for the Mg particles to prevent them from aggregating during milling according to SEM observation. Carbon additives for milling can lead to smaller crystal size, and the particle size of the material can be further reduced by extending ball milling time in a certain range by TEM observation. Also, the carbon can improve the adsorption and desorption properties of materials, and improve the MgH2 decomposition enthalpy change and heat absorption. Compared with magnesium-nickel hydrogen storage materials, adding carbon makes the hydrogen absorption and desorption properties of the materials improving. DSC analysis shows that adding carbon makes the hydrogen desorption temperature of the material reducing 20oC. According to the p-c-T curves and the van't Hoff equation, it is found that the addition of carbon reduces the hydrogen absorption plateau, and decreases the enthalpy change by 25 kJ/mol, thus reducing the phase stability of materials, and enhancing the ability of dehydrogenation of the system, and ultimately improving the hydrogen release performance of materials

28.3- Preparation of Micro-Mesoporous Composite Sieves Catalyst and Its Catalytic Cracking Performance of Coal Tar

He Xiaoxiao, Meng Zhuoyue, Xue Wenying，Zhaojingjing, Xi'an University of Science and Technology, PR CHINA.

At present, China's large amount of coal tar is relatively crude and its low processing and conversion capacity is low. Catalytic pyrolysis is an effective way to improve the quality of the coal tar, heavy components in tar to be divided into BTX, PCX, and other light aromatics components, in order to improve the quality of the tar. In this paper, SBA-15 mesoporous molecular sieves were prepared mainly by hydrothermal synthesis and microwave hydrothermal synthesis. The main use of triblock copolymer P123 as template, tetraethyl orthosilicate as silicon source, and the synthesis conditions were studied under the condition of acid, the influence of the crystallization time on the synthesis effect was discussed. The synthesis conditions under acidic conditions were carried out to explore the influence of the synthesis effect by using different crystallization time. The traditional hydrothermal method was optimized by ultrasonic dissolving, the temperature water bath was 40℃, the crystallization temperature was 90℃, and the crystallization time was 24h. The microwave hydrothermal method can improve the crystallization efficiency, and shorten the crystallization time to 2h. The micro-mesoporous molecular sieves were obtained by mechanical mixing microporous molecular sieve ZSM-5. The SBA-15 prepared by hydrothermal synthesis has a hexagonal column structure with moderate pore size, thicker pore walls, and higher hydrothermal stability. In addition, the isothermal adsorption curve and pore size distribution of N2 adsorptiondesorption also verified that SBA-15 indeed has the structural properties of mesoporous materials. Finally, the catalytic cracking experiment was used to study the application of ZSM-5/SBA-15 composite molecular seive in the catalysis of coal tar cracking. It was found that the ZSM-5/SBA-15 has a good catalytic effect.

28.4- Hydrogenation of Aromatic Components over NiMo/Mesoporous Analcime Carbide Catalyst

Chenguang Jiang, Haiyong Zhang, Yonggang Wang , Ning Chang, China University of Mining & Technology (Beijing), PR CHINA.

A series of mesoporous analcime zeolite supported NiMo carbide catalyst were developed and utilized forhydrogenation ofaromaticson a fixed bed reactor. The results demonstrate that the synthesized analcime as supportwith good crystal structure stability, which can provide a part of medium-strong acidic sites. Therefore, analcime zeolite supported NiMo bimetallic carbide catalysts have a good hydrogenation performance on model compounds and coal tar.

28.5- Partial Oxidation Cracking of Coal Tar Over Fe-Ni Mixed Metal Oxides for Production of Light Fuels and Hydrogen Rich Gas

Dechao Wang, Lijun Jin, Yang Li, Haoquan Hu, Dalian University of Technology, PR CHINA.

The clean and efficient utilization of coal tar, a by-product of coal pyrolysis, is an important field for the comprehensive use of coal. In this study, a novel process, partial oxidation cracking, was proposed for upgrading of coal tar to produce light fuels (< 360 oC) and hydrogen rich gas. A serial of Fe-Ni mixed metal oxides was prepared as oxygen carrier. In this process, oxygen species including lattice oxygen and adsorbed surface oxygen react with coal tar to improve the cracking of coal tar. As a result, more heavy oil fractions (> 360 oC) are decomposed to produce light fuels. Due to the supply of oxygen species on the Fe-Ni mixed metal oxides, CO2 and CO were detected in the gas product, which confirms the catalytic cracking of coal tar follows a partial oxidation mechanism. The gas stream is rich in hydrogen, and the hydrogen concentration is over 50 vol% when the Fe-Ni mixed metal oxides are added. The mixed metal oxide of Fe1Ni (the atom ratio of Fe and Ni is 1:1) showed the best catalytic performance in terms of high light fuels content and high concentration of hydrogen gas. The Fe-Ni mixed metal oxides were characterized by XRD, N2 adsorption/desorption, Raman, H2-TPR, and XPS to reveal the correlation between the catalytic performance and the physicochemical properties.

SESSION 29
GASIFICATION TECHNOLOGIES - 5

29.1- Development of New Technology for Controlled Underground Coal-Coalbed Gas Fluidized Co-Mining

Zuotang Wang, China University of Mining and Technology (CUMT), PR CHINA.

Mainly introduce the development of new technology for controlled underground coal-coalbed gas Fluidized co-mining used in the industrial demonstration in Pan county, Guizhou province.

29.2- Effects of Microwave Irradiation and Hydrothermal Treatment on the Gasification Characteristics of Brown Coal

Lichao Ge, College of Energy and Electrical Engineering and Zhejiang University; Hongcui Feng, HUATIAN Engineering & Technology Corporation, MCC; Jingyu Guan, Harbin Boiler Company Limited; Chang Xu, College of Energy and Electrical Engineering; Yanwei Zhang, Zhihua Wang, Zhejiang University; PR CHINA.

Microwave irradiation (MI) treatment is a typical evaporative dewatering process, which has many advantages, such as: non-contact heating, energy transfer instead of heat transfer, rapid heating, selective material heating, volumetric heating and so on. While hydrothermal dewatering (HTD) is a typical non-evaporative process, which can remove water in the liquid form, saving the latent heat of vaporization. HTD has also been considered as the simulation of the coal maturing process in nature. Literatures contain many investigates about the dewatering and upgrading effects caused by MI or HTD. But few studies report the differences and comparisons between MI and HTD. This paper investigates the effects and comparisons of MI and HTD on yield of solid products, coal composition, pore structure, and gasification characteristics of two Chinese brown coals. Results shown that both the upgrading processes significantly decreased the coals' inherent moisture and oxygen content, and increased their calorific value and fixed carbon content. Based on N2 adsorption results, coal particle was broke to pieces, coals' hardness and brittleness increased; pore distribution of upgraded coal developed to the microporous region after each upgrading process. Compared with HTD, MI process carried out rather quickly and intensely. Process time needed for MI were minutes, but

more than ten hours for HTD. After MI upgrading process, surface area and pore volume always increased, while them increased at first but then decreased as the HTD treatment temperature increased. In general, similar effects were observed for MI and HTD at mild upgrading temperature, but more obvious effects were gained for HTD at relatively high temperature. Thermo-gravimetric analysis shown that the gasification process of HTD upgraded coals were delayed towards high temperature region, the temperatures when carbon conversion rate reaches 50% increased. From the results of kinetic calculation, activation energy increased after HTD treatment, and the reaction order of mechanistic model increased. However, the temperature when carbon conversion rate reaches 50% decreased, and the maximum gasification rate increased, indicating the increase of gasification activity for MI upgraded coals. Activation energy decreased after MI treatment, and the reaction order of mechanistic model decreased. The differences caused by the two upgrading processes may be attributed to the completely different modification mechanisms. Besides, all the changes caused by MI and HTD are more obvious when the upgraded temperature increased.

29.3- A Novel and Yet Simple Methodology Based on the use of Inclined Plane for the Measurement of Slag Viscosity

Baiqian Dai, Lian Zhang, Monash University, AUSTRALIA.

Slag viscosity has a broad implication in glass production, geophysical phenomena, metallurgical processes, fly ash vitrification, combustion and gasification. The current technologies for viscosity measurement face the challenges of cost and difficulty in operation. Numerous studies have also tried to establish slag viscosity prediction models by using chemistry compositions base on the CaO-Al2O3-SiO2 system, which is normally suitable for slags from high-rank bituminous coal. However, the slag from low-rank coal and biomass are rich in alkaline metals, which have been rarely investigated by the scientific community. Additionally, the existing empirical models are unable to predict the viscosity for slags from low-rank coal and biomass. This study aims to develop a novel and yet simple methodology for high-temperature slag viscosity measurement by using a simple inclined plane method. Four ash samples with known viscosity were used to establish and validate an empirical equation for slag viscosity calculation. The key factors that affect the viscosity, including ash mass, temperature and residence time have been examined systematically. The relationship between the slag travel length and viscosity has been clarified. Four different inclined angles, including 25o, 45o, 60o and 90o, have been used to investigate the effect of inclination angle on the slag flow-ability. The results confirmed a linear relationship between the slag travel length per unit mass and cosβ. Additionally, the results demonstrated an Arrhenius-type relationship for the variation of slag viscosity temperature. Finally, an empirical equation was established for viscosity calculation by multiple linear regression. The established method was further applied to a variety of low-rank coal and biomass ash samples. The results will be discussed in detail in this presentation.

29.4- Mechanism for Calcium Species Enhancing Hydrogen Production during Steam Gasification of Modified Coke from Calcium Carbide Slag Added Coal Blending Coking

Jiang Guo, Haili Jiao, Dong Yan, Meijun Wang, Jiao Kong, Weiren Bao, Taiyuan University of Technology, PR CHINA.

The production of coke for gasification by coal blending coking is one of the effective ways to relieve the excess capacity of coking industry. However, low reactivity and hydrogen production restrict the wide application of coke for gasification. In-situ addition of additives during coal blending coking is benefits removal of these restrictions. Calcium carbide slag (CCS) is a suitable additive which is supposed to interact with carbon both in coking and gasifying process. In this study, an optimized coal blending scheme was employed as basic blended coal from previous studies. The modified cokes were prepared from blended coals which were added different amount of CCS (3%, 5%, and 7%) by stamp-coking at a heating rate of 3 oC/min to 1150 oC with holding time of 30 minutes in a muffle furnace. Isothermal gasification of cokes with CO2 or steam was conducted on a laboratory fixed-bed system at 1000 oC and the gaseous products were analyzed by an on-line gas analyzer. The forms of calcium species in coal blending and cokes were identified by X-ray diffractometer (XRD) to reveal the interaction between CCS and carbon. CCS is found to have significantly promotional effect on the reactivity of cokes with coke reactivity index (CRI) of CCS-7% being 3.5 times higher than that for no CCS added coke. It is observed that H2 production is significantly enhanced while the CCS is added in the coal blending. CaCO3 and CaO are detected in the modified cokes by XRD. It is speculated that calcium species interact with carbon to form intermediate complexes CaO-C, which act as active centers to adsorb more gasifying agent so that the gasification reaction rate is accelerated. In the presence of steam, the formation of a new intermediate complex CaO-H2O-C on active center benefits for the improvement of H2 production, which can intensify water gas shift reaction by absorbing CO.

29.5- The Impact of Coal Seam Methane in Underground Coal Gasification

Cliff Mallett, Jianmin Zhang, CUMT International UCG Research Centre, PR CHINA.

This presentation examines the impact of coal seam gas at the UCG Pilot conducted at Bloodwood Creek in Australia. The UCG Pilot was conducted in a coal seam around 13m thick at a depth of 200m and produced syngas 2008-2012. The pressure in the underground UCG gasification chamber was 1200kPa or higher, apart from some short periods. The seam contains coal seam methane at around 2-3m3 /t and the UCG site is surrounded by an extensive CSG field.

During UCG syngas production the coal seam gas was of little significance to operations. The only coal seam gas incorporated into the UCG process, is that in the coal that is gasified. Methane was not released from surrounding coal as the gasification chamber pressure was generally above that required for the desorption of coal seam gas. A tonne of coal at the Bloodwood Ck UCG site produced syngas containing 17GJ of energy, which includes 0.09GJ from 2.5 Sm3 of methane.

During syngas production there were short intervals when pressure in the production well was reduced. When it fell below 750kPa there was an increase in methane concentration in the syngas which disappeared when pressure was increased to 800kPa, indicating the trigger point for significant methane desorption from the surrounding coal.

During the decommissioning phase of UCG, coal seam gas plays a more significant role. When production ceases the pressure in the gasification chamber is dropped to atmospheric to encourage inflow of groundwater. This cools the cavity, and as water is converted to steam by the hot rocks and vented to flare on the surface, it strips the cavity of volatile organic contaminants. The pressure drop also stimulates the desorption of methane from surrounding coal as the pressure falls. At the UCG Pilot, within a week after decommissioning coal seam gas methane comprised 75% of the gas in the cavity, and was at 98% after two months. This effectively inertises the hot cavity and ensures no ongoing gasification or combustion of the coal.

As the inflow of water into the depressurised cavity proceeds, it creates a significant drawdown in groundwater pressure around the cavity. As this extends, the area of coal capable of desorbing methane increases. The desorbed methane flows at speed through the fractures in the coal, and sweeps water towards the low pressure cavity. This results in a loss of the standing water level in water monitoring wells in the area where the methane is rapidly desorbing. Water samples cannot be obtained in the vicinity of the cavity until groundwater pressure is restored, methane desorption is suppressed and the cavity fills with water.

Although not an issue at the Bloodwood Ck UCG Pilot, it is noted that coal seam methane and syngas have been associated with underground explosions where gas compositions have not been controlled during ignitions. These events can damage the integrity of the UCG panel wells and wellhead facilities.

SESSION 30
COAL SCIENCE - 5

30.1- Correction Method of Mercury Intrusion Test Result on Coals

Dangyu Song, Henan Polytechnic University, PR CHINA.

The pores and fissure in coal are the effective space for the absorption and migration of coalbed methane (CBM), so determination the volume, surface, and structure of pore is important work in coal reservoir evaluation. Mercury intrusion Porosimetry (MIP) is one of the most effective methods for pore analysis of porous materials. Many researchers determined the pore volume, specific area, and their pore size distribution in coal with MIP. However, due to the obvious compressibility of the coal matrix and the influence of interparticle void effect, the MIP results of coal tend to have large deviation. Some researchers had proposed a correction method on MIP result of coal, but this correction method is very complicated, and need some parameters determined by CO2 and N2 adsorption/desorption test. In this paper, we established a simple method to correct the MIP data of coal, and also discussed the effect of sample size and pore shape on the results of MIP data analysis. The main understanding and conclusions are as follows.

1. A correction formula for mercury intrusion data is proposed, based on the compressibility of pores and coal matrix in mercury intrusion process

$$V_{\mathrm{pore}}(P_i) = V_{\mathrm{Hg}}(P_i) - \frac{V_{\mathrm{a}} - V_{\mathrm{Hg}}(P_{i-1})}{V_{\mathrm{a}}} \times \frac{\mathrm{d}V}{\mathrm{d}P} \times P_i$$

where Vpore (Pi) is the accumulate pore volume under pressure Pi, ml/g; VHg(Pi) is the accumulate mercury intrusion volume under pressure Pi, ml/g; Va is the coal matrix volume of unit mass, ml/g; VHg(Pi-1) is the accumulate mercury intrusion volume under pressure Pi-1, ml/g; dV/dP is the compressibility of coal matrix, ml/MPa; Pi is the mercury intrusion pressure. The MIP data of four coals with different rank were corrected using above formula, the corrected results are shown in right figure. Comparing the calibration results with Li's results (1999), it was found that they were basically the same. From the right figure, we can find that when the pressure exceeds 10

MPa, the pore volume deviation caused by the matrix compress effect is gradually obvious. When the pressure reaches 200 MPa, the pore volume deviation can account for 30%-60% of the total pore volume.
2. The shape of pores in coal also has great impact on mercury intrusion test results. In calculation model of national standards for mercury porosimetry, it is assumed that the pores in the porous media are cylindrical. we analyzed the development and structural characteristics of pores in four coal samples, by observing more than 3,000 argon polished SEM images magnified hundreds to tens of thousands of times. We found that although there are vast of pores developed in coal, most of them are closed pores, and the connected pores in the coal matrix are mainly fissures and micro-cracks. Therefore, in the analysis of mercury intrusion data, the relationship between the pressure and the pore diameter should be based on the plate pore model rather than the cylindrical pore model.
3. When the coal particle size is too small, the inherent fissures in the coal matrix will be destroyed during the sample crushing, and the pore volume will be reduced, while the interparticle void effect will increase the pore volume in low pressure regime. Comparing mercury intrusion curves of 200 mesh, 60-80 mesh, 3-6 mm, and 10 mm coal particles, we found that the mercury injection curve of the 3-6 mm sample can not only overcome the interparticle void effect, but also can effectively reflect the development of fissures in the coal samples.

30.2- Study on Surface Structure and Drying Characteristics of Semi-Coke

Shiyong Zhao, Xiao Liang, Shaopeng Gao, Shuzhan Lv, Xi'an University of Science and Technology, PR CHINA.

In the industrial productive process of semi-coke, the moisture of the semi-coke after industrial coke quenching is generally at the range of 20% to 25%, which not only produces the transportation burden, but also limits the application of the semi-coke. Scanning electron microscopy (SEM), N2 adsorption-desorption and X-ray photoelectron spectroscopy (XPS) analysis were used to study the surface structure of Shenmu semi-coke, and the drying and dehydration of semi-coke (medium grain, small-sized grain and fine grain) was studied by air-blast drying. The dehydration rate of three kinds of semi-coke at different drying temperature and time was discussed. The results show that the pores of the semi-coke are developed, but the oxygen functional groups of the semi-coke are obviously reduced compared with the raw coal, and the moisture of the semi-coke is mostly physically adsorbed in the pores, and the moisture can be evaporated fully by air-blast drying. What's more, the higher the drying temperature, the faster the moisture loss of the same size semi-coke, and the shorter the drying time. When drying temperature is less than 200℃, the dehydration rate is fine grain > small-sized grain > medium grain. When drying temperature is 250℃, the dehydration rate is fine grain > medium grain > small-sized grain, and when temperature is more than 300℃, the dehydration rate of the three kinds of semi-coke is close, and the total drying time is 50min. Considering the issue of heat efficiency, the drying temperature should be 200℃~250℃. After drying, the semi-coke will reabsorb about 1.0%~ 1.6% of water. And finally, the whole moisture content will be controlled at about 2.0%.

30.3- The Effects of Supercritical CO_2 on Pore Structure in High-rank Coal

Shiqi Liu, China University of Mining and Technology and CUMT National University Science Park; Shuxun Sang, China University of Mining and Technology; Tian Wang, Yi Du, Huihuang Fang, China University of Mining and Technology and CUMT National University Science Park; PR CHINA.

The effects of supercritical CO2 (scCO2) on coal pores play a critical role in CO2 geological storage-enhanced coalbed methane recovery (CO2-ECBM). To investigate the effects of scCO2 on the pore structure in high-rank coals, CO2 sequestration processes were replicated using a scCO2 geochemical reactor. Two coal samples were exposed to scCO2 and water for 240 h under 45 °C and 10 MPa. Mercury intrusion porosimetry, nitrogen adsorption tests, and CO2 adsorption tests were used to identify the pore volume (PV), pore specific surface area (SSA), and pore size distribution (PSD) of the coal samples before and after scCO2-H2O treatment. The increase in the macropore volume caused by the scCO2 is mainly controlled by the pores 1-30 μm in diameter, resulted from the dissolution of carbonate minerals with large grain size in organic matter. The high-rank coal is more significant for macropore volume than SSA. The changes in the mesopore volume in the high-rank coal are caused by changes in the pores <20 nm; additionally, many pores <3 nm are generated by the scCO2, due to the formation of dissolution-created pores in minerals and reactions between scCO2 and organic groups. The SSA of the mesopores increased at a faster rate than macropore. The changes in the micropore volume and SSA in the high-rank coal are caused by changes in the pores >0.5 nm; additionally, volume and SSA of micropore <0.5 nm decreased by the scCO2, resulted from the increase in the interlayer spacing of aromatic layers in high-rank coal.

30.4- Impact of Interaction between Coals on Coking Property of Blends

Haili Jiao, Meijun Wang, Jiao Kong, Jiang Guo, Dong Yan, Liping Chang, Professor, Taiyuan University of Technology, PR CHINA.

The inferior coking coals as feedstocks for the preparation of char used for fixed bed gasification is an effective way to realize the utilization of excess coking capacity and the lower rank coal. Coking property is important to the properties and structures of the resultant char, which is affected by the interactions between the component coals in blends. In this study three different coals were selected to investigate the effect of interaction on the coking property of the blends. The coking property is evaluated by the GR.I. The interaction is obtained by the degree of GR.I of the blend respectively greater or less than expected if the coals had acted independently. The results indicate that the most examined blends showed both significant positive and negative interactions, and the interaction between coals varies with the content and type of the components in blends. The interaction between coals is mediated by interchange of volatile matter, the physical adsorption and the superposition of plastic temperature interval. Besides, the interaction between coals is also affected by the chemical composition and structure of the blends such as O/C and H/C. The study is of great significance for the blending coking that use blends of inferior coking coal as feedstock.

30.5- Study on Ash Fusion Behaviors and Physico-Chemical Characteristics of Semi-coke and its Blended Fuel with Coal

Maobo Yuan, Chang'an Wang, Pengqian Wang, Zichen Tao, Yongbo Du, Defu Che, Xi'an Jiaotong University, PR CHINA.

With the rapid development of coal chemical industry in China, a large number of low-volatile carbon-based fuels such as semi-coke are in urgent need of combustion and utilization, and the co-combustion with high-volatile coal shows the potential to realize the large-scale utilization of semi-coke in coal-fired power plant. Because the blending coal can hardly match the design coal, it is easy to aggravate the degree of deposition and slagging on the heating surface and affect the operation of the boiler. However, the melting behavior of ash produced by blended coal with semi-coke combustion needs further study. In this paper, the ash melting behavior and physico-chemical characteristics of semi-coke and its blended fuel with coal were experimentally studied. Firstly, the relation of ash composition and ash melting behavior was observed by comparing the ash composition and ash fusion point of semi-coke and raw coal. Secondly, the influence of blending ratio and blending mode on the ash melting behavior of semi-coke blended fuel was studied by micro-computer ash melting point meter. Finally, the microstructure and physico-chemical properties of the melted ash at the softening temperature were evaluated by scanning electron microscope (SEM) technique with X-ray spectrometer (EDS) and X-ray diffractometer (XRD) technique. The experimental results showed that the mineral composition and oxide content in the semi-coke were different from the raw coal, which led to the change of coal ash fusibility. Meanwhile, the ash fusion point of semi-coke blended fuel could not be expressed linearly by the ash fusion point of its raw coal, and the influence of blending mode including in-furnace blending and out-furnace blending on the ash fusion point could be neglected. While the microstructure and physico-chemical properties were affected by the blending mode. Compared to the in-furnace blending, the carbon content was lower in out-furnace blending. Furthermore, the blending mode had a significant influence to the mineral composition.

SESSION 31
CARBON MANAGEMENT - 3

31.1- Enhanced CO_2 Sorption Performance of $CaO/Ca_3A_{l2}O_6$ Sorbent with Steam Addition

Qing Li, Jieying Jing, Xuewei Zhang, Zehua Wei, Wenying Li, Taiyuan University of Technology, PR CHINA.

CO2 enhanced sorption methane steam reforming (SESMR) for hydrogen production is a potential approach to economically provide hydrogen and to reduce CO2 emission. The key point for this process is to develop a kind of proper CO2 sorbents with high adsorptive capacity. CaO/Ca3Al2O6 sorbents have been proved to be a promising sorbent for CO2 sorption in our previous investigation. However, the sorbents still suffer from low CO2 sorption capacity. There have reported that the presence of steam during carbonation would influence the CO2 capture performance. Considering the abundant existing steam in real SESMR process, it is necessary to understand its effect on the CO2 sorption performance of the home-made CaO/Ca3Al2O6 sorbents. In this work, the effect of steam addition during carbonation were investigated over CaO/Ca3Al2O6 sorbents in a thermogravimetric analyzer and a fixed bed reactor system. Various concentrations of steam up to 10 vol% were provided during carbonation process. Results showed that superior CO2 sorption capacity could be achieved as the steam

concentration increased, which was derived from the increased surface area and pore volume. the sorbent reactivity was significantly increased for all concentrations of steam injected during carbonation step. The presence of 10vol% steam increased the CO2 capture capacity by 37%. The steam promotion mechanism in the carbonation process was ascribed to the production/transient of $Ca(OH)_2$ and the improvement of CO2 molecular diffusion

31.2- Molecular Basket Sorbents for CO_2 and NO_x/SO_x Capture from Flue Gas of Power Plants and CO_2 Utilization for Fuels and Chemicals

Chunshan Song, Pennsylvania State University, USA and Dalian University of Technology, PR CHINA; Xinwen Guo, Dalian University of Technology, PR CHINA; Xiaoxing Wang, Pennsylvania State University, USA.

Carbon dioxide (CO2) management is at the center of contemporary global technical and political discussions on global energy challenges and the use of energy resources including coal, oil and gas. There are also ongoing efforts to turn renewable energy sources such as biomass and solar energy into carbon-based chemicals, fuels, and materials. These carbon-based energy resources are projected to be dominant in our primary energy portfolio in the 21st century. Thus carbon dioxide (CO2) has become a plentiful source of carbon, and CO2 capture has been an active focus area of separation process and engineering research [1]. CO2 can be captured from industrial flue gases using more energy efficient processes recently developed. One of the new processes for CO2 capture is based on solid "Molecular Basket" sorbent (MBS) being developed at Penn State [1]. MBS consists of functional polymers and nano-porous materials. There are long-term merits in using CO2 as a feed for chemicals and materials and as a carrier for energy. Capturing CO2 and converting it into chemicals, fuels, and materials using renewable energy, is an important path for sustainable development and a major challenge in 21st century [1,2]. The captured or concentrated CO2 can be used for catalytic conversion for manufacturing chemicals (lower olefins such as ethylene and propylene, methanol, and carbonates), clean fuels (such as transportation fuels or synthetic natural gas), organic and inorganic materials. New bimetallic catalysts have been shown in our recent research to be active and selective for CO2 conversion to C2-C4 olefins and C5+ higher hydrocarbons [2,3]. Effective use of catalysis and adsorption over nano-porous materials can decouple the traditional link between energy utilization and negative environmental impacts. Recent research at Penn State University and at Dalian University of Technology (in conjunction with the PSU-DUT Joint Center for Energy Research) on novel bimetallic catalysts will be discussed as examples to show the technical feasibility.

31.3- High Efficiency Injection Technology in Deep Anthracite During CO_2-ECBM Process

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This work is based on self-designed CO2-ECBM experimental simulation system and the northern Shizhuan CO2-ECBM demonstration projects in the Southern Qinshui basin. This experimental simulation system has a function for simulating the continuous geologic process of CO2 injection, adsorption-desorption replacement, diffusion-seepage displacement and CH4 production under the conditions of reservoir temperature, pressure, moisture and stress. The northern Shizhuan CO2-ECBM demonstration projects, which contain three CO2 injection wells and seven CBM production wells, were carried out for four years and 4491 t CO2 were injected. According to the data obtained by above experimental simulation and demonstration projects, we concluded a high efficiency injection technology as an example of deep anthracite in Qinshui basin and optimized injection parameters using self-developed numeral simulation software, COMET3, SIMEDWin Ⅱ and other commercial software. Firstly, by controlling CO2 injection rate and pressure to maintain CO2 injectivity, we hold a constraint on the increase and rate of coal swell and its derived stress field variation near injection well, further resulting in a controllability of permeability attenuation. The liquid CO2 injection rate was 5-10 t/h and the maximum pressure was 15-18 MPa. Then, the intermittent CO2 injection procedure was adopted, resulting in some recovery and adjustment for coal swell and its derived stress field variation near injection well. Of those different injection procedures with 45, 90 and 180 days injection-interval period, the injection procedure of 90 days performed a best comprehensive effectiveness. For a long-term broken down and a better injectivity, some N2 deserved to be injected for weakening coal swell and stress field variation derived from CO2 injection and adsorption and therefore the permeability can recover to a certain extent. The experimental results indicated that the permeability of coals can be improved by dozens to hundreds of times and approached to 90% of the original permeability as N2 replaces CO2.

31.4- Enhanced CO_2 Photocatalytic Reduction through Simultaneously Accelerated H2 Evolution and CO_2 Hydrogenation in a Twin Photoreactor

Zhuo Xiong, Yongchun Zhao, Junying Zhang, Huazhong University of Science & Technology, PR CHINA.

The photocatalytic reduction of CO2 utilizes solar energy to mitigate CO2 emissions and is a promising technology for renewable fuel production. In this study, a novel twin reactor was developed to hydrogenate CO2 into hydrocarbons by using H2 directly produced from photocatalytic water splitting. The twin reactor was further modified to simultaneously perform the CO2 hydrogenation and water splitting reactions in the gas and liquid phases, respectively. Moreover, two photocatalysts, Pt/TiO2 and Cu/TiO2, were used to improve the photo-hydrogenation performance in the reactor. The results indicate that the H2 produced from water splitting effectively enhanced the CO2 hydrogenation in the gas phase, and we found that the highest CO2 reduction activity was achieved by using Pt/TiO2 and Cu/TiO2 as the H2-generating and CO2 hydrogenation photocatalysts, respectively, which promoted H2 evolution and CO2 hydrogenation and resulted in enhanced CO2 photoreduction.

31.5- Preparation and Photocatalytic Properties of Bracts Like Ti/Li/Al-LDHs Using Chitosan Guiding Agent

Xiao-ling Zhao, An-ning Zhou, Jia-xin Wang, Dong-qiang Lei, Yi-fan Dong, Xi'an University of Science and Technology; Wen-Ying Li, Taiyuan University of Technology; Ya-gang Zhang, Xi'an University of Science and Technology; PR CHINA.

Ti/Li/Al-LDHs is a kind of hydrotalcite-like compounds with CO2 photocatalytic performance. This paper carries out a new preparation method of bracts like Ti/Li/Al-LDHs using chitosan as guiding agent and urea as precipitant in hydrothermal synthesis. The growth trend of Ti/Li/Al-LDHs crystal was controlled by the complex adsorption of chitosan and Ti4+.The results show that the morphology of Ti/Li/Al-LDHs is in the shape of bract, and has bigger pore volume and pore size. The addition of chitosan and urea and the ratio of metal ions can affect the crystal morphology and UV absorbance. However, the UV absorbance of Ti1Li3Al2-LDHs and Ti1Li3Al4-LDHs is not significant. The reaction products of photo-catalytic reduction of CO2over Ti/Li/Al-LDHs are mainly CO and CH4. The bracts like Ti/Li/Al-LDHs has higher catalytic activity due to its highly ordered bract like structure, which provides more active surfaces. The photocatalytic efficiency of bracts like Ti1Li3Al4-LDHs is better than that of bracts like Ti1Li3Al2-LDHs.

SESSION 32
CLEAN COAL AND GAS TO FUELS – 1

32.1- Study on the Coating Internal Filtration Technology for Slurry Bed Fischer-Tropsch Reactor

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In this paper, we describe efforts to develop fouling-resistant coatings for filters used in slurry-bed Fischer-Tropsch (FT) reactors. We begin with laboratory experiments using a low surface energy polymer coating on sintered stainless steel filter supports. The supports were coated using a two-step process. First, a polymer primer layer was deposited to ensure good adhesion between the substrate and functional layer. This was followed by a finishing coat to tune the surface properties and minimize adhesion of catalyst particles. The coats were applied by sequentially infiltrating a polymer emulsion under vacuum, followed by sintering. The thickness of the coating can be adjusted using the emulsion concentration, coating conditions, or the number of coating layers. The porous filters were sintered at 150-180℃ for 10 min for the primer, and 380-390℃ for 10 min for the finish. Pore size analysis and flux measurements showed reductions in pore size and apparent changes in the flow regime. Simple CFD calculations were performed to estimate the potential benefits of the coating under field conditions.

32.2- A Single-phase Study on the Turbulence Models of Cyclonic-static Micro-bubble Flotation Column by CFD and PIV

Shiqi Meng, Xiaokang Yan, China University of Mining and Technology, PR CHINA.

Cyclonic-static micro-bubble flotation column (FCSMC) is one of the most important development in column flotation technology in recent years, especially for the separation of fine particles. FCSMC integrates several different flow regimes into one cylinder, so its internal flow field has an essential influence on flotation performance. PIV and CFD are often used in the flow field research. However, in the research on FCSMC, the PIV

test is incomplete and the numerical simulation of turbulence model is controversial as well. Therefore, in this paper, the single-phase swirl field in the FCSMC are measured by PIV and the common turbulence models are used to perform numerical simulation. According to the PIV test results, the RSM model can accurately predict the distribution of water velocity in the single-phase swirl field of a flotation column. Both Standard k-ε model and RNG k-ε model can predict the tangential velocity and the trend of radial velocity, but the error is unsatisfactory while predicting radial velocity. The distribution of axial velocity calculated by the two models is inconsistent with the results of PIV, so they can't predict axial velocity. Realizable k-ε model can predict the axial velocity, radial velocity and tangential velocity in the single-phase swirl field of a floatation column. But the predicted results of axial velocity and radial velocity are greatly biased, and only the prediction of tangential velocity is reliable.

32.3- Low Temperature Synthesis of Ni_2P/Al_2O_3 Catalysts for Naphthalene Hydrogenation

ZhiQiang Qie, Jieying Jing, Zhifen Yang, Ziyi Zhang, Wenying Li, Taiyuan University of Technology, PR CHINA.

The hydroaromatics and cycloalkanes obtained by hydrogenation of aromatics are ideal components for high performance aviation jet fuel. The key point for this process is to develop a kind of efficient catalyst for enhancing the reaction activity and selectivity. In this work, a series of Ni2P/Al2O3 catalysts were synthesized at low reduction temperature with nickel acetate as nickel source and ammonium hypophosphite as phosphorous source. The effect of reduction temperature on the formation of active phase Ni2P and the performance of the catalyst naphthalene hydrogenation was investigated. Results showed that the nickel acetate affected the reduction of ammonium hypophosphite. The pure phase of Ni2P was generated between 300-500°C, and the particle size increased with the increasing temperature. Its catalytic performance was evaluated with naphthalene as a model compound in a fixed-bed reactor at 300 °C, 4Mpa. Catalytic evaluation showed that the Ni2P/Al2O3 prepared at 400°C possessed the highest hydrogenation saturation activity, which was ascribed to the small particles of Ni2P and suitable acidity.

32.4- Integrated Process of Coal Pyrolysis and Steam Reforming of Methanol over Ni Based Catalysts

Xin-Fu He, Xiao-Qin Zhang, Jun Zhou, Hong-Ju Wu, An-ning Zhou, Xi'an University of Science and Technology, PR CHINA.

Coal pyrolysis for tar production is one of the most important utilization technologies of low rank coal. However, the existing pyrolysis technologies have the problems of low tar yield and high content of heavy components in tar. In this study, the integrated process of coal pyrolysis (IPCP) and steam reforming of methanol (SRM) for improving tar yield was put forward. The effects of different catalysts (Z111, Z205 and FFT-1B) and pyrolysis temperature were investigated, and the optimal process parameters were obtained. The results show that IPCPSRM process can significantly improve the tar yield. The highest tar yield of 16.1% can be achieved under Z111 catalyst, at 550 oC, water methanol mole ratio of 1.2 and total flow rate of 300 mL/min, and under this condition, the light fractions (benzenes, phenols) of tar have the highest relative content. Tar yield and the relative content of the main components of tar increase first and then decrease, having a maximum value at 550 oC in the integrated process under Z111 as the temperature increases.

32.5- Hydrodeoxygenation of Dibenzofuran over Ni/ordered Mesoporous SiO_2-Al_2O_3 Catalysts

Ru Wang, Zhen-yi Du, Hua-wei Peng, Jie Feng, Wen-ying Li, Taiyuan University of Technology, PR CHINA.

This work has been undertaken with the aim of designing promising noble-metal-free catalysts for efficient hydrodeoxygenation (HDO) of dibenzofuran (DBF) into fuel grade hydrocarbons. For this, Ni/ordered mesoporous SiO2-Al2O3 catalysts were synthesized and their catalytic performance was tested for HDO of DBF in a batch reactor at 280 oC , 6.5 MPa for 9 h. The catalysts were systematically characterized using XRD, N2-adsorption desorption, H2-TPR, NH3-TPD, and Pyridine-IR techniques. Firstly, Ni was loaded onto ordered mesoporous alumina (OMA), SBA-15 and γ–Al2O3 as the supports. By comparing the catalytic performance, the role of the pore structure and Lewis acid were elucidated. Our results indicated that hydrodeoxygenation of dibenzofuran with only the hydrogenation (HYD) reaction route was present on three catalysts. Ni supported on OMA showed better performance in the reaction than Ni/SBA-15 and Ni/γ–Al2O3. The excellent catalytic performance was attributed to the combination of Lewis acid and mesoporous structure in OMA. Lewis acid can promote the breakage of C-O bond and mesoporous structure was conducive to the mass transfer of reactants. Secondly, the effect of Brønsted acid by silica doping (10 wt%, 20 wt%, 30 wt%) in the synthesis of ordered mesoporous alumina was investigated. The silica doping not only regulated the support acidity, but also changed the pore structure and surface area of support. A significant observation noticed in this study is that the incorporation of SiO2 into Ni/OMA results in an outstanding improvement in the yield of the bicyclohexane product. Among the catalysts tested, the Ni/20 wt%SiO2-Al2O3 catalyst showed the highest efficiency, with superior yield of 84.5% for bicyclohexane and 98.2% conversion of dibenzofuran. However, excessive silica (30 wt%) doping proved to be detrimental to the catalytic activity, since the blockage of support and decrease of metal dispersion. The obtained structure-activity results reveal the concentration of Brønsted acidic sites had a significant effect on the yield of the desired products.

SESSION 33
COAL BED AND SHALE GAS - 3

33.1- Origin of High and Variable Heavy Hydrocarbon Gases of Coal in Enhong Syncline of Yunnan Province in China

Fengjuan Lan, China University of Mining & Technology, PR CHINA.

Coalbed gases in Enhong syncline are characterized by high concentration of heavy hydrocarbon gases (C2+). The C2+ distribute variably in Enhong syncline, which can be divided in to "dry gas area" and "wet gas area". In the "wet gas areas", the concentrations of heavy hydrocarbon gases are between 2.9 and 36.98%, which are nearly zero in the "dry gas area". Pyrolysis simulation experiments (Py-Gc) with coal samples in Enhong syncline are carried out to prove that the coals can product lots of h eavy hydrocarbon gases. Lots of oil and bitumen produced in the coal maturation process are found through the coal maceral and calcite thin section observation. Barkinite are supposed as the material basis of lots of heavy hydrocarbon gases production in this place because the process of barkinite changing into oil and bitumen are observed under the microscope. But the C2+ distribute variably in the place with different origin of thermogenic gas in the "wet gas area" and biogenic gas in the "dry gas area". The different gas characteristic may be related to the different preservation condition such as coal pore structure. Coals in the "wet gas area" have more pore specific surface area and micropore, but less macropore. Under the effect of both parent material and pore structure, high and variable concentrations of heavy hydrocarbons are existed in Enhong syncline.

33.2- Characterization of Multi-Scale Microfractures of Coals Related to Coal Rank

Xinghua Shi, Jienan Pan, Henan Polytechnic University, PR CHINA.

Microfractures in coal seams are the key factor in the context of enhanced coalbed methane (ECBM) recovery as they determine permeability and productivity. Although significant progress has been made in the study of cleats in coals, the detailed structural and fractal characteristics of microfractures of different rank coals (especially high-rank coals in China) are poorly understood. This study aims to analyze the characteristics of microfractures combined with X-ray micro-computed tomography (X-ray μCT), nano-CT, and fractal theory, to reveal the effects of coal rank on the microfracture structures, and to discuss the relationship between fractal dimensions and permeability. The results show that for the experimental coals, micron-scale fractures are dominated by type B microfractures, followed by type A microfractures, while the nanoscale fractures are dominated by type D microfractures but lack of type C microfractures. Additionally, coal rank has significant effect on microfracture structures. The microfracture network in low-rank coals is usually well-connective, whereas the connectivity and scale of the microfracture network reduces with increasing coal rank. The average microfracture length, width and volume reduces but quantity increases as coal rank increases, and these downward trends can be divided into three stages: rapid decline stage (0.59% < Ro, ran < 1.25%), slow decline stage (1.25% < Ro, ran < 2.25%), and stable stage (Ro, ran > 2.25%). The average aperture first decreases but then slightly increases with coalification. Furthermore, the fractal dimension (D) of these microfractures increases as coal rank increases in the range of 1.64–1.78, indicating that the microfracture structure gets more complicated with coalification. Connectivity analysis interprets a highly connected pore network resolved by nano-CT with a total 4945 pore bodies, 7194 pore throats and a connected porosity of 1.96%. The CT porosity displays a 'U-shaped' trend as the fractal dimension increases: first decreases from 2.12% to 0.94% and then increases from 0.94% to 1.49% (turning point at D=1.72). These Chinese coal samples have very low to medium permeability, with highly variable values ranging from 0.004 to 1.465 mD. A negative correlation between permeability and fractal dimension was found and such a relationship is especially apparent for coals with higher ranks. Fractal dimension plays a significant role in assessing the exploitation potential of a coal seam, and coals with higher fractal dimensions are not favorable for CBM exploitation. This investigation not only assists in understanding the mechanism of CBM migration, but also provides certain guidance for the improvement of CBM production.

33.3- The Applicability Analysis of Determination Model in Nanometer Pore Using Low Pressure CO_2 and N_2 Adsorption in Coal

Yunbo Li, Dangyu Song, Henan Polytechnic University, PR CHINA.

The characteristic of nanopore (pore size less than 200 nm) distribution in coal is a key factor affecting the occurrence and migration of coalbed methane (CBM). The appropriate determination method and calculation model are the basis for accurating pores. Based on the CO2 (at 273K) and N2 (at 77K) gas adsorption experiments of four different metamorphic coals, Our forced on the adaptability of different models (such as the Langmuir, D-R, D-A, BET and NLDFT model) to accurately describe the gas adsorption processes and pore distribution (PSD), and then the optimal model was obtained; finally, the Beiloutian coal was selected as an example to analyze the development characteristics of NPSD. The results showed that: (1) the Langmuir model is only suitable for the gas adsorption at low relative pressure condition (P/P0<0.01), and the error value increases with the relative adsorption pressure rising; the D-R and D-A model have the approximate results at low CO2 relative pressure condition (P/P0<0.01), and D-A model has more accurate fitting results; The BET model is only accurate when the relative adsorption pressure is 0.05<P/P0<0.35 by N2 adsorption; the data also showed that the NLDFT model can keep the higher fitting accuracy by CO2 and N2 adsorption processes at the relative adsorption pressure from 0.001 to 0.9996; (2) The specific surface area (SSA) and pore volume of micropores were obtained using CO2 adsorption by Langmuir, D-R, D-A, and NLDFT model, and the SSA and pore volume in the range of 66.9570-248.6736 m2/g and 0.0201-0.0997 cm3/g, respectively; the meso- and macropore SSA and pore volume of N2 adsorption were 0.0007-2.3398 m2/g and 0.0036-0.04 cm3/g calculated by BET and NLDFT model. Our results also showed that the fitting accuracy were in descending order of D-R, D-A, Langmuir and NLDFT models; (3) In combination with the applicable range of the model, CO2 adsorption and NLDFT model are recommended for micropore to analyze the coal pore sizes of 0.36-1.1 nm, and NPSD of pore size from 1.1-200 nm can be obtained by N2 adsorption combined with NLDFT model; (4) The characteristics of pore development in Beiloutian coal were analyzed using CO2 and N2 adsorption combined with NLDFT model. It was found that pore volume and SSA less than 1 nm accounted for 88.82% and 98.05% of the total pore volume and the total SSA, indicating that the micropores in coal are the main space for coalbed methane storage and are key physical factors for the occurrence and migration of coalbed methane. The conclusion of the article will provide a basis for the accurate calculation of nanopores in coal.

33.4- Prediction and Validation of Organic Carbon Content in Shale Reserves Based on Back Propogation Neural Network

Zhen Zhang, Shuheng Tang, Songhang Zhang, Zhaodong Xi, China University of Geosciences (Beijing), PR CHINA.

Many factors should be considered in the process of shale gas exploration and development. The TOC content is one of the important parameters of the geological conditions for the accumulation of hydrocarbons. The accurate control of its numerical values is of paramount importance. This article takes the Lower Cambrian Niutitang Formation in Fenggang area of the Northern Guizhou Province as the research object. Through observing the correlation coefficient between TOC content and each logging parameter the natural gamma, bulk density and natural potential, photoelectric cross-sectional index and five log curves of lateral resistivity are preferably chose as the basic eigenvector which is used as training, test and prediction data with the measured results of the organic carbon content of the samples. From that, a back propogation neural network prediction model is established, and the analysis results are compared and analyzed with classical △lgR method, conventional well-logging curve (uranium curve and volume density curve) fitting and the kerogen content prediction of TOC. The results show that the back propogation neural network model has a very small deviation between the predicted and measured results. After removing the only outliers, the average absolute error is 0.09, and the average relative error is 5.4%. It is superior to other methods in terms of the error. Besides, it also has the characteristics of quickness and wide application.

SESSION 34
VALUE-ADDED PRODUCTS FROM COAL - 6

34.1- Study on Adsorption Properties of HZSM-5 Modified by Chemical Liquid Phase Deposition in Separating of M-Cresol and P-Cresol

Meng-yao Li, Yi Luo, Wen-jun Fan, Jie Feng, Wen-ying Li, Taiyuan University of Technology, PR CHINA.

Cresols (o-cresol, m-cresol and p-cresol) from coal liquid or coal tar are traditional chemical products whose prices depend on their purity. However, the sepeartion of cresol monomer is still a hard work, for their close boiling points and similar polarities. This study is about the modification of HZSM-5, which is expected to separate p-cresol from m-cresol as an adsorbent. We choose a mixture of m-cresol-cresol and tetramethyl orthosilicate as adsorbate, which pass through static adsorption, and then is detected by gas chromatography. The results show that: the orifice size is closely related to the deposition agent's amount, reaction time, and Si/Al ratio. When the addition amount of tetramethyl orthosilicate is 200μL, the total adsorption capacity is 0.04 g/g and the selectivity was 90%.

34.2- Preparation and Capacitive Properties of Carbon Materials from Direct Coal Liquefaction Residue and Phenolic Resin

Jiangtao Cai, Yating Zhang, Guoyang Liu, Anning Zhou, Xi'an University of Science and Technology; Jieshan Qiu, Beijing University of Chemical Technology and Dalian University of Technology; PR CHINA.

Effectively utilizing direct coal liquefaction residue (about 20-30wt. % of the raw coal) for preparing high performance advanced carbon materials with low cost has important scientific significance. The ordered mesoporous carbons (OMCs) were prepared by using the mixture of asphaltene extracted from coal liquefaction residue and phenol-formaldehyde resin (PF) as carbon precursors, SBA-15 as template. The microstructures of the as-made OMCs were studied by X-ray diffraction, field emission scanning electron microscopy, and N2 adsorption techniques. Electrochemical workstation was used to analyze the electrochemical characteristics of the OMCs. The as-made OMCs also have high specific surface areas (627-742 m2/g) and pore volumes of 0.50-0.63 cm3/g respectively. The electrochemical characteristics of the capacitors from the OMCs were studied with 6mol/L KOH as electrolyte in three-electrode system. It has been found that the specific capacitance of the OMCs can reach above 248 F/g at the current intensity of 1A/g, and a long cycling durability with a capacitance retention over 95.4 % after 1000 cycles at the current intensity of 2A/g.

34.3- Study on Competition Relationship and Influencing Factors of Cresol - Butylated Products

Yi Luo, Meng-yao Li, Wen-jun Fan, Jie Feng, Wen-ying Li, Taiyuan University of Technology, PR CHINA.

2,6-di-tert-butyl p-cresol (BHT) is a popular antioxidant from p-cresol, and m-cresol is an important organic chemical intermediate. Both of them can be produced from coal tar, while p-cresol can be separeted hardly from m-cresol for their close boiling points. Traditionly, they are converted into tert-butyl derivatives, and then are separated by their larger boiling points'difference. In our study, p-cresol and m-cresol mixture are expected to be converted into only 6- tert-butyl-m-cresol and BHT. The realtionships of cresol's structure and their tert-butyl substitution shows that the solubility and acid concentration are the key factor in the tert-butylation process. Under an optimal conditions, their yields are 94.79% BHT and 49.56% 4,6-di-tert-butyl-m-cresol (DMC).

34.4- Prediction of Metallurgical Coke Thermal Properties and Analysis of Influencing Factors

Shi-Zhuang Shi, Zhen Xu, Jin-Hui Zhou, Gong-Er Wang, Yong-Hui Luo, Yan-Gao Mao, Qi Zheng, Shuai Lu, Zhi-Long Lin, Wuhan University of Science and Technology, PR CHINA.

In order to predict, improve and regulate the thermal properties of metallurgical coke in accordance with the demands, and also to make clear the effect of various factors on the thermal properties, prediction models of coke thermal properties were proposed on the basis of analysis of influence rules of the various factors and by means of ninety six runs of test for sixteen blending schemes, using bulk density (d), coalification degree index (Vdaf), caking property indices (G and Y) and mineral catalytic index (MCI) as input variables. The models simultaneously concern the two kinds of coke making processes, i.e. coal top-charging and coal side-charging, reveal intrinsic rules of influencing coke thermal properties by various factors, determine the optimal value of various factors and the best attainable value of coke thermal properties. The models make prediction with higher accuracies, apply to wider areas, and could be used not only to the traditional coke making process but also to the tapping coke making process. The impact of various factors, ways to improve coke thermal properties and the method of high reactive coke development were also analyzed.

34.5- Effect of N- and O-compounds on the Performance of NiWCx Catalysts for Hydrogenation of Naphthalene

Haiyong Zhang, Ning Chang, Chenguang Jiang, Genwei Chen, Longyin Liu, China University of Mining & Technology (Beijing), PR CHINA

The aromatic components in the coal tar are catalytically hydrogenated to produce cycloalkanes and hydro-aromatics, which can be used to make high performance jet fuels. Among them, the stability of the catalyst is undoubtedly of concern. Several

Al2O3 supported NiW carbide catalysts modified with TiO2 or citric acid were prepared using incipient wetness impregnation method and temperature programmed carburization. These catalysts were characterized by XRD and evaluated on a fixed bed reactor for hydrogenation of naphthalene with quinoline and phenol in different concentrations. The hydrogenated products analyzed by GC-MS and GC indicate that quinolone is more poisonous than phenol at the same concentration. Grafting TiO2 on alumina reduces the effect of quinoline and the decalin selectivity is higher compared than alumina supported catalysts.

SESSION 35
GASIFICATION TECHNOLOGIES - 6

35.1- Characteristics of Coal Gasification Using Chemical-Looping with MoO_3 as Gaseous Oxygen Carrier

Jing-xian Kang, Qun Yi, Taiyuan University of Technology; Guo-qiang Wei, Chinese Academy of Sciences (CAS); Yi Huang, Wen-ying Li, Jie Feng, Taiyuan University of Technology; PR CHINA.

Conventional coal gasification techniques are often suffered with parasitic energy inefficiencies and additional capital expenses because either pure oxygen feed stocks or subsequent nitrogen separation are necessary, which also resulted in amount of indirect CO2 emissions. Chemical-looping gasification (CLG) of coal to yield syngas is a clean and effective coal gasification technology. In this study, a novel concept of coal gasification using chemical-looping technology with MoO3 as a gaseous oxygen carrier was proposed. Compared to the traditional gasification technology, this CLG process consists of fuel reaction and air reaction two steps, resulting in cascade release of chemical energy of coal thus effectively reducing the exergy loss in gasification, and also avoids air separation process. MoO3 was used as gaseous oxygen carrier due to its high oxygen carrying capacity and special physical properties. MoO3 is in the vapor phase at the temperature and pressure within the fuel reactor, but reduced form of MoO2 or Mo is solid under the same conditions. Thus, the metal oxide vapor and the coal react as in gas-solid reaction, thereby ensuring rapid kinetics and enhancing carbon conversion. The reduced carrier mixed with ash is transported to the air reactor where the carrier is re-oxidized. The solid materials are heated to produce the metal oxide vapors that subsequently fed back into the fuel reactor. The circulation of oxygen carrier MoO3 accelerated coal gasification reactions and eliminated barriers associated with ash-carrier separation. The energy saving benefits from improvement of gasification efficiency, avoidance of air separation process and high separation efficiency of ash-oxygen carrier in the new CLG of coal presents huge potential in large numbers of indirect CO2 emissions reduction compared to traditional coal gasification.
The thermodynamic analysis of the reaction between coal and molybdenum trioxide (MoO3) were investigated by ASPEN PLUS and HSC based on the Gibbs free energy minimization principle. The equilibrium composition of product gas under different reaction conditions was obtained. The Ellingham diagram was used to distinguish the oxidation ability of MoO3, and the result showed that MoO3 was suitable for chemical-looping gasification. The experimental study was carried out in a vertical fixed bed reactor with multi-zone heating. Effects of critical parameters (lattice oxygen equivalence ratio, feedstock to steam (F/S), gasification temperature and reaction time etc.) that have significant effects on gasification performance such as cold gas efficiency, carbon conversion, syngas yield and composition were performed. The above researches are benefit to acquire a suitable syngas for downstream production through source controlling of gasification process. Besides, the reactivity and physico-chemical properties of the MoO3 oxygen carrier particles after multi-cycle reactions were also investigated.

35.2- Char Conversion in a Drop Tube Reactor: Numerical Modeling and Detailed Validation

Andreas Richter, Fengbo An, Bernd Meyer, TU Bergakademie Freiberg, GERMANY.

The KIVAN reactor, operated at TU Bergakademie Freiberg, is a drop tube reactor for measuring reaction kinetics of carbonaceous feedstock under gasifying conditions. The operating pressure can reach 100 bar, the temperature is limited to 1400 K. Several sampling tubes in the reactor allows for measuring the temperature and the gas composition along the reactor. In comparison to measurement systems that provide only global char conversion data, the use of local distributions of temperature and composition allows for a more detailed validation of reaction models. In the present work, a CFD model of the KIVAN gasifier is applied to study the gas flow (e.g. gas velocity, temperature, composition) and the char conversion in detail. Based on the experimental results, the accuracy of different char conversion models is analyzed and compared. It can be shown that an advanced modeling of the intrinsic heterogeneous reactions together with an appropriate modeling of the changes in density and particle diameter is necessary for providing reliable results at different operating conditions.

35.3- Carbon Footprint of the Exergy UCG™ Technology: Unminable Coal to Products

Michael S. Blinderman, Ergo Exergy Technologies Inc.; Simon I. Maev, Cvictus Inc.; CANADA

Long-term viability and public acceptance of any fossil fuel based technology are in a large degree determined by its carbon footprint.
It has been widely claimed that Underground Coal Gasification (UCG) may be considered as a coal-based technology with a potential of significantly reducing GHG emissions and earning the status of a truly clean coal technology.
Carbon management methods conceived, developed and, in part, implemented in the Exergy UCG™ (εUCG™) technology include four specific in situ techniques, namely, CARBON RETENTION™, CARBON REFLUX™, CARBON QUENCHING™ and CARBON INTERMENT™. Applied together, they modify the well-established εUCG™ technology so that the combined carbon footprint of the εUCG™ process and the syngas-fed end-use plants is demonstrably lower than those of currently dominant industrial processes.
These novel carbon management techniques, based on a substantial body of experimental and modeling work, are presented here in terms of their conceptual design, impact on the plant carbon cycle, effect on overall energy and carbon efficiency of the process and the capital and operational cost of their implementation.
To illustrate the significance of carbon management, an example of the εUCG™ based commercial plant being developed in Alberta, Canada is treated in substantial technical, environmental and economic details.

35.4- Development of a New Dynamic Reduced Order Model for a Shell Coal Gasifier Integrating the Slag Flow Model

Mukyeong Kim, Insoo Ye, Geun Sohn, Changkook Ryu, Sungkyunkwan University; Bongkeun Kim, Doosan Heavy Industries & Construction; SOUTH KOREA.

Reduced order model (ROM) for entrained flow coal gasifier provides fast prediction of key operation characteristics which can be used to improve the design and operation of the process. It typically adopts one-dimensional approach for the gasifier in which the coal and gasifying agent are injected at the first control volume. However, such approach is not appropriate for Shell coal gasifier. It has a unique configuration of coal burners installed on the sidewall of the cylindrical reactor, which splits the coal and gas flows upward and downward on the burner level. The downward flow circulates the lower part of the gasifier and then moves upward along the wall. Coal particles are concentrated more on the downward stream by gravity, whereas the gas flows upward more due to the buoyancy induced by rapid temperature increase. Without considering this flow pattern, the conventional approach may lead to unrealistic prediction of temperature profile and slag thickness on the wall. In particular, the slag thickness at the slag tap is an important parameter for the gasifier operation, of which the calculation requires adequate prediction of gas temperature simultaneously.
In this study, a new gasifier ROM for dynamic simulation for Shell coal gasifier was developed based on the two stream arrangement of control volumes considering the flow pattern and other key characteristics identified through detailed computational fluid dynamic (CFD) analysis. The ROM includes submodels for devolatilization and char conversion of coal particles, gaseous reactions, radiation, and convection heat transfer. It also incorporates the numerical slag flow model previously developed by the authors, which interacts with the gasifier model to find converged solutions of gas temperature, slag thickness, and heat transfer at each time step. The ROM was validated by comparison with CFD results for the steady-state conditions of Taean IGCC (300 MWe) gasifier in Korea. It was then applied to the actual operation conditions of the gasification plant, and transient responses predicted by the model were compared with the measured data.

SESSION 36
COAL SCIENCE – 6

36.1- Toward the Advanced Coal Science –Strategic Production of Fine Chemicals

Masakatsu Nomura, Faculty of Engineering, Osaka University; Satoru Murata, University of Toyama; JAPAN.

The authors had published a review titled with possibilities of new coal chemistry-feedstocks for carbon fiber and fine chemicals in the journal of Chemistry (41, 442 (1986), Kagaku Doujin). Now, due to environmentally less acceptable coal fired power plant, above subjects are attracting much attention in the field of R&D of coal utilization. The authors guided one student to summarize two debates (about coal structure) published in Fuel journal. Then, a unit coal structure model was proposed by him based

on the detailed analyses of SRC (95% quinoline soluble at 420℃). Then the work of Leon Stock et al. concerning Ruthenium ion catalyzed oxidation reaction on anthracite had stimulated the authors because the authors pointed out the importance of the knowledge about bridge bonds and above oxidation reaction clarified types of bridged bonds connecting aromatic moieties. However, this oxidation was limited to anthracite in view of quantitativeness. The authors have succeeded in getting satisfied material balance of bituminous and subbituminous coals in oxidation by devising the extraction of benzene polycarboxylic acids. With the help of these coal structural studies the authors joined the project study of clarifying the coking process, then having assumed that the amount of transferable hydrogen in coal and types of bridge bonds of the coal are closely related to the softening of coking coal. The authors propose here that coking coal has much amount of transferable hydrogen and much branched bridge bonds than non-coking coal. A. Tomita et al. have published the direct observation of layered structure of coals using high-resolution transmission electron microscopy. During past decade, Artificial Intelligence has been developed so the authors strongly expect that interdisciplinary joint project (AI scientists, coal chemists, synthetic organic chemists, and pharmaceutical scientists) will be organized to attain coal molecular structure at atomic level then coal must be valuable feedstocks to produce polycyclic aromatic compounds, heterocyclic aromatic compounds and so on. including carbon nano material source

36.2- Geochemistry and Mineralogy of Coal and Gasification By-Products from Two Entrained-Flow Coal Gasification Plants in Ningdong, China

Yafeng Wang, Yuegang Tang, Baolin Wang, Xin Guo, Xi Pan, Binbin Huan, China University of Mining and Technology (Beijing), CHINA; Robert B. Finkelman, University of Texas at Dallas, USA.

The rapid development of coal chemical industry in China has resulted in increased generation of coal gasification by-products including coarse residues and fine residues of various properties. In this study, coal and coal gasification residue samples, collected from two coal gasification plants (coal-to-methanol plant and coal-to-olefin plant) located in Ningxia Hui Autonomous Region, China, were characterized to understand their distribution, migration, transformation, and potentially environmental impacts. The samples from coal-to-methanol plant included feed coal (GEFC), coarse residue A (GECRA), coarse residue B (GECRB), and fine residue (GEFR). The samples from coal-to-olefin plant included feed coal (GSPFC), coarse residue (GSPCR), and fine residue (GSPFR). Using inductively coupled plasma mass spectrometry (ICP-MS), concentrations of Be, F, V, Cr, Co, Ni, Cu, Zn, As, Se, Sr, Mo, Cd, Sb, Cs, Ba, Hg, Tl, Pb, Th, and U, were determined in coarse residue, fine residue, and coal samples. The mineral phases in samples were determined using X-ray diffraction (XRD) and scanning electron microscope with associated energy-dispersive X-ray spectrometer (SEM-EDX). For hazardous trace elements in all the residues from coal-to-methanol plant and in the sample GSPFR, Sr has the highest concentration followed by Ba. However, the concentration of Sr was slightly lower that Ba in the sample GSPCR. To evaluate the potentially environmental impacts of hazardous trace elements, the relative enrichment index was calculated for all the elements in coarse residues and fine residues. Generally, the potentially hazardous trace elements tended to be enriched in the fine residues that had a smaller particle size and consequently larger specific surface areas. Fluorine, Cd, As, Se, Sb, and Tl were markedly enriched in the fine residues. Among these elements, maximum enrichment was observed for Se in the fine residue from the coal-to-methanol plant. Various minerals, such as quartz, calcite, kaolinite, illite, pyrite, etc. in coal, were detected by XRD and SEM-EDX. However, glass was the dominant phase in the residues by SEM observation. During the gasification, most of the minerals were transformed except for quartz that has high fusion temperature of ＞ 1700 ℃. Calcite detected in the residues was the recrystallization product of liquid slag during the cooling process. Other neoformed mineral phases, such as rutile, pyrrhotite, albite, augite, etc., were detected in the residues. To some extent, the gasification process was similar to magmatism because of the crystallization of those minerals.

36.3- Behavior of Trace Amount of Crystalline Minerals in Coal by TEM, TG-DTA and XRD

Atsushi Ishihara, Karin Uemura, Shunsuke Koyabu, Tadanori Hashimoto and Hiroyuki Nasu, Mie University, JAPAN.

Coal is mainly used as a raw material for coal-fired power generation fuel and iron-making coke. Trace elements in coal have a problem of affecting the high temperature corrosion of gas turbine blades in thermal power generation and the production and property of coke used in iron making.1-3) For the reasons, it is important to know the change in behavior of trace elements with treating temperature and heating rate. Therefore, in this study, we investigated the change in the behavior of trace elements in coal with changing atmosphere and treating temperature.

36.4- Research on Methods to Differentiate Coal and Gangue Using Image Processing and Machine Learning

Weidong Wang, Ziqi Lv, Hengrun Lu, Hequn Li, China University of Mining and Technology (Beijing), PR CHINA

Based on the issues for coal and gangue online recognition, in order to improve the degree of automation of separating coal and gangue, this paper proposes several methods that can be used to improve the differentiation of coal and gangue via image processing and machine learning. Images of coal and gangue were converted to grayscale, the background was segmented, and the contrast was stretched. A basic eigenvalue was then determined based on the contrast between the grayscale mean and the gray-level co-occurrence matrix in each image. The biorthogonal wavelet was then used to expand coal and gangue images based on discrete wavelet transforms in two dimensions (2-D), while the supplementary eigenvalue is comprised of the mean variance of the wavelet coefficient at different scales. The eigenvalue of coal was then contrasted with each gangue eigenvalue, as well as the basic and the supplementary eigenvalue to construct a mathematical recognition model based on image processing and use of a support vector machine (SVM). At the same time, coal and gangue images were directly taken as input, and a recognition model was established based on a convolutional neural network (CNN). Experimental results indicate that for coal and gangue images collected in different conditions, the recognition model based on SVM is more suitable for the recognition of small samples of coal and gangue under laboratory conditions (at a rate up to 94%). The recognition model based on CNN performs better for image recognition of large samples of coal and gangue under complex conditions (at a rate up to 99%).

36.5- Classification of Water Forms in Lignite and Energy Consumption Analyses during Microwave Drying Technology

Junjie Liao, Chao Li, Liping Chang, Weiren Bao, Taiyuan University of Technology, PR CHINA.

Differential scanning calorimetry (DSC) was conducted to classify the water forms in Yunnan lignite and Inner Mongolian lignite. The result shows that the water in lignite mainly contains freezable water and non-freezable water, and further the freezable water can be divided into free water and freezable bound water. More than 40% db of water is free water; 27%~40% db is freezable bound water; and less than 27% db is non-freezable water. The theoretical dewatering energy consumptions of Yunnan lignite and Inner Mongolia lignite obtained through the DSC under N2 are 2080±19 J/g H2O and 2084±16 J/g H2O, respectively, which are nearly independent of coal type. The dewatering energy consumptions of lignite under CO2 are 2652±8 J/g H2O and 2448±27 J/g H2O, respectively, which are concerned with coal type and larger than the theoretical dewatering energy consumption under N2. The result shows that CO2 can interact with oxygen containing groups on coal surface and water molecules, thereby affecting the dewatering energy. The microwave drying device was employed to dry lignite. The result shows that it is difficult to completely drying the lignite in 450 W microwave field. When the microwave power is larger than 700 W, the lignite is prone to slight pyrolysis. The atmosphere has little effect on drying characteristics of lignite when use a relatively large amount of coal sample (> 50 g). The Inner Mongolia lignite will release volatiles in microwave field and needs to be humidified. The dewatering energy of total moisture in microwave field under 500~600 W is 8.6~15.3 kJ/g H2O, and the dewatering energy of freezable water is 8.7~12.5 kJ/g H2O. The dewatering energy of non-freezable water is 8.5-21.8 kJ/g H2O. The dewatering energy consumption of total water in Inner Mongolian lignite with particle sizes of 1.00-3.00 mm and 3.00-6.00 mm is 6.5~16.7 kJ/g H2O and 6.1~16.6 kJ/g H2O, respectively.

SESSION 37
SUSTAINABILITY AND ENVIRONMENT - 1

37.1- Air Pollution and Coal Consumption in China: A Perspective from Space

Kai Qin, China University of Mining and Technology, PR CHINA.

China is suffering from serious air pollution dominated with aerosol particles in autumn and winter, and Ozone in summer that adversely affects human health. Coal consumption as an important energy for the Chinese economy is evident in the exacerbating harmful pollution levels in China. Due to its large spatial coverage, satellite remote sensing provides opportunities to monitor the large-scale variabilities of air pollution. In additional, China has built near 1500 ambient monitoring stations over 367 cities to supervise the air quality improvement. Hourly average concentrations of air pollutants including PM2.5, NO2, SO2, and O3 from these stations are available in the National air quality publishing platform. This gives us an unprecedented opportunity to improve the space-borne estimation of air quality over China. In this presentation, firstly, aerosol optical depth (AOD) data from Moderate Resolution Imaging Spectroradiometer (MODIS) and Geostationary Ocean Color Imager (GOCI) are used to estimate ground-

level PM2.5 concentration. Tropospheric NO2 and O3 columns from Ozone Monitoring Instrument (OMI) are used to estimate ground-level NO2 and O3 concentrations. Secondly, the tempo-spatial characteristics of the tropospheric NO tropospheric columns and the SO2 planetary boundary layer columns from 2005 to 2016 in China are quantitatively analyzed. Furthermore, the relationship between air pollutant changes and coal consumptions in provincial-levels in China is revealed. The results have profounding implication for improving our understanding of China's efforts to decrease pollution levels by cutting fossil fuel consumption to achieve clean energy goal.

37.2- A Novel Application of Palm Kernel Shell Derived Carbon to Magnesium-Based Hydrogen Storage Materials

Yeboah Martin Luther, Zongying Han, Xinyuan Li, Ruiqian Jiang, Shixue Zhou, Shandong University of Science and Technology, PR CHINA.

The utilization of waste biological resources to synthesize value added products benefits the world by reducing environmental pollution. In recent years, carbon has gained much attention as a functional material used for various applications, mainly including water purification, hydrogen storage and electrode manufacturing. However, various sources of carbon i.e. petroleum coke, coal and pitch are not environmentally friendly and well as non-renewable, therefore the need to explore new alternatives such as biomass. In this work, carbon derived from palm kernel shell (later denoted as PKSC in this text) was introduced into the milling of magnesium as an additive after which the resulting composite was hydrogenated by high pressure hydrogen absorption. Through X-ray diffractometry analysis, it was discovered that, increasing the content of PKSC increases the conversion percentage of Mg into MgH2, which is attributed to the highly dispersed and reduced particle and grain size of Mg after ball milling. Analysis of differential scanning calorimetry curves depicts a decreasing trend in peak desorption temperature as the content of PKSC is increased. PKSC acts as an anti-agglomerate, helping in the achievement of a more dispersed composite due to its layered carbon structure.

37.3- $Ti_1Li_3Al_4$-LDHs@Activated Carbon with Enhanced Photocatalytic CO_2 Reduction Performanc

Dong-Qiang Lei, An-Ning Zhou, Xiao-Ling Zhao, Wen-Ying Li, Xi'an University of Science and Technology, PR CHINA.

In this study, we prepared Ti1Li3Al4-LDHs@actived carbon (AC) composites by means of impregnation-precipitation and using coconut-based activated carbon (BAC) or coal-based activated carbon (CAC) as supporting material. Ti1Li3Al4-LDHs@ACs were characterized by means of X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier transform infrared (FTIR) and ultraviolet-visible (UV-Vis) spectra analysis, the parameters of preparation such as the type and amount of activated carbon on photocatalytic performance of Ti1Li3Al4-LDHs@ACs in photocatalytic reduction of CO2 were investigated. The results show that the characteristic crystal-face (003) and (006) diffraction peaks of Ti1Li3Al4-LDHs are clearly observed in Ti1Li3Al4-LDHs/BACx (x represents mass ratio of LiCl and BAC), the absorption wavelength thresholds of the composites are relative lower that of Ti1Li3Al4-LDHs. It also has been found that catalytic reactivity of Ti1Li3Al4-LDHs@BAC3/1 in photocatalytic reduction of CO2 to CO is more active than Ti1Li3Al4-LDHs. That is because that the large band gap of Ti1Li3Al4-LDHs@BAC3/1 can reduce the recombination of photogenerated electron-hole pairs in photocatalytic reactions.

37.4- Pyrolysis Behaviors of Five Agricultural Wastes with a Focus on Liquid Product

Shiqi Wan, Nan Zheng, Jie Zhang, Jie Wang, East China University of Science and Technology, PR CHINA.

Agricultural waste is an important biomass energy source because of its abundant availability, renewability, non-conflict with the food chain, and environmental gain. Pyrolysis is an efficient way to convert biomass to higher grade products including gas, bio-oil and bio-char via thermal treatment. The purpose of this study is to investigate the pyrolysis behaviors of five agricultural residues (peanut straw, cotton straw, sorghum stalk, corn stalk and reed) using a gas-sweeping fixed-bed reactor. All biomasses were collected from a rural village in Lian Yun Gang city, China. The study is focused on the different compositions of these biomasses and their relationships with pyrolysis products, especially liquid product. Pyrolysis was carried out in an inert gas stream at a heating rate of 10 °C min-1 from room temperature to 700 °C. GC-TCD (gas chromatography equipped with thermal conductivity detector) was used to determine the main gases (CO2, CO, H2 and CH4). GC-FID (flame ionization detector) was used to determine hydrocarbon gases (C2–C3) and some typical liquid compounds. GC-MS (mass spectrometry) was used to characterize liquid compositions. The fiber analysis showed that peanut straw had the highest content of neutral extractives, and reed and cotton straw had the highest contents of cellulose and hemicellulose, and corn stalk and sorghum stalk was the most enriched with lignin. The pyrolysis results showed that the yields of bio-oil (water-excluded, dry biomass basis) were 31.5%, 27.6%, 28.0%, 24.9%, 24.3% for reed, sorghum stalk, corn stalk, cotton straw and peanut straw, respectively. It was interesting to see from GC-MS analysis that the bio-oils derived from sorghum stalk and corn stalk contained a higher proportion of long-chain fatty compounds including hydrocarbons and oxygenates (mainly unsaturated C16 and C18 acids), distinct from three other biomass species. These two bio-oils also had higher proportions of guaiacols, indicating a correspondence to their higher contents of lignin. The bio-oil derived from reed stalk showed the highest proportion of furfural and saccharides, in line with its highest content of cellulose and hemicellulose. Peanut straw produced the highest gaseous products (especially high for CO2) and the lowest yield of bio-oil. The bio-oil derived from peanut straw was composed of many nitrogenous compounds. Quantitative analysis by GC-FID demonstrated that peanut straw had the higher yields of both BTX (benzene, toluene and xylene), while sorghum stalk and corn stalk had the higher yields of PCX (phenol, cresol and xylenol). In the presentation, we will further report on the contents of alkali and alkaline earth metals (K and Ca) inherent in the five biomass species and their effects on the pyrolysis behaviors.

37.5- Preparation of Activated Carbons from Anthracite by CO_2 Activation Coupled with KNO_3 Catalyst for CO_2 Adsorption

Zhang Shuangquan, Sun Cong, Yang Xiaoqin, China University of Mining & Technology, PR CHINA.

The preparation of activated carbons (ACs) from Chinese Taixi anthracite with CO2 as an activation agent coupled with KNO3 catalyst was studied for their application in separation of CO2 from gas mixtures by pressure swing adsorption (PSA) method. The influences of the preparation conditions on the pore structure and the CO2 adsorption capacity of the ACs were investigated. The results showed that the ACs had higher CO2 adsorption capacity than those of the ACs with H2O activation or H2O/CO2 activation. It was found that the volume of pores smaller than 1.0 nm for the ACs prepared by CO2 activation was higher than that prepared by H2O or H2O/CO2 activation, which strongly determined the CO2 adsorption capacity. KNO3 catalyst could effectively promote the formation of much smaller micropores and shorten the activation time. The CO2 adsorption capacity of the ACs increased with increasing the catalyst amount, and 3 wt.% was more suitable. Excessive activation temperature was not in favor of the development of small micropores and the suitable activation temperature was 920 °C. The specific surface area, total pore volume, microporosity, average pore diameter and CO2 adsorption capacity of the AC under the optimal conditions of 3 wt.% of KNO3 amount, 920 °C of activation temperature and 40% of burn-off were 1071 m2·g–1, 0.45 cm3·g–1, 89%, 1.67 nm, and 2.65 mol·kg–1 (25 °C, 0.101MPa), respectively.

SESSION 38
CLEAN COAL AND GAS TO FUELS - 2

38.1- Candle Soot as a Novel Collector for Coal Flotation

Wencheng Xia, China University of Mining & Technology, PR CHINA.

The mixture of candle soot and hydrocarbon oil (dodecane) was used as a novel flotation collector in the flotation of coking coal and low rank coal. X-ray photoelectron spectroscopy (XPS) and contact angle measurements were used to indicate the surface properties of candle soot. Scanning electron microscopy with energy dispersive spectrometer (SEM/EDS) and attachment time measurer were used to show the adsorption of candle soot on coal particle surface. XPS and contact angle results showed that the candle soot was very hydrophobic. SEM/EDS results showed the candle soot consisted of plenty of carbon nanoparticles which could attach and adsorb on the coal particle surface and hence shortens the attachment time of coal particle and bubble. The flotation recovery of both coking and low rank coals using the mixture of candle soot and dodecane as a collector were higher than that using solo dodecane as collector. The adsorption of candle soot and other ultra-fine particles on coal particle surface enhanced the surface hydrophobicity and floatability of coking and low rank coal particles.

38.2- Methanol Synthesis over $Cu/Zno/Al_2O_3$ Catalysts Prepared Using Reverse Microemulsion Method

Panpan Yang, Yulong Zhang, National Institute of Clean-and-Low-Carbon Energy (NICE), PR CHINA.

Reverse microemulsion is an effective way to prepare metal nanoparticles. We proposed a reverse microemulsion system to prepare a series of Cu based catalysts for methanol synthesis, using hexadecyl trimethyl ammonium Bromide (CTAB), n-pentyl alcohol, cyclohexane and metal salt solutions. Characterization of structure, morphology and catalytic activity were studied respectively. The results indicate that the aging temperature, alkali concentration and the ratio of H2O/CTAB have substantial influence on the particle sizes and activity, which provided a new preparation method of methanol synthesis catalysts.

38.3- The Application of Gas Separation Membranes to Coal Gasification Process

Ivy Huang, Richard Baker, Tim Merkel, Membrane Technology and Research, Inc., USA.

Gasification of coal to produce syngas for coal-to-chemicals or hydrogen for IGCC power production is an area of growing interest. These applications require large gas separation plants as part of the flow scheme. Despite advances in conventional separation technologies over the past several decades, costs of gas separation systems remain high. Membrane gas separation is an emerging new process that is an often overlooked by plant designers but has a number of useful attributes: low cost, straight forward flow sheet, small foot print, ease of operation and no hazardous chemicals to worry about. There are a number of established and new applications of these membranes in coal gasification processes.

In general membranes are best used to perform a low cost bulk separation. Sometimes this type of separation is all that is needed but more frequently a second separation technology will be used in a subsequent polishing step. Examples of this type of combination processes are: membranes plus cryogenic fractionation, membranes plus pressure swing adsorption and membranes plus absorption processes. Examples of the application of these processes to coal gasification streams will be used to illustrate the technology.

The technology can be expanded to perform the separation required for gasification streams from a variety of coals and other feedstocks (including biomass and municipal/industrial wastes).

38.4- High Demand Ethylene Formation from CO_2 Hydrogenation over Efficient and Stable Fe-Co-K/ZrO_2 Catalysts: Promotional Mechanisms of Oxygen Vacancies

Jie Ding, University of Wyoming, USA and Nanjing University of Science and Technology, PR CHINA; Liang Huang, Wuhan University of Science and Technology, PR CHINA; Maohong Fan, University of Wyoming, USA and Georgia Institute of Technology, USA; Qin Zhong, University of Wyoming, USA; Armistead G. Russell, Georgia Institute of Technology, USA; Hao Gu, University of Wyoming, USA; Haijun Zhang, Wuhan University of Science and Technology, PR CHINA.

The objective of this research is to convert the increasingly concerning CO2 and renewable H2 to bulk chemical and industrial materials, ethylene, over a novel family of catalysts, which creates a win-win scenario for simultaneous climate change prevention and sustainable economic development. The catalytic activities of the novel FexCoyKz/ZrO2 catalysts as well as conventional FexCoyKz/Al2O3 and FexCoyKz/SiO2 catalysts were compared under various reaction temperatures. The FexCoyKz/ZrO2 catalysts with only 5% metal loading presented the best activities at 300 oC, while the conventional catalysts achieved the best ones at higher reaction temperature (320 oC). The new catalysts achieved 11.4~164.9% higher CO2 conversion, 50.8~133.7% higher selectivity of ethylene than the conventional FexCoyKz/Al2O3 catalysts and showed better stability. The improved catalytic properties were mainly resulted from the higher concentrations of oxygen vacancies on the FexCoyKz/ZrO2 catalysts, which promoted the adsorption and activation of CO2 as well as the conversion from CO2 to CO. It is a promising catalyst for conversing the captured CO2 and renewable H2 to high demand ethylene with a green route.

38.5- Impact of Nanobubbles on Mechanical Coal Flotation Process

Ahmed Sobhy, Dongping Tao, University of Science and Technology Liaoning, PR CHINA.

A bank of three 10-liter mechanical flotation cells integrated with nanobubble technology was investigated to assess the impact of nanobubbles on coal separation performance at different operating variables. The most significant operation parameters such as fuel oil collector dosage, methyl isobutyl carbinol (MIBC) frother concentration, flow rate to nanobubble generator, feed solid concentration, and feed flow rate were studied individually. Nanobubbles are generated selectively on the hydrophobic particles, which should have a positive effect on flotation separation efficiency. It has been shown that frother concentration, collector dosage, and flow rate to nanobubble generator had a positive and significant effect on coal recovery and separation efficiency while maintaining the product grade. Solids concentration had modest influence on flotation performance, while feed flow rate showed a negative impact on flotation performance.

SESSION 39
COAL BED AND SHALE GAS - 4

39.1- Pore Characterization and Its Impact on Methane Adsorption Capacity for Organic-Rich Marine Shales

Yang Wang, China University of Mining & Technology, PR CHINA.

Shale matrix pore structure controls the gas storage mechanism and gas transport behaviors. We employed various techniques to characterize the complex pore structures of shale samples collected from two marine shale formations in upper Yangtze area in China. The characterization techniques include field emission scanning electron microscopy (FE-SEM), high pressure mercury intrusion porosimetry (MIP), and low-pressure N2/CO2 adsorption. The excess methane adsorption capacity was measured for each samples and results were modeled using Langmuir model. Based on the FE-SEM image analyses, micro- and meso-pores within organic matter and inter-particle pores between or within clay minerals are the most commonly developed in these shale samples. Both uni- and multi-modalpore size distributions (PSDs) were observed, and a significant portion of pores are in the pore size range between 3 and 100 nm. It was also found that the micropore (< 2 nm) is the major contributor to the overall specific surface area (SSA), whereas most of the pore volume is occupied by mesopores (2~50 nm). Methane adsorption capacity increases with the increase of both micropore volume and micropore surface area, and this confirms that microporosity is the governing factor on methane adsorption capacity and storage.

39.2- Geochemistry of Coal Seam Gas Co-produced Water and its Potential Effects on the Ecosystem in southern Junggar Basin China

Meng Li, Jienan Pan, Xinghua Shi, Yawen Wu, Henan Polytechnic University, PR CHINA.

Coalbed methane (CBM) or coal seam gas (CSG) is becoming an increasingly important source of energy around the world. In China, a rise in the demand of natural gas and a decline in these conventional energy resources, along with issues such as climate change have encouraged a nationwide interest in alternative sources of energy like CSG. However, there are important environmental concerns associated with the large volume of co-produced water with undesirable composition in the CSG industry. The Junggar Basin is one of the largest producers of CSG in Northwest China. Most of its produced water is disposed of in unlined surface impoundments. Data were collected from a network of 35 observation wells to investigate the effects of CSG discharge waters on the environment, the freshwater ecosystem and human health. Chloride, sulfate, bicarbonate, sodium, and kalium were the dominant ions in all areas, but substantial variability existed in relative concentrations; pH varied from more than 7 to less than 9, and total dissolved solids concentrations ranged from less than 7600 to greater than 20,000 mg/L. Heavy metals such as barium, manganese, vanadium and arsenic are found at concentrations of 6700 μg/L, 95 μg/L, 25 μg/L and 2.5 μg/L respectively. The concentration of barium is two to three orders of magnitude greater than those other heavy metals, which contributes to the significant source of pollutants.

The mean SAR values ranged from 600–2800 which poses significant threats to the soil ecosystem. Besides, these problems become more destructive due to the arid climate of northwestern China where evaporation rates speed accumulation of salt on the surface. These findings suggest that CSG waters could affect agricultural production operations and long-term water quality.

39.3- Moisture Occurrence and Its Influence on Methane Adsorption Capacity of Coal

Feng Wang, Yanbin Yao, Xuehao Yuan, China University of Geosciences and Beijing Key Laboratory of Unconventional Natural Gas Geological Evaluation and Development Engineering, PR CHINA.

In this study, a new NMR fluid typing method was applied to identify different occurrence states of water and multiphase methane (adsorbed, porous-medium confined, and bulk methane) and to investigate the effect of water occurrence on methane adsorption capacity of long flame coal and anthracite coal. At first, isothermal adsorption experiments from NMR method is compared with those from conventional volumetric methods, based on several parallel contrast experiments on the same coal samples. The results show that the deviation in Langmuir volume from two methods is generally within 2cm3/g, indicating that the NMR method is capable in calculating the amount of adsorbed methane, and it is also applicable in monitoring the transform and phase change between adsorbed and bulk methane due to the adding of water into the samples. Then, the influence of adsorbed water, and non-adsorbed water (including capillary-bound water and free water) on methane adsorption were simulated based on a set of costume-designed NMR simulation experiments. The results show that for anthracite coal, the

methane adsorption capacity emerges a decrease trend with increasing contents of both adsorbed water and non-adsorbed water content. Specifically, the Langmuir adsorption volume for anthracite decreases by 28.97cm3/g and 3.42cm3/g per unit mass of adsorbed and non-adsorbed water respectively. In contrast, for long flame coal, although the adsorbed water can induce the reduce of the Langmuir adsorption volume, from 22.78cm3/g to 11.35cm3/g, the adsorption capacity maintains a stable level at 11.29cm3/g with the adding of non-adsorbed water content, especially when the non-adsorbed water over 1.42g. Adsorption competition between water and methane in coal has been validated by many scholars for decades, the adsorbed water occupies the adsorption sites in the coal matrix surface, which constrains the further adsorption of methane. Nevertheless, the non-adsorbed water and adsorbed water are distinct in terms of migration mechanism and reaction with methane molecular. The influence of non-adsorbed water on methane adsorption for low rank coal is negligible, whereas for high rank coal, the methane adsorption capacity continuously decreases. The reasonable explanation is that although free water in macro-pores do not have contribution to the gas adsorption, the water film restricts the gas diffusion and migration through the pores network, even the Jamin effect will occur when the water droplet blocks the throats completely, which is extremely unfavorable for CBM production.

39.4- Research on Key Techniques for Improving Coal Bed Methane Recovery by Combustion of Coal Seam

Xianjie Shao, Yingming Peng, Feng Li, Dickens Oyaka, Mingfeng Li, Zeheng Liu, Yanshan University, PR CHINA.

Heat and CO2 are produced when coal is burned under the ground, which can increase coal seams temperature, reduce adsorption, increase desorption and diffusion rates. As the coal seams are roasted at high temperature, the physical properties of the coal are changed and the permeability is improved. The methane can be replaced and displaced by CO2, which in turn increases CBM production and recovery. Through theoretical research and physical simulation experiments, the key technologies of the combustion of coal seam and the conditions and timing of the geology suitable for the technology are demonstrated in detail. Injecting the oxidizer based on the electric ignition method is the best way in the ignition technology. The fire control technology can be achieved through the adjustment of the working system of fire wells and gas recovery wells. Specific measures for controlling fire in input wells include adjusting the amount of air injected, water injection, high-temperature foam, and other measures. Adjustment of drainage working systems are the measures for fire control in gas recovery wells. In addition to the conventional parameters such as temperature, pressure, air injection volume, and daily gas production, monitor wells to be drilled between injection and production wells are also required. Through the monitoring parameter of temperature, the propulsion speed and distance of the burning front are calculated. Coal seams suitable for fire technology should be simple in structure, with no faults in the area, coal seam thickness greater than 5m, formation inclination less than 30°, burial depth greater than 500m, low moisture content, stable cover coat, and good sealing conditions. Daily gas production declining to below the economic limit, and daily water production below 0.5t/d is the best time for burning. At this time, the formation pressure is relatively low, and there is almost no formation water. Both in air injection and ignition, they are favorable.

39.5- Coalbed Methane Enrichment Pattern and Screening of Favorable Areas in Western Guizhou, China

Chu Qingzhong, Yan Yi, Peng Yingming, Yanshan University; Jin Liuqing, Guizhou Shale Gas Co, Ltd; PR CHINA.

Based on the study of regional background, lithology and sedimentary structure, through the phase analysis of vertical and horizontal wells in a single well, it is believed that in the Late Permian, the area was in the transitional zone between sea and land, and the coastline was advanced from east to west. The deltaic and lagoon-tidal depositional environments were mainly developed. Using the principle and method of sequence stratigraphy, the sequence interface was determined. The upper Permian system was divided into three sequences, and the coal seam is mainly developed in the transgressive system domain of the mid-term sequence SQ2 and the later sequence SQ3. There are two kinds of coal-forming models in this area, namely, the deltaic coal-forming environments and the lagoon-tidal plate coalification coal-forming environments. The coal formed in the deltaic environment has good coal quality and a large thickness, but its stability is poor, and coal seams are interrupted and bifurcate in the horizontal direction. The coal seams formed by the lagoon-tidal environment have a wide distribution area and good continuity, but their thicknesses are relatively thin. Through studies on the types of coal and rock, metamorphism, burial conditions, physical properties of coal, hydrogeological conditions and adsorption capacity, 14 indicators had been optimally selected. By using the analytic hierarchy process and the grey clustering method, a coalbed methane resource evaluation model was established in the western part of Guizhou, and the mining area was divided into groups of Level I, Level II, and Level III coalbed methane pools according to three levels: best, moderate, worst. The evaluation results provide the basis and target area for coalbed methane development planning and deployment.

SESSION 40
COAL MINING AND BENEFICIATION - 1

40.1- Scientific Coal Mining and Education

Jiachen Wang, China University of Mining and Technology (Beijing), PR CHINA.

China become the largest energy consumer in 2010, and the primary energy consumption accounted for 23% of the world's total in 2016. China's total energy consumption is 3,053 Mtoe, where coal consumption takes 62%. China produced 3.2 billion tons of coal in 2017, accounting for 45% of world coal production. So there are four parts are discussed in the paper: 1. Significance of Coal Energy in China. 2.Scientific Coal Mining. 3.Progress in Scientific Coal Mining Techniques. 4.Industry and College Mining Education in China. The Energy status of China, Mining technology history, Technical problems of scientific mining, Definition of Scientific mining, Comparison with US mining industry and education in University are also proposed in the presentation.

40.2- Detection and Monitoring of Underground Coal Mine Gases at Lakhra Coal Mines, Pakistan

Niaz Muhammad Shahani, Zhijun Wan, Muhammad Ali, Barkat Ullah, China University of Mining & Technology, PR CHINA.

Coal or coal-bearing strata, especially in underground coal mines covers the substantial amount of gases. These mine gases are very dangerous when mixed with air. Most commonly found gases such as CO, CO2, CH4, and H2S etc. are the combination of atmospheric air or oxygen. A total of eight most promising regions of naturally ventilated Lakhra Coal Mine No. 28, C-Block have been examined by using portable Multi-Gas Detector (IMR-2800). The concentration of CO and CO2 is reported as 388 ppm and 0.7% respectively. The study proposes an appraisal of the efficient ventilation system. The mine locations with high concentration of gases may be supplied with adequate air or should be permanently sealed off and isolated from the working environment. It has been found that detected concentration of gases may cause serious health problems or even fatal accidents, therefore, proper ventilation system for the mine has been suggested.

40.3- Flow Field Evolution during Gas Depletion with Consideration of Creep Deformation

Yang Zhao, Baiquan Lin, Ting Liu, Qingzhao Li, Yuannan Zheng, China University of Mining and Technology, PR CHINA.

Unsteady creep of the coal seam and its resultant abnormal flow of coal seam gas are the main causes of dynamic disasters in deep mines. In this paper, to study the evolution of creep inducing seepage in deep mines, the flow field evolutions during gas adsorption and desorption were simulated first based a multi-field (namely, coal deformation field, diffusion field and seepage field) coupling model considering the creep deformation. Then, the spatial and temporal evolutions of matrix and fracture gas pressures, coal permeability and equivalent stress during gas adsorption and desorption were analyzed. Finally, laboratory experiments were performed to verify the simulations. The results show that at the initial stage of adsorption, gas in fractures undergoes a rapid increase in its pressure under the pressure gradient. Afterwards, it gradually diffuses into matrix pores and raises the matrix gas pressure, which results in a swelling deformation of coal matrix and alters the fracture aperture. As a result, the evolutions of coal permeability and equivalent stress were affected. During the desorption process, the fracture gas pressure drops rapidly at first and then falls at a lower rate. The gas diffusion into fractures gradually leads to matrix shrinking and an increase in coal permeability. With a decrease in fracture gas pressure, the equivalent stress of coal declines rapidly first, followed by a slow rise induced by the diffusion of matrix gas. Furthermore, changes in the amount of gas desorption was analyzed by fitting the experimental test data in a specific time, which verified rationality of the simulation. This study can provide theoretical guidance for the prevention and control of dynamic disasters in coal mines and the pre-drainage of borehole gas in deep mines.

SESSION 41
GASIFICATION TECHNOLOGIES - 7

41.1- Evaluation Method of the Energy Conversion Efficiency of Coal Gasification and Related Applications

Tianhong Duan, Zuotang Wang, China University of Mining and Technology, PR CHINA.

Traditional gasification parameters, such as cold gas efficiency, hot gas efficiency, or thermal efficiency, only evaluate the heat energy utilisation efficiency of gasifiers, and do not take into account the gasification processes expending electricity and other types of energies. Therefore, the energy conversion efficiency cannot be assessed using these parameters. The calculation process on the energy conversion efficiency of underground coal gasification (UCG) is the basis for obtaining quantitative data of carbon emission reduction and establishing the carbon trading methodology of UCG. Moreover, the energy conversion efficiency both for surface coal gasification and UCG is a key research topic because it directly affects the economic and environmental benefits of gasification projects. This study proposed that two parameters, the integrated gasification efficiency (hcom) and the hot gas integrated gasification efficiency (h′com) should be included into the coal gasification parameters and used to evaluate the energy conversion efficiency of coal gasification. In addition, the calculation methods of these two parameters for both surface gasification and UCG were established. Using the method, hcom and h′com of the UCG and Texaco gasification under the same scale was compared and that of various UCG processes was calculated. The results proved the necessity and reasonability of the two parameters and suggested that a certain amount of CO2 was favourable to improve hcom and h′com of UCG. However, a certain amount of pure O2 can improve hcom of UCG without direct influences on h′com. Under the condition of each process, to maximise hcom and h′com, there must be an optimal steam (CO2) to O2 rate.

41.2- Designing of Intelligent Flexible Gasification Unit Using Excel and Aspen Simulation Workbook

Jianwei Li, Bai Feng, Jiaojiao Lei, Xingxin, Xi'an University of Science and Technology, PR CHINA.

China innovates few proprietary coal gasification technologies after import and digestive absorption with the rapidly development of coal chemical industry. But there is still weak in the gasification process design, control and monitoring. In this article, BP artificial neutral networks is used and realized into Excel templet to estimate the heat value or melt point, which as well as the coal ultimate and proximate analysis data will be used as the perform parameters of gasifier. This Excel templet is also used as an interface to conduct the coal gasification unit automatically design and sizing by using Aspen Simulation Workbook invoking an embedded Aspen flowsheet simulation model. The Aspen simulation model reads in the original coal analysis data and estimated parameters from the Excel templet and writes the output return after a pre-build in simulation and optimization function. Through which the Excel templet file can give correct stream information, gasification efficiency, and automatically calculates the reasonable geometric size for the equipment design even the coal properties is changed. These equipments include gasifier, scrubber, flash evaporator and necessary pipes.

41.3- Process Analysis of RDF Gasification Integrated with Coal Boiler

Aleksander Sobolewski, Marek Sciazko, Institute for Chemical Processing of Coal; Tomasz Chmielniak, AGH University of Science and Technology and Institute for Chemical Processing of Coal; Joanna Bigda, Institute for Chemical Processing of Coal; POLAND.

Poland has significant amounts of low-quality fuels, including waste coal, combustible waste (with calorific value over 6 MJ / kg) separated from municipal waste and also chemically contaminated waste wood. Effective use of them could bring both economic and ecological effects. Low-quality fuels gasification in fluidized bed systems integrated with coal boilers seems to be interesting and efficient method of its processing. The integration of low-quality fuels gasification with low capacity 200 MWe boiler units is of particular interest, because it gives opportunity to increase their use, as well as economic and ecological efficiency. The presentation demonstrates results of the simulation of low-quality fuels gasification in the system integrated with power boiler. Mass and energy balance calculations were carried out using the developed process model (ChemCAD) of fluidized bed reactor (based on SES technology) which was verified on the basis of real operational data (Figure. 1).

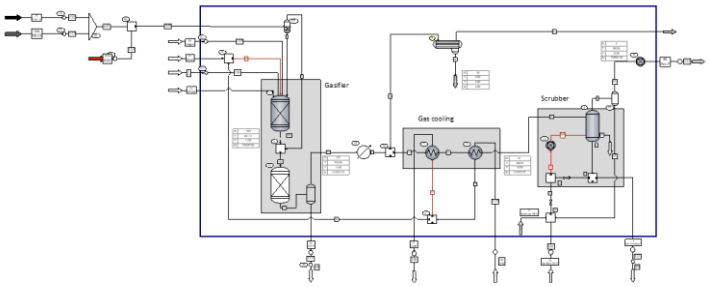

Figure 1. Process calculation diagram

In addition, the concept of a RDF (Refuse Derived Fuel) gasification system integrated with coal boiler, model of the gasification process and the results of its verification will be shown and discussed. The presented concept assumes the integration of a gasification system with a 200 MWe class multifuel fired boiler. The proposed solution is the only one that meets the assumed criteria for fuel costs and CO2 emissions and it minimizes the impact of formal and legal restrictions under the Act on Thermal Treatment of Waste. The gasification system has 1 production line processing about 60 t of RDF per hour and is equipped with deep gas cleaning system. The gas is supplied to the boiler in which the fuel mixture of coal, waste coal and biomass is fired. The proposed configuration allows to achieve the assumed goals of the analysis, i.e.

The formal separation of RDF gasification from the power unit, as long as the gas is purified to a level that allows obtaining natural gas emission during combustion (According to the Polish and European regulations the boiler is not incineration plant, only gasification island, and the solid by products from the boiler could be a valuable product).

Low CO2 emission. The plant offers the possibility to reduce CO2 emissions to the level of 550kg / MWh (the emissivity of the block will be adjustable by using biomass in the amount justifying the expected CO2 emissions).

Obtaining the average fuel cost at the entrance to the block not higher than at present.

41.4- 3D TFM-Tracer Approach to Simulate a Lab-Scale Fixed-Bed Gasifier

Massoud Massoudi Farid, Sebastian Kriebitzsch, Andreas Richter, Bernd Meyer, Technische Universität Bergakademie Freiberg, GERMANY.

Conversion of solid or liquid hydrocarbon feedstocks into synthesis gas using gasification/partial oxidation with the aim of power generation, or production of chemicals, hydrogen, substitute natural gas (SNG), and transportation fuels [1] is a promising solution to decrease the greenhouse gases emissions. Furthermore, the possibility of low-grade feedstock utilization, such as low rank coals and wastes, makes the gasification even more attractive as a flexible technology. One of the most appropriate gasification technologies to gasify wide range of solid feedstocks including different coal ranks and opportunity fuel blends with RDF/municipal waste/domestic waste, tires, and wood waste is British Gas Lurgi (BGL) Fixed/Moving Bed slagging gasifier. However, particles agglomeration and over packing with fines, which are results of non-uniform flow, can lead to problems such as poor interphase mixing, unreacted carbon, hot spots and lower conversion rate in these types of reactors [2]. To optimize and upscale the reactor, better process understanding is necessary. In this regards, visualization of the aforementioned problems has been always one of the challenging steps. To overcome this challenge, modelling tools such as computational fluid dynamics (CFD) which provides spatially and temporally resolved information of the system could be of great importance. As the first step towards the simulation of an industrial scale BGL slagging gasifier, a CFD model is developed to simulate a fixed bed gasification process using a 3D Two Fluid Model (TFM)-Tracer approach. In this approach TFM is used as a ground base to lagrangian tracer particles through them distribution of different properties such as size, solid fuel spices, reaction rates, and so on are simulated. The results are validated with the results obtained from a lab scale experiment [3] and detailed temperature, pressure, and gas species distributions are presented.

41.5- Kinetic Study of High-Temperature Co-Gasification of Petroleum Coke and Coal

Xin Yu, Dunxi Yu, Professor, Huazhong University of Science and Technology, PR CHINA.

As a by-product of petroleum processing, petroleum coke production keeps growing steadily with the increase in oil consumption. High calorific value, low ash content, and low price make petroleum coke as an alternative fuel extremely attractive. Gasification is one of the promising ways to make full use of this fuel. However, due to the very high carbon content (over 90 wt%) and very low alkali and alkali earth metals (AAEMs) contents, the gasification efficiency of petroleum coke is usually low. Therefore, how to improve the gasification efficiency of petroleum coke is one of the scientific issues to be solved urgently.

In this work, we proposed the co-gasification of petroleum coke with coal, which aims

to introduce AAEMs from the coal as catalysts to improve the gasification efficiency of petroleum coke. Experiment was carried out in a thermal gravimetric analyzer (TGA) to study the co-gasification kinetics of petroleum coke and coal. Raw petroleum coke, two coals (a high AAEMs coal and a high silica-alumina coal), and their blends with different ratios were gasified at a wide temperature range (1000-1300°C). Based on this study, the kinetics of co-gasification of petroleum coke and coal were derived, and were compared with those of raw petroleum coke and coal. Besides, the optimum co-gasification condition was derived. The above research can provide technical support and theoretical guidance for the use of this technology.

SESSION 42
COAL SCIENCE - 7

42.1- Optimization of Illinois Basin (USA) Coals by Coal Preparation

Allan Kolker, U.S. Geological Survey; Liliana Lefticariu, Southern Illinois University; Maria Mastalerz, Agnieszka Drobniak, Indiana Geological and Water Survey; Anne Scott, Clint Scott, U.S. Geological Survey; USA.

The Illinois Basin, in the State of Illinois and adjoining parts of Indiana and Kentucky, comprises the third largest U.S. coal producing region, after the Powder River Basin and the Appalachian Basin. With greater adoption of scrubbers in U.S. coal-fired utilities, the high sulfur contents of Illinois Basin coals are no longer an impediment to their use. Whereas front-end sulfur reduction is no longer essential, Illinois Basin coals are still commonly prepared prior to delivery, in order to reduce mineral matter and optimize heating value, thereby improving overall coal quality. In the present study we sampled thirteen cleaning operations preparing Illinois Basin coals in Illinois and Indiana to track benefits in coal quality, and to determine co-benefits in reduction of mercury and other toxic substances. Samples include feed coal, prepared coal, and refuse coal at various stages of the cleaning process. Some operations have mixed or multiple products, if more than one coal bed is mined. In addition to proximate and ultimate determinations, samples were analyzed for mercury, trace elements, sulfur forms, and organic petrology to track the behavior of these parameters in the coal preparation process.
Results show co-benefits in mercury, trace element, and pyritic sulfur reduction corresponding to reductions in ash yield and increased heating values. For eight preparation circuits in Illinois, coals feeding the circuit have mercury contents ranging from 0.05 to 0.48 ppm, whereas the cleaned product has mercury ranging from 0.04 to 0.09 ppm. All of these cleaned coals are below the world average mercury content for coal (0.10 ppm; Yudovich and Ketris, 2005, Int. J. Coal Geology 62, 107-134). Reduction of mercury for these eight circuits ranges from -26.9 to 82.5 percent on an as-received basis, with a mean reduction of 32 percent. As a result, coal preparation reduces the proportion of mercury and toxic trace elements that must be captured from the flue gas under the U.S. EPA Mercury and Air Toxics Standards. In most cases, mercury and some trace elements are correlated with pyritic sulfur reduction, confirming a pyritic host for mercury. Further quantification of mercury and trace element distribution in pyrite by laser ablation ICP-MS is anticipated in the next set of geochemical analyses. These results form part of a larger collaborative study of element variation and its controls in Illinois Basin coals.

42.2- Characterizing Nanoscale Pores and Pore Networks in High-Rank Coal

Difei Zhao, Yujie Wang, Yinghai Guo, China University of Mining and Technology, PR CHINA; Geoff Wang, The University of Queensland, AUSTRALIA.

The coal-bearing strata of China are rich in high-rank coalbed methane(CBM) reserves. However, the structural characteristics of high-rank coal are complex, and the reservoir space is mainly comprised of micro-nano pores with poor micro-seepage ability within the coal matrix. This affects the migration of gas in high-rank coal, which influences the efficiency and productivity of CBM reserves. The accurate characterization of the micro-porosity and pore networks of these deposits can provide the scientific basis for improving the development efficiency and productivity of CBM reserves. Furthermore, studying the pore structure of the coal matrix can provide guidance for the development of underground greenhouse gas storage and CBM resource evaluation.
In this study, the characteristics of pores and pore networks in high-rank coal deposits, including pore size distribution, pore type, and connectivity, are investigated by combining qualitative and quantitative testing techniques. The pores were photographed using an argon ion polishing and field emission scanning electron microscope (AIP-FESEM), which allowed the pore types to be identified with an Energy Dispersive Spectrometer(EDS). The structural parameters of the micro-nano pores of high-rank coal were then obtained by exploiting image processing techniques.
However, the AIP-FESEM images can only capture images of the pores with diameters greater than 10 nm. Therefore, a direct observational method for imaging pores with diameters less than 10 nm is still required. Hence, for the first time, argon ion polishing technology was used to obtain high-quality observations of the pores' surfaces, and furthermore observe pores with an atomic force microscope (AFM) to obtain the images of nano pores with diameters of less than 10 nm. This surface treatment technology, combined with AFM observations has the advantages of strong repeatability and high-quality surface observations. The results show that pores smaller than 10 nm are mainly metamorphic and intermolecular pores, and the morphology is mainly in the form of surface defects on organic matter.
Through image processing, the diameter distribution and other parameters of the pores were obtained, and the results compared with observations from high-pressure mercury injection and low-temperature nitrogen gas adsorption. The results revealed a high proportion of pores with diameters over the range of 3 to 50 nm, and the poor development of meso-porosity. The main pore types over different scales are summarized to relate pores to the pore network. The pores are divided into adsorptive pores and seepage pores, according to gas migration processes and a fractal model. The major types and morphologies of the adsorptive and seepage pores are summarized according to the results of the image characterization.
Based on the above experimental study, the characteristics of micro-nano pores and pore networks in high-rank coal deposits are explored. The meso-porosity of high-rank coal was poor, while the nanoscale reservoir space of thermal pores and residual microstructural pores were well developed, which leads to a high storage capacity, but weak microscopic seepage capacity in the coal matrix. The structural characteristics affect the seepage and release capacity of CBM in the coal matrix, and thus influences the productivity of high-rank CBM.

42.3- The Study on Inter-Particle Interaction and Its Effect on Coal Flotation

Yuexian Yu, Xi'an University of Science and Technology; Liqiang Ma, China University of Mining & Technology (Beijing); Zhen Li, Anning Zhou, Xi'an University of Science and Technology; PR CHINA.

Good hydrophobicity of coal surface is the prerequisite for a successful flotation. Slime coating, defined as fine and ultrafine hydrophilic particles coat coal surface, prevents the contact between coal and collectors/air bubbles, giving rise to a low flotation recovery. In this work, the behaviors of aggregation and dispersion between coal and clays (kaolinite, montmorillonite and illite) or original coal slimes (refer to the fine particles of <45 μm in flotation feed) were studied by using zeta potential distribution analysis, micro flotation test, focused beam reflectance measurement and the extended Derjaguin–Landau–Verwey–Overbeek (DLVO) theory. Firstly, the effect of clay coatings on coal flotation was studied. It is shown that, in the presence of clays, the acidic condition exacerbates clay coatings, which greatly depress coal flotation. However, in neutral condition, clays slightly coat coal surface, which only impacts the concentrate ash. In alkaline condition, clays do not depress coal flotation. Insufficient collectors during flotation result in low-density (<1.3 kg/L) coal slime coating which significantly depress coal flotation due to preferential affinity of these slimes to collectors and air bubbles. On the contrary, the hydrophilic high-density (>1.8 kg/L) slime only has a slight impact on coal flotation owing to its partially coating on coal. However, the middle-density (1.3~1.8 kg/L) coal slime dramatically decreased flotation recovery due to severe coating of these slimes on coal caused by the hydrophobic force. These middle-density coal slimes are heterogeneous. The hydrophobic patches of slime particle attach to coal surface dominantly through strong hydrophobic force. While their hydrophilic patches face outward to the water, preventing the contact between coal and collector/air bubble. The extended DLVO theory calculation shows that van der Waals force and electric double-layer force determine the clay coatings on coal surface. However, the mechanisms of original coal slime coatings on coal surface are different. The high-density slimes coat coal through weak van der Waals force. Middle-density and low-density slimes coat coal by both van der Waals force and hydrophobic force. Therefore, the adhesion forces between coal and low/middle density slimes are stronger than that of high-density slimes, which accounts for the different flotation results obtained above.

42.4- Mechanism of Influence of High Intensity Conditioning on the Interaction between Coarse and Fine Coal Slime during Flotation

Chao Deng, China University of Mining & Technology (Beijing); Liqiang Ma, China University of Mining & Technology; PR CHINA.

The intermediate density (1.4~1.8 g/cm3) fine-grained coal slurry below the particle size of 0.074 mm was mixed into the coarse-grained slime (> 0.074mm) to carry out the flotation test including the pretreatment step of the high intensity conditioning, and the effect of the intermediate density fine-grained coal on the coarse-grained slime during the flotation process was studied. The force between intermediate density fine coal slurry particles and low gray coarse granular coal was determined by AFM, and the surface shape of coarse coal in flotation clean coal and tail coal was observed by SEM. The appearance and the mechanism of its influence are discussed in combination with EDLVO theory. The results show that the inhibition effect of intermediate density fine-grained coal slurry on coarse-grained coal slurry in the flotation process involving pretreatment of the high intensity conditioning is better than that of conventional flotation which mainly depends on the high intensity condition can purify of the surface of the coal particles and disperse the collector, so that the collector has a greater collision probability and better adhesion to the coarse coal slurry.

42.5- Effect of Nitration on Indian Bituminous Coals: A Study by X-ray Diffraction and FT-IR Techniques

Prabal Boral, Sudip Maity, Ashok K Singh, Pradeep K Singh, CSIR-CIMFR; Atul K Verma, IIT- ISM; INDIA.

Coal can be used as a feedstock for aromatic chemicals like activated carbon, specialty carbon materials such as graphite, fullerene, graphene, humic acid etc. The study of structural parameters of coals and their structurally modified counter parts by nitration is very much essential to understand their basic nature and to decipher their suitability towards more meaningful industrial utilization. In this context, five Indian bituminous coals are treated with nitric acid in glacial acetic acid and aqueous media to find out the chemical and spatial structure of the organic mass by X-ray diffraction and FT-IR techniques.

X-ray parameters of coal like interlayer spacing (d002), crystallite size (Lc), aroamticity (fa), average number of aromatic layers (Nc), and coal rank (I26/I20) have been determined using profile-fitting software. Considerable variation is observed in treated coals in comparison to the raw (demineralized) coals. The d002 values of treated coals have increased in both the media showing increase in disordering of organic moieties. The Lc and Nc values have decreased in treated coals corresponding to raw coals. The present study shows that nitration in both the media is capable of removing the aliphatic side chains from the coals and aromaticity (fa) increases with increase in rank. The corresponding I26/I20 values are least for treated coals in glacial acetic acid medium followed by raw and then to treated coals in aqueous medium.

FT-IR studies show that coal arenes of the raw coals are converted into nitro-arenes in structurally modified coals (SMCs) in both the media, the corresponding bands at 1550 – 1490 cm-1 and 1355 – 1315 cm-1 respectively. FT-IR study confirms that nitration is the predominant phenomenon, though, oxidation and nitration phenomena takes place simultaneously during treatment with nitric acid to form SMCs. In comparison to raw coals, the SMCs show higher aromaticity and may be easily converted to coal derived products like activated carbon and specialty carbon materials.

SESSION 43
SUSTAINABILITY AND ENVIRONMENT - 2

43.1- Effect of Size and Surface Chemistry of AuENPs on the Uptake of the ENPs into the Sediment-Dwelling Lumbriculus Variegatus

Ping Luo, China University of Mining and Technology, PR CHINA.

With increased production, usage and disposal of engineered nanoparticles (ENPs), there is growing concern over the fate of ENPs in the environment. One of the major concerns is the bioavailability and the unknown toxicity of ENPs after the potential uptake by organisms. It is assumed that bioavailability and uptake depend on the environmental conditions as well as physiochemical properties of ENPs, such as particle size or surface coating. This study focuses on how different sizes and surface coatings of specially produced AuENPs influence the uptake of ENPs in the organisms. Uptake and depuration experiments were performed with the sediment-dwelling worm Lumbriculus variegatus. Characterisation of AuENPs in organisms including imaging and qualitative analysis by Synchrotron as well as their behaviour in natural sediment were performed. Studied AuENPs were coated with either citrate (AuCIT), mercaptoundecanoic acid (AuMUDA) or Bovine Serum Albumin (AuBSA) and featured size ranges of 5 nm and 30 nm. A control sample of ionic Au (Au3+) was also included. Surface coating and particle size were both found to be factors affecting the uptake and depuration of ENPs in Lumbriculus variegatus. Comparing these results to exposure with Au3+, the results showed that AuENPs settled more slowly in the sediment matrix, showed faster uptake rates during exposure and also faster elimination rates during depuration. Eventually the uptake and retention of Au ENPs and Au3+ in Lumbriculus variegatus ranked with regards to size in the following order: Au3+ > 5 nm > 30 nm. Surface coating influenced the uptake and retention of AuENPs in Lumbriculus variegatus in the following order: AuBSA > AuCIT > AuMUDA. However, synchrotron XRF imaging suggests a higher uptake of AuMUDA in Lumbriculs variegatus than of AuCIT.

43.2- TGA-FTIR Study on Co-Pyrolysis of Coal and Herb Dregs

Zhou Lu, Sun Shaojie, Wu Jianjun, China University of Mining and Technology, PR CHINA.

Chinese medicine dregs is the waste in the processing of Chinese herbal medicines, the production of Chinese Patent Medicines and the other Chinese medicine related products. The co-pyrolysis study in blended samples containing both Shenmu coal and traditional have been synthesized and characterized by thermogravimetric analyzer and Fourier transform infrared spectroscopy. The effects of different proportions of biomass on low-order coal pyrolysis process have been investigated. The results show that the co-pyrolysis of coal and dregs is not a simple superposition of the pyrolysis characteristics of individual coal and individual wood chips, but a synergistic effect. During co-pyrolysis, as the proportion of dregs in the blended sample increases, the apparent activation energy decreases continuously, but the reactivity increases. The analysis of infrared absorption spectra reveals that coal is blended with different proportions of dregs. The gas composition and content of the post-combustion heat analysis are also different. The co-pyrolysis is beneficial to the precipitation of combustible gases such as hydrocarbons in the coal, namely the volatile combustible gas, and the precipitation tendency of HCl decreases at first and then increases with the increasing of dregs content. Increasing dregs could add combustible gas escape, promote the premixed combustion of post-combustion, improve diffusion mixed conditions greatly.

43.3- Study on Water Reduction of Coal Pyrolysis Product over Perovskite Catalysts

Wang Qingyu, Demin He, Jun Guan, Dalian University of Technology; Xueqiang Li, Jianxuan Shang, Shanxi Coal and Chemical Industry Group Co. Ltd; Qiumin Zhang Dalian University of Technology, Dalian; PR CHINA.

The coal resources in China are relatively abundant. In many technology routes of coal chemical industry, the polygeneration system based on coal pyrolysis can make a reasonable comprehensive utilization of low-rank coal, to realize the complete conversion of coal in pyrolysis process, obtaining semi-coke, gas and coal tar. However, a large amount of waste water will be generated in pyrolysis process due to its high moisture contents, which would bring a great trouble on the subsequent treatment. Therefore, a catalyst suitable for the water-gas shift reaction under high temperature condition is prepared to remove the water vapor and CO produced by the coal pyrolysis process.

However, the temperature of coal pyrolysis is generally at 450-600°C, which is far beyond the scope of traditional shift reaction catalysts. Besides, the pyrolysis products contain a large amount of aromatic compounds and sulfur organic compounds, which may affect reactive activity of the catalysts.

Since the perovskite composite oxide (ABO3) presents a definite advantage in terms of thermal and chemical stability and exhibits a higher catalytic activity, a series of perovskite catalysts are prepared by citrate complex method and the catalytic activity was compared under the same conditions. In addition, the perovskite catalysts are partially replaced by A site and B site, and the effects of temperature, water-carbon ratio, space velocity, pressure and other conditions on the activity of the catalysts are investigated. The specific surface area of the catalysts is measured by BET, and its crystalline phase structure was determined by XRD, and the amount of carbon deposited on the catalysts was measured by using TGA.

43.4- A Research on Problems and Corresponding Strategies in Application of Integrated Membrane Techniques to Advance treatment and Recycling of Coking Wastewater

Shuguang Ouyang, Guanghua Wang, Wuhan University of Science and Technology, PR CHINA.

Coking wastewater mainly comes from primary cooling of coke oven gas and coking production process, purification and recovery process of coking chemical products. About 0.7 ton of wastewater is produced with production of 1 ton of coke. In 2017, 300,000,000 tons of coking wastewater was produced from the production of 431,426,000 ton of coke in China. As coking wastewater contains many toxic, biodegradable substances, it is considered as a hard-to-handle organic wastewater. Very often, direct emission of the pre-treated and biochemically treated wastewater, whose amount of pollutants is still high, can impose serious harmful impact on water bodies. Therefore, advanced treatment and recycling of the biochemically treated wastewater becomes a general trend in the field of wastewater treatment. Membrane process, together with its integration of other relevant techniques, is considered as one of the most promising methods of many advanced treatment and recycling methods. In general, the main problems in application of integrated membrane techniques to advance treatment and recycling of coking wastewater include high cost, instable effluent quality, secondary pollution caused by chemical cleaning of membrane and treatment of concentration liquid. Targeted at these problems, the author puts forward the following strategies: improving efficiency and stability of pre-treatment and biochemical treatment, improving fouling resistance and the antibacterial properties of the membrane, exploring new environment-friendly cleaning method of the membrane, salt extraction of concentration liquid for coking coal blending.

43.5- Comparison of Air Pollutant Dispersion around Buildings Using Computational Fluid Dynamics

Hesheng Yu, China University of Mining and Technology, PR CHINA; Jesse Thé, University of Waterloo and, Lakes Environmental Software, CANADA.

The accurate prediction of pollutant distribution near buildings is important in both indoor and outdoor air quality management. The commonly used Gaussian dispersion models such as AERMOD and CALPUFF do not perform well in the near field of constructions due to complex turbulence characteristics. Computational fluid dynamics (CFD), which resolves the obstacles, is an excellent alternative to modelling pollutant dispersion within built environment. A CFD dispersion modelling includes primarily flow simulation and the distribution of pollutant concentration based on the resolved flow field. This paper comparatively reviews different models in the CFD dispersion modelling around buildings. Firstly, it describes various widely accepted turbulence models such ask-ε family, k-ω SST, detached eddy simulation (DES), and large eddy simulation (LES), followed by the cross-comparison of performance between turbulence models in different cases from an isolated building and street canyon to complex city environment. The standard k-ε model is inadequate to simulate dispersion around constructions. The RNG k-ε model and SST k-ω model are appropriate RANS methods for air dispersion within urban settings. The advanced LES approach are more accurate than the RANS counterparts at a higher computational cost. Its implementation depends largely on grid density and inflow conditions. The hybrid DES is a bridging technique that delivers accurate results at a reasonable computational demand. Finally, this paper summarizes the best practices of CFD models in air quality management

SESSION 44
CLEAN COAL AND GAS TO FUELS - 3

44.1- Effect of Pretreatment Methods on Oil Agglomeration Performance

Jie Sha, China University of Mining & Technology, PR CHINA.

In this study, oil agglomeration of Chinese low rank coal (jet coal) was carried out using diesel oil as a bridging liquid. The study contains two stages. In the first part the optimal parameters of this experiment were investigated, such as solid concentration, amount of oil, stirring speed, agitation time and the dosage of the active agent on the agglomeration process. It has been found that without the improvement of activators, the difficult-to-float Chinese jet coal with low natural hydrophobicity could hardly ever been agglomerated. However, the adoption of isooctanol remarkablyfacilitated the growth of the spherical agglomeratesand thus increased the yield and the combustible matter recovery. On the second stage, the effects of the agglomeration operating methods were discussed. The conventional oil agglomeration was operated in the sequence of the slurry conditioning followed by oil adding. The article provides new procedures rely on direct contact between pure bridging oil and surfactant with dry coal followed by addition of water. The investigations showed that, the oil pre-wetting procedure provided better yield of the low-rank coal than conventional one. It was also concluded that, lower oil consumption could be achieved in oil pre-wetting procedure when choosing same yield and combustible recovery as criteria. Thus, oil agglomeration of hydrophilic low-rank coals can be successfully and economically accomplished by applying the oil pre-wetting procedure.

44.2- Internal Heat Transfer Characteristics of Pulverized Coal during Pyrolysis

Hongzhi Ni, Demin He, Jun Guan, Associate Professor, Dalian University of Technology; Xueqiang Li, Jianxuan Shang, Shaanxi Coal and Chemical Industry Group Co. Ltd; Qiumin Zhang, Dalian University of Technology; PR CHINA.

A 2D transient heat transfer model was established according to pyrolysis of single coal cylinder in the designed reactor. In this model, the effects of cylinder diameter size and final heating temperature on pyrolysis of coal were considered. Temperature gradient in small-particle coal could be overlooked during pyrolysis under low heating rate, but heat transfer in large-particle coal could not be neglected in industrial production. After boundary conditions like heat convection of samples in the reactor were determined, the developed model was solved by using Comsol multipysics software, to explore the effects of thermal conduction on internal and external temperature difference, thus getting temperature distribution and its variation with time. The composition of coal will change as the reaction continues, which will further influence heat transfer in coal. Water and organic matters evaporation during the pyrolysis also will affect heat transfer process and temperature distribution in lump coal. The effects of diameter size and final heating temperature on temperature distribution in lump coal were investigated. The calculated results are reasonably agreed with actually measured temperature. Moreover, a new reactor was designed based on the analysis of reaction kinetics, heat and mass transfer processes, for the pyrolysis process in lump coal. The efficient, economic, and clean use of coal is the inevitable way for future development.

44.3- Development of the Integrated Gasification Fuel Cell Power Generation System with CO_2 near Zero Emission

Dong Binqi, Shenhua Group Corporation Limited; Li Pingping, Li Chufu, National Institute of Clean and-Low-Carbon Energy; Yang Zhibin, China University of Mining and Technology (Beijing); Yuan Ming, Shenhua Group Corporation Limited; Wei Chang, National Institute of Clean and-Low-Carbon Energy; Peng Suping, China University of Mining and Technology (Beijing); PR CHINA.

Integrated gasification fuel cell power generation (IGFC) technology can greatly improve the efficiency of coal to electricity, reduce the cost of CO2 capture and realize the near zero emission of CO2 and pollutants. Under the support of National Key R&D Program of China, Shenhua Group combines some units, such as National Institute of Elean and-low-carbon Energy, China University of Mining & Technology, Tsinghua University, Suzhou HuaTsing Power and China Huaneng Group, to develop the IGFC technology with CO2 near zero emission. The IGFC technology developments will focus on system design and optimization, novel coal gasification and syngas purification, high temperature fuel cell power generation with syngas, tail gas pure oxygen combustion & CO2 capture and system integration & demonstration. The works will develop a 100 kW level solid oxide fuel cell (SOFC) and another 100 kW level molten carbonate fuel cell (MCFC) system with 50% electrical efficiency using coal syngas, and will build a MW level IGFC system with 91% CO2 capture ratio in early 2021, which will be the first high temperature fuel cell power generation system demo with syngas and CO2 capture in the world. Based on the system demo data, a 100 MW level IGFC system with 47% total efficiency and 90% CO2 capture ratio will be designed.

44.4- Structural Features and Pyrolysis Behaviors of Extracts from Microwave-Assisted Extraction of a Low Rank Coal with Different Solvents

Yankun Xiong, Haoquan Hu, Lijun Jin, Yang Li, He Yang, Dalian University of Technology; PR CHINA.

Microwave-assisted extraction of a low-rank Naomaohu (NMH) coal was carried out by two types of solvent, namely cyclohexanone (CYC) and tetrahydrofuran (THF), to obtain extracts (ECYC and ETHF) and residues (RCYC and RTHF). The raw coal, extract, and residue were characterized by elemental analysis, TG, FTIR, GPC, 1H NMR and solid-state 13C NMR. The results showed that CYC exhibits high total extract yield of 8.3 wt.% than THF being 4.7 wt.%. Moreover, CYC is more efficient in extracting organic components of NMH coal, especially condensed arenes and macromolecular compounds. The average molecular weight of ECYC is obviously higher than that of an average cluster of NMH raw coal. Online pyrolysis-vacuum ultraviolet photoionization mass spectrometry (Py-VUVPI-MS) was taken to investigate initial volatile products from pyrolysis of NMH coal, RCYC and ECYC. The distribution of initial volatile products suggested that NMH coal and ECYC possess same basic structures and ECYC is rich in macromolecular cluster with lots of side chains and bridge bonds. The chemical structures of the compounds in ECYC could reflect the macromolecular network structure of NMH coal to some extent. This work provides a way to study and construct the organic structure of coal.

SESSION 45
COAL SCIENCE - 10

45.1- Research on the Motion Characteristics of Fine Coal in Centrifugal Force Field

Zhang Jun, Tao Youjun, Shi Zhengxiang, Wang Yipeng, Zhao Younan, China University of Mining and Technology, PR CHINA

This paper described motion characteristics of fine coal in centrifugal force field, and introduced the working principle of the Falcon concentrator. By calculating the force and the settling final velocity of the fine particles in the centrifugal force field, it was obtained the relationship between the settling time of the fine particles and the centrifugal acceleration. The calculation result shows that the larger of centrifugal acceleration, density gap between the particle and the medium, diameter of fine particle, the shorter settling time of the particle. By calculating the tangential velocity of fine particle in the fluidization zone, it was found that the variation of the tangential velocity of the particles in the different flow film microlayers. The results show that the tangential velocity of each microlayer in the flow film gradually increased with the increase of the radius in the radial direction. At the end of the paper, taking -0.5mm fine coal of Wennan Coal Mine as an example, compared the actual effect of Falcon separator and flotation timed-release test on desulfurization and ash reduction, it was found that sulfur removal of fine coal in centrifugal force field was better than froth flotation.

45.2- Hydrogen Sorption Properties of MG-C Composites Prepared by Nickel Ball Milling

Ruiqian Jiang, Ruiqian Jiang, Xinyuan Li, Xiaojing Liu, Shixue Zhou, Shandong University of Science and Technology, PR CHINA.

In this paper, hydrogen sorption properties of Mg-coal based carbon (Mg-CBC) composites prepared by nickel ball milling were investigated. The CBC acts as a good solid lubricant during ball milling, efficiently suppressing the cold welding and agglomeration of Mg powders. During ball milling, the Ni atoms fall from the grinding balls when the grinding balls collide with each other. Element distribution analysis shows that Ni appears on both Mg and CBC particles. The pressure-concentration-temperature (p-c-T) test points out that the sorption plateau pressure of as-obtained Mg-CBC composites is reduced compared to that without carbon additive. Moreover, the hydrogen sorption kinetic of Mg is also enhanced due to the particle size reduction and Ni catalytic. As the particle size decreases, the distance of hydrogen diffusion inside the particles can be reduced.

45.3- Study on the Preparation of Coal Slurry by Ultra Low Ash Pure Coal

Shaopeng Gao, Shiyong Zhao, Xiao Liang, Xi'an University of Science and Technology, PR CHINA.

The energy structure of china is rich in coal, lack of oil and lack of gas. China's abundant coal resources are the safest, most economical and most reliable energy. Developing coal based liquid fuel and replacing oil with coal is an important way to ensure sustainable and reliable supply of energy based on domestic resource advantages. Therefore, the ultra-low ash clean coal (ash 0.74 %, yield 85.74 %) selected from Taixi Coal Separation Plant is taken as the research object. The research on the preparation of coal water slurry, oil coal slurry and oil coal water slurry, as well as concentration, viscosity, stability and rheology of coal slurry are carried out to analyze the slurry property of coal slurry. The results show that the concentration of coal water slurry is 61%, the shear rate corresponding viscosity is 1151mPa·s in 100s, and the amount of additive is 0.5%, which belongs to the swelling plastic fluid. The viscosity of the oil-coal slurry with coal, water and oil ratios of 45.9%, 12.7%, and 41.4% corresponding to a shear rate of 100s was 763.5 mPa·s, the viscosity of coal-water slurry prepared with coal and oil ratios of 50% and 50% corresponding to a shear rate of 100s is 687.8 mPa·s, both of them belong to a typical pseudoplastic fluid.

SESSION 46
COAL MINING AND BENEFICIATION - 2

46.1- High-Efficient-Fast Driving of Roadway by Bolting System in Practice

Guichen Li, China University of Mining and Technology, PR CHINA.

(1) Background: The General situation of roadway driving in China, the relation between coal mining and roadway driving, Consumption time of driving, the introduction of high-speed driving in economy and effectiveness.
(2) Theory and technology for high-efficient-fast driving: Continuous beam theory background, the requirement of support, the concept of transboundary support, the concept of large-bolt supporting technology, Technical characteristics of large-bolt supporting, Support effect of large-bolt, reducing the coefficient of stress concentration, and the construction process of large-bolt-support technique.
(3) Engineering practice: Geological conditions in 21204 longwall face, Hulusu coal mine, the comparison of original support and Large-bolt support scheme, Effect analysis and Support effect.

46.2- Prevalence of Musculoskeletal Disorders and Assessment of Workplace Factors: A Case of Coal Mine in Pakistan

Izhar Mithal Jiskani, Zhou Wei, China University of Mining and Technology, PR CHINA; Saleem Raza Chalgri, Mehran University of Engineering and Technology, PAKISTAN; Cai Qingxiang, China University of Mining and Technology, PR CHINA; Paras Behrani, Universiti Teknologi PETRONAS, MALAYSIA; Raheel Aziz, Balochistan University of Information Technology, PAKISTAN.

Mining is considered one of the dangerous and risk involving industries of the world. When considering the underground coal mining, it is unique in its health and safety issues. Musculoskeletal Disorders (MSDs) are one of the major rising issues in the mining industry. Many countries have developed their regulations and framework to overcome this risk but least development in the mining sector of Pakistan has put this issue at back. MSDs in coal miners have not been extensively studied in Pakistan. Thus, this cross-sectional study was conducted in order to find frequencies of musculoskeletal disorders and to assess workplace factors at the underground coal mine. The results open an avenue about the health and safety scenario in Pakistan's one of the crucial industries i.e. Mining. Results show that MSDs have been found in underground coal mine workers and an important issue emerging from these findings is inadequate working conditions and lack of awareness about ergonomics, which may be one of the root causes of health and safety problems.

46.3- Study on Utilization of Mine Drainage Water from Abandoned Coal Mines in Jiawang as Urban Water Source

Xiangdong Li, Bo Fei, Qiyan Feng, Ping Lu, China University of Mining and Technology, PR CHINA.

Xuzhou is a coal-based city with prominent contradiction between supply and demand of water resources. Increasing population industrial development and urbanization have led to the growing scarcity of drinking water. Jiawang mine area is one of Xuzhou many mining areas, due to over-exploitation of resources has been basically depleted, mine basically closed all the mines. However, a large amount of mine water generated from the exploitation of coal mines directly discharges without treatment, flooding the surrounding farmland and polluting the local environment.
The purpose of this study is to analyze the indicators of mine waste water quality, in order to reach the national drinking water standard after treatment, and be used for the utilization of water resources in Xuzhou. Utilization of mine water resources can not only greatly reduce the destruction of environmental resources caused by over-exploitation of groundwater resources in the mining area, but also alleviate the water shortage in Xuzhou urban area, which has hugly significance on the comprehensive utilization of mine water produced by coal mining in China.

46.4- A Closer Look at Large-Scale Coal Research Projects Sponsored by the National Energy Technology Laboratory

Thomas A. Sarkus, National Energy Technology Laboratory/ U.S. Department of Energy, USA.

Fouling of heat transfer surfaces plays a significant role in the efficiency and greenhouse gas emissions of a coal-fired utility, particularly in those plants utilizing nearby bodies of unprocessed water such as rivers or oceans for cooling. Buildup of either biofilms or scale deposition can significantly increase the effective thermal resistance within the condenser unit, turbine backpressure, fuel consumption, and greenhouse gas emissions. In order to mitigate these factors, every plant must adopt some form of cleaning and mitigation strategy, all of which require significant operational expense and/or regular required offline time.
This paper details the adaptation of a novel, fouling resistant surface treatment to improve the heat transfer performance of a prototypical shell-and-tube exchanger unit. The surface treatment, unlike most conventional epoxy coatings, was applied at a thickness of less than 100μm, and was shown to have a negligible effect on thermal energy transfer in a liquid-liquid model system. Characterization of biofilm growth and attachment on the treated surface was shown to be significantly reduced, both in static and dynamically controlled testing conditions. Additionally, despite the extremely thin application, the surface treatment showed excellent abrasion and erosion resistance, even when applied to a previously worn/cleaned substrate, indicating its potential for refurbishment of existing, in-service units.
The surface treatment was applied both on a laboratory coupon scale as well as on a pilot basis, in order to demonstrate both suitability at the micro- and macro-scale. This paper will detail the changes in exchanger performance and behavior after application, along with outlining the expected improvement both in operational efficiency. Additionally, initial trials on applying the coating on the vacuum-side of a condenser unit in order to promote more efficient drop-wise condensation shall be discussed, and an estimate on the overall effect on plant operations and estimated backpressure penalty shall be determined.

SESSION 47
GASIFICATION TECHNOLOGIES - 8

47.1- Progressive Reaction between Na/Ca and Silica during Gasification of Low Rank Coal

Ge Yu, Yu, Huazhong University of Science and Technology, PR CHINA.

Coal gasification is widely developed nowadays. The low rank coal (such as the Zhundong coal), which is of low ash and high content of sodium and calcium, is particularly suitable for gasification. It is well-known that sodium and calcium can catalyze the gasification process. Nevertheless, the silica existed in the coal can also

react with them, which will decrease their catalysis and change the char or ash properties. Temperature and atmosphere may be the key factors that affect the reaction. However, the progressive reactions between silica and sodium/calcium during gasification is still unclear. This work aims to investigate the progressive reaction between the Na/Ca and silica during the gasification process. Experiment was conducted in a novel thermo-gravimetric reactor (TGR, Figure 1). The Ca-loaded coal, Na-loaded coal, and Ca/Na-loaded coal were mixed with silica, and then reacted in pure N2 (pyrolysis), CO2 + N2, H2O + N2, or CO2 + H2O + N2 (gasification) at different temperatures. The partially reacted samples were extracted at different reaction time and subjected to analyze the characteristics by SEM-EDS, XRD and N2 adsorption measurement. In addition, the volatilization of Na and Ca were obtained by ICP-OES. Based on the data obtained, the progressive reaction between the Na/Ca and silica during gasification is better understood.

47.2- U.S. DOE's Gasification Systems Program - An Overview

K. David Lyons, National Energy Technology Laboratory; Massood Ramezan, KeyLogic Systems; USA.

The U.S. Department of Energy's (DOE) Gasification Systems Program has a history of success in technology development and demonstration. The Gasification Systems Program supports the development of technologies that will advance the use of coal while benefitting the global environment. To accomplish this, the primary program focus is converting coal into clean synthesis gas (syngas) that can in turn be converted into electricity, chemicals, hydrogen, and liquid fuels to suit market needs while reducing pollutants. In the past the program's research and development (R&D) portfolio focused on deployment of the clean and affordable energy systems required for growing energy markets. The program supported several major projects, such as demonstrating novel, efficient, and cost-effective high-temperature gas cleaning technology, as well as developing a non-cryogenic air separation technology with lower capital cost and energy requirements than conventional cryogenic processes to produce high-temperature/high-purity oxygen from air by using ceramic ion transport membranes. These and other projects supported DOE's vision of near-zero emissions power generation by reducing the cost and improving the efficiency of energy production from coal.

The Gasification Systems Program is currently transitioning to and focusing on smaller, lower-cost, profitable, gasification-based energy systems that will support a significant reduction in emissions from coal. These efforts will also produce technologies for increasing plant reliability and improving the product and byproduct creation for increased value. Benefits from this approach include:

Reduced cost: Small, modular plants with common components could be built prefabricated, which reduces construction time and costs.

Improved environment: New and innovative technology designs will help to reduce water use and all emissions, including carbon dioxide (CO_2).

Market: The right-sizing of plants to local markets by coupling several small, prefabricated modular units can open the market for coal-based plants.

Opportunity feedstocks: Opportunity fuels, such as waste coal and coal fines, municipal solid waste (MSW), and local biomass, will reduce the cost of products.

This paper provides an historical overview of DOE's Gasification Program, features the Modular Energy Systems R&D, and provides detailed discussion of advances in technologies that will serve as the foundation for future low-cost, coal-based energy systems that will enable new applications for coal worldwide.

47.3- R-GASTM Coal Gasification Technology Development and Demonstration

Zhiwu Feng, Yangquan Coal Chemical Group, PR CHINA; Zhong Eric Zhou, Gas Technology Institute, USA.

GTI's R-GAS™ technology offers a pathway for direct gasification of high ash content, high ash fusion temperature (AFT) coals. With an efficient, high-performance design that eliminates the need for feedstock blending and/or fluxant addition – as is required with existing commercial technologies – R-GAS™ provides a cost-competitive solution for the clean utilization of China's large reserves of high AFT coals. Together with Yangquan Coal Chemical Group (YQ), the R-GAS™ technology is being scaled to a commercially viable size and demonstrated in an 800MTPD unit at YQ's plant in Taiyuan, China.

Based on propulsion combustion technology, R-GAS™ establishes plug flow in the gasifier reactor through rapid and efficient mixing, eliminating large scale recirculation in the reactor, allowing the gasification reactions to occur at high temperature. This reduces residence time, providing peak performance in a compact design. The gasifier pressure vessel is protected by a water-cooled liner designed for high heat flux, keeping the metal at safe temperatures during operations with gasification temperatures above 2,700°C in the reactor and maintaining the liner-exit temperatures above AFT (1,500 ~1,690°C). The partial-quench design allows for both dry and wet removal/recovery of fine ash. Wet recovery process will be employed in the current demonstration plant, making use of the existing blackwater system at the facility. The ability to retrofit a total quench configuration will also be available if desired. Another key technology that will be demonstrated is the ability to split coal feed in an ultra-dense phase flow regime (<55% transport gas fraction by volume) from one to multiple lines to enable the use of multi-element feed injection.

YQ, as a top 3 coal chemical company in China striving to become a leading force in the field, has been operating and developing modern plants of methanol-to-olefins, coal-to-ethylene glycol, coal-to-ethanol, coal bed methane-to-olefins, and coal bed gas-to-glycine, etc. YQ have partnered with GTI to demonstrate direct gasification of high AFT coals, which account for about 50% of China's total coal reserves and more than 70% of the total coal reserves of Shanxi Province. Test runs have been carried out using GTI's 18TPD pilot R-GAS™ facility to evaluate three different varieties of YQ high AFT coal: #15 coal, Xinjing coal, and Xinyuan coal. Over 300 hours of pilot plant operation with these coals had demonstrated carbon conversion up to 99%, operations both with and without steam injection, and direct utilization of feed stocks with ash fusion temperatures exceeding 1,600°C and ash content exceeding 28wt%, dry-basis.

The success of the pilot plant studies has led to the current demonstration program, in which a commercial-scale R-GAS™ unit is being designed for 800MPTD of #15 coal, with the ability to operate on the Xinjing and Xinyuan coals as well. Having completed the process design package and HAZOP analysis, the project partners are presently engaged in detailed engineering, procurement and construction activities, with commissioning and startup anticipated in 2019. The demonstration unit is projected to achieve carbon conversion and cold gas efficiency (CGE) up to 99.9% and 80%, respectively. Successful demonstration of the R-GAS™ gasification technology will provide a new solution for the efficient and clean utilization of high-AFT coal in China. Moreover, this demonstration will prove the commercial viability of R-GAS™ technology, paving the way for scale-up to larger units and deployment for use in future plants with both high AFT and traditional-rank coals, for which performance is estimated to exceed 84% CGE (IL#6 coal). Once fully commercialized, R-GAS™ gasification technology would help the Chinese coal chemical companies to tap into their local coal reserve of high AFT for more effective and economic utilizations.

47.4- Design Basis of 1 MWth Calcium Looping Gasification Pilot Unit

Zekun Jia, Haibing Li, Bingfei He, Bin Xu, Limin Shao, Haozhe Chen, Kezhong Li, ENN Group Co., Ltd.; Liang Zeng, Tianjin University and Collaborative Innovation Center of Chemical Science and Engineering; PR CHINA.

The calcium looping gasification (CLG) process decouples the coal gasification and combustion in two fluidized bed reactors, including the gasifier and the regenerator. CaO-based sorbent is used to link the two reactors by CO2 soprtion/desorption and heat transfer. In the gasifier, the coal is gasified, and the sorbent is added to capture CO2 and enhance the quality of the synthesis gas. In the regenerator, CaCO3 decomposes into CaO and CO2. The energy required for calcination is provided by the combustion of unreacted coke from the gasifier. There are many advantages of the CLG process, including:

The gasification process efficiency can be optimized by adjusting the carbon conversion between the two reactors.

The coke which is hard to be gasified is burned in the regenerator, thus improving the overall carbon conversion and reducing the gasifier size (residence time) at the same time.

The regenerator uses air instead of oxygen, therefore the air separation unit is avoided and the capital investment is reduced.

CaO sorbent can be used to in-situ separate CO2 and directly adjust the ratio of H2/CO which is beneficial for the downstream applications.

The operation of CLG process is challenging because of the matching of two pressurized fluidized bed reactors. The mass balance, energy balance and pressure balance between the two reactors are interrelated key factors. ENN has investigated the influence of these key factors, and conducted experiments and simulations to design 1 MWth pilot scale unit. The CLG process was designed to produce synthetic natural gas (SNG) from lignite or sub-bituminous coal. In this work, Buliangou sub-bituminous coal was used for both simulation and experiment. The effects of temperature and the ratio of reactants on carbon conversion and gas composition were studied. The results of thermodynamic simulation have shown that the decrease of gasification temperature favored the formation of methane. However, when lower than 750oC, the molar ratio of H2 and CO was too high to further produce methane and chemicals. Therefore, an operation temperature around 800oC was appropriate for gasification. Lab-scale fixed bed experiment was conducted to verify the simulation results, from which a similar conclusion was drawn. The effect of calcium oxide to coal ratio was also investigated. The addition of calcium oxide was helpful on improving the product gas quality and reducing the carbon dioxide emission from the gasifier. The carbon conversion increased along with the increment of calcium oxide to coal ratio. Based on the fixed bed results, the mass balance and energy balance of the whole system was calculated. Two adiabatic reactors were operated at optimized temperature, and the heat balance between them was satisfied, with the circulation of calcium oxide and ash. A cold model test was also carried out, and related parameters were obtained by a series of experiments and modifications, which provide the foundation for the design and construction of 1 MWth CLG pilot-scale unit.

47.5- Dry Solids Pump – Full-scale Development and Testing at 500 psi

Timothy W. Saunders, Joseph Caravella, Gas Technology Institute; Greg Weber, University of North Dakota; USA.

The gasification and clean coal industry has been seeking a solution for feeding carbonaceous materials into high gas pressure environments for many years. Existing feeding technology handicaps the implementation of such advanced combustion systems. These limitations include pressure levels below that desired by the system manufacturers, unreliable and inaccurate feed control, and the need for very large footprints and structure heights to incorporate the stacked lock hoppers that are the only feed solution. These attributes contribute to high capital cost, high operating cost and a proven low level of feed reliability. Additionally, existing feed systems are very inflexible in their ability to handle a wide range of coal types, particularly low rank coals such as sub-bituminous and lignite. For advanced combustion systems to achieve the objectives expected for them, highly controlled and accurate feeding along with flexibility in feedstock is critical to reduce cost of operation and make the combustion systems competitive with traditional power plants. Further, an efficient and inherently compact feed system enables modularization through factory manufacture and scalability.

This requirement for a high-pressure feed solution has in major part been developed and funded by the US Department of Energy National Energy Technology Laboratory (NETL). The project was taken up by Pratt and Whitney Rocketdyne (PWR), later becoming Aerojet Rocketdyne, and then acquired by the Gas Technology Institute (GTI), who is finishing the development program. PWR initially designed and manufactured a full-scale Dry Solids Pump (DSP) at the request of NETL. This direct-to-commercial scale approach was intended to reduce the development time to market for the DSP system. The full-scale DSP was manufactured and installed in a test stand at the Energy & Environmental Research Center (EERC) in Grand Forks, North Dakota. Following DSP commissioning, a test program was undertaken to verify the pump's ability to inject pulverized coal into high gas pressure. The test team found there to be a challenge to this development approach arising from the time to dismantle, cost to modify, and time and cost to reassemble the commercial-scale pump to support iterative changes required for development. Hence the ability to modify the feeder as lessons were learned in its operation became very expensive and time consuming. To address this challenge, a program was instituted whereby a subscale version of the DSP was built to allow rapid and lower cost optimization of the internal mechanisms of the machine and enhancements to the configuration to improve performance and efficiency. As part of this subscale program the DSP was tested using a range of coals from anthracite through bituminous to sub-bituminous, lignite and biomass blends with the previous coal feeds. The subscale DSP was able to confirm its ability to handle these coals and coal-biomass blends and allow injection into a high-pressure environment (150 psi for the subscale DSP). The DSP design and configuration was developed and optimized through the subscale program to handle these various and wide-ranging fuel types. The design data generated by the subscale test program was then incorporated into a modification of the original full-scale DSP. The design upgrades were incorporated into a revised full scale DSP which was commissioned early in 2018. Following commissioning the DSP has been tested at a range of pressures up to 500 psi, the hardware's design pressure limit.

This paper will present the results of the subscale pump test program and the resulting design modifications made to the full-scale DSP. Test results from the full-scale pump program will be reviewed along with the anticipated commercial DSP configuration. The anticipated commercial DSP configuration is based on these test results, consistent with the general objectives originally laid out by the DOE for the feed system.

SESSION 48
COAL SCIENCE - 8

48.1- New Direction of High Efficient Utilization of Coal-Research Process of All Group Component Separation and Applied Technology

Zhihong Qin, Xiaoqin Yang, China University of Mining and Technology, PR CHINA.

The history of coal utilization is reviewed briefly. On the basis of above, a new method of all group component separation and a new idea of petroleum processing and utilization of coal group components for classification and utilization which was presented expressly. I introduced the following aspects. Coal - based composite carbon films were prepared by using coal group components. The coal - based intermediate carbon microspheres and intermediate semi-coke were prepared based on the source material. Coal-based carbon foam and supercapacitor were prepared by group components. And a new method of coking coal blending based on all group component separation. Finally, the new model of coal embedded structure model is summarized.

48.2- Model Research on the Main Process Parameters of Heavy Medium Separation

Deng Jianjun, Chen Ming, China University of Mining & Technology; Guo Congtao, Huaibei Mining Group; Sun Qingfang, Wang Chuanzhen, China University of Mining & Technology; PR CHINA.

In the actual production process, the structure parameters of the heavy medium cyclone can't be changed, the change of the raw coal nature is uncontrollable. So the stability and optimization of process parameters is the key factor to the full realization of heavy medium cyclone separation. The main process parameters affecting the cyclone separation are: heavy medium density, magnetic material content, the medium inlet pressure, the feeding quantity, etc. The effect of process parameters on the separation is mainly through affecting the actual separation density. Based on the analysis of the influence of process parameters on the separation density, firstly establish the mathematical model between the actual separation density and the various process parameters, then establish the relationship model of product structure and the actual separation density, in order to determine the best separation process parameters in accordance with the requirements of product structure. The actual production situation shows that the model can better reflect the actual production to some extent, but there is a certain deviation, so it also needs to be improved.

48.3- Experiment and Mechanism Study on Floatation of Fine Coal by Nano Bubble Flotation Column

Fangyuan Ma, Doctoral Student, China University of Mining and Technology; Doping Tao, Liaoning University of Science and Technology; Youjun Tao, China University of Mining and Technology; PR CHINA.

Flotation is a fine particles separation technology that is the most effective and the most widely used.The range of narrow flotation particles is the defect of traditional flotation technology,it is about between 10mm to 100mm.Too large particles or too fine particles will result in low flotation efficiency.The main reasons are the collision probability between fine particles and bubbles is small and the probability of loss large particles,the attachment probability of coarse particles and bubbles is small ,and the probability of coarse particles falling off the bubbles is large. There are many ways to form nanobubbles, Venturi tubes are used to form nanobubbles by hydrocavitation .Flotation column has good performance, and it is widely used in the flotation field.For the fine coal,venturi tubes are used to create nanobubbles,and the flotation recovery effect of nanometer bubbles on fine-grained coal is studied by changing the conditions of flotation column.On this basis, the recovery mechanism of nanometer bubble to fine coal is described.Experimental results show that the recovery rate can be increased by 10% to 39%. Under the condition of adjusting flotation factors,.and the dosage of conventional bubble flotation agents is reduced by more than 1/2. The nanobubbles can concentrate on the surface of hydrophobic particles in the flotation system.Due to the collision and adhesion probability of particles and bubbles is increased by nano bubbles and the probability of particles and bubbles falling off is reduced by nano bubbles,the flotation is optimized.Nano bubbles play a role that is secondary collector because they are preferentially formed on the surface of hydrophobic particles.nanometer bubbles can improve the surface hydrophobicity of particles, which is beneficial to improve the flotation efficiency and recovery.In addition, The nano-bubbles can selectively agglomerate hydrophobic fine particles,increase fine particles size, combine the collision and attachment process into one, increase the rate of mineralization, and increase the probability of collection.

48.4- Process Factors for Preparing Ultra-low-ash Low-rank Coal using Oil Bubble Flotation

Jinzhou Qu, Quan An, Li An, Anning Zhou, Zhen Li, Wei Yu, Lijun Liu, Meili Du, Chao Yang, Xi'an University of Science and Technology, PR CHINA.

Ultra-low-ash low rank coal is an important raw material for chemical industry. In order to utilize the fine-grained low rank coal effectively and solve the problem of poor floatability, severe entrainment, and high consumption of oil collectors in flotation, the oily bubble flotation method was introduced. Based on the atomization and flash evaporation method, the new oil bubble generation device was designed. Then, it was used for the oily bubble flotation test of the Cuner coal samples, Shendong Mining Area. Therefore, the optimum process conditions for the oil bubble floatation were explored. The results showed that the best ultra-low-ash concentrate with ash content of 3.02% and combustible matter recovery of 94.47% was obtained at the pulp concentration of 66.7g/L, the frother dosage of 0.77 kg/L and the collector dosage of 0.90 kg/L. It seems that the selectivity of flotation concentrate is improved and the consumption of flotation reagents is reduced by oily bubble flotation. These works could contribute to the preparation of ultra-low-ash low rank coal and the expansion of coal flotation method.

48.5- Exploration on the Process Characteristics of Oily-Bubble Flotation of Low Rank Coal

Tao Xiu-xiang, Chen Song-jiang, Yang Zhao, Li Lu-lu, China University of Mining and Technology, PR CHINA.

China is rich in low-rank coals that account for 45.68% of existing coal reserves in China. The clean and efficient utilization of low rank coals is of great significance for ensuring the effective energy supply and promoting economic development and environmental protection. In order to solve the difficult problem in flotation of low rank coal, it has become the focus of research in the related field that oily bubbles instead of air bubbles are taken as a carrier in flotation to improve the attachment efficiency and recovery of low rank coal. In this paper, low rank coal slime collected from Shendong mining area was used as the experimental material, and it focused on the characteristics of oily-bubble flotation process of low rank coal. Additionally, difference in conventional flotation and oily-bubble flotation was discussed.
The induction time between air bubbles, oily-bubbles and fine low rank coal particles was measured. The results indicated that the induction time between oily-bubbles and coal particles was obviously lower than that of air bubbles. By comparing the foam height of air and oily bubbles, it was found that the amount of oily bubbles is less than air bubbles, causing relative low flotation rate of oily-bubble flotation at initial stage. Besides, the maximum foam height and half-life of air bubbles and oily-bubbles were measured respectively. The results showed that the stability of oily-bubbles was higher than that of air bubbles, which is benefit for the enrichment of concentrates. The clean coal water recovery of oily-bubble flotation is lower than that of air bubble flotation, which indicated oily-bubble flotation is lower in water entrainment.

SESSION 49
SUSTAINABILITY AND ENVIRONMENT - 3

49.1- Indonesia's Coal Production Forecast using System Dynamics: The Impact to the Environment

Firly R. Baskoro, Katsuhiko Takahashi, Katsumi Morikawa, Keisuke Nagasawa, Hiroshima University, JAPAN.

Indonesia plays an important role in global coal supply, it was proved by the ranking of Indonesia in terms of coal production and export amount. In 2017, Indonesia is the 5th largest coal production and ranked 2nd in the amount of coal export in the world. In the same time, the amount of coal production in Indonesia is around 461 million tons. However, only 97 million tons of coal production that accounted for domestic utilization. In the future, the Indonesia's coal production is expected to be increased due to the growth in coal demand for electricity generation. In contradiction with the production, the amount of Indonesia's coal reserves (128.1 billion tons of coal resources and 28.5 billion tons of coal reserves) is only 2.2% compared to the world coal reserves. This condition leads to a concern over the security of coal supply in the domestic market, as well as the impact of coal utilization to the environment. To overcome the concern, study for predicting the future of coal production in Indonesia is necessary. This research is conducted with an aim to estimate the amount of Indonesia's coal production to achieve the target of primary energy demand, as well as to examine the interaction between primary energy sources in determining the national energy mix, and analyze the impact of coal production to the carbon emission. A lot of research has been conducted to predict the future of coal production using time series forecasting method. The method only considering the historical production data as the variable, which means it was unable to be directly applied in decision-making due to limited knowledge of the factors that affect the production. By using system dynamics, it is possible to understand the parameters that affecting the coal production and it is possible to discover the behavior of coal production. In addition, system dynamics also allows us to conduct simulation and provide a better result for policymaking. This feature is important to develop energy policy regarding the economic and environmental aspects. To produce a result that has a closer similarity to the real system, the model will be arranged based on the energy structure in the real system. The interaction between coal and its substitution will be analyzed to understand the behavior of energy sources in the energy mix. Export will also be accommodated in the model, as a significant factor for coal production and economic growth in Indonesia. Coal production strongly influenced by the number of available reserves, which also related to the coal price. This research will incorporate the impact of several factors, such as coal reserves, the interaction between coal and its substitution, and coal price, to estimates Indonesia's coal production in supporting economic growth. This model of Indonesia's coal production will provide an insight for coal policy regarding the market structure, economic aspect, and environmental issue.

49.2- Product Distribution Control and Reaction Mechanism Study of Isobutanol Conversion into Aromatics

Wen-yi Yang, Bin-bin Zhang, Zhen-yi Du, Wen-ying Li, Taiyuan University of Technology, PR CHINA.

Isobutanol can be produced in large scale by biomass fermentation as a renewable energy source. Production of low-carbon olefins and light aromatic hydrocarbons using isobutanol as the raw material is a very promising process. In this work, the conversion pathway of isobutanol to olefins and aromatics was studied over parent and Ga impregnated ZSM-5 zeolites. In contrast to olefins, the selectivity of aromatics and alkanes can be increased byreducing the Si/Al ratio and increasing the residence time. The results showed that isobutanol were firstly dehydrated to isobutene on ZSM-5 zeolite, and then polymerized to form high-carbon alkenes which can be further converted to aromatics and alkanes through hydrogen transfer route. This reaction mechanism was confirmed byintermediate species detected with in-situ FT-IR method. After Ga2O3loading, the aromatics selectivityincreased, which suggested that the high-carbon alkenes produced by polymerization from low-carbon olefin were preferentially dehydrogenated into aromatics with the presence of Ga species.On the other side, the cracking activity to form ethylene and propylene was weakened. The amount of Brønsted acid sites in the Ga impregnated samples decreased because the Ga species replaced the H+ on Brønsted acid sites at the surface of zeolite, forming BAS-Ga structure and promoting the dehydrogenation route through the synergistic effect.

49.3- Insight into Ce-Fe Binary Oxides for Oxidative Dehydrogenation of Ethylbenzene to Styrene with CO_2

Kechen Song, Xueqi Guo, Deping Xu, China University of Mining & Technology (Beijing), PR CHINA.

The oxidative dehydrogenation of ethylbenzenewith carbon dioxide (CO2-ODEB) has received much attention because it is characterized in high efficiency, energy-saving, and effective utilization of the greenhouse gas of CO2. It has been reported that the utilization of CO2 could reduce the required energy from 6.27×106 to 7.9×105 kJ/ton of styrene produced [1]. The reaction may follow the Mars-van Krevelen redox mechanism involving the lattice oxygen over Ce-Fe binary oxides [2]. Meanwhile, introducing Fe ions with undersized and low valence in Ce lattice or vice versa could increase the thermal stability and cause strong lattice structural distortion, then lead to rapid oxygen transport and high OSC property.
Nano-sheets Al2O3 (NSA) supported Ce-Fe binary oxides with different molar ratio were synthesized by vacuum impregnation and interpreted by XRD, N2 physisorption, and H2-TPR. Then comparatively evaluated as catalysts for the CO2-ODEB, under atmospheric pressure, T = 550 oC, CO2/EB mole ratio = 20, W/F= F=7.25 g-cat•h/mol, to investigate their catalytic activity.

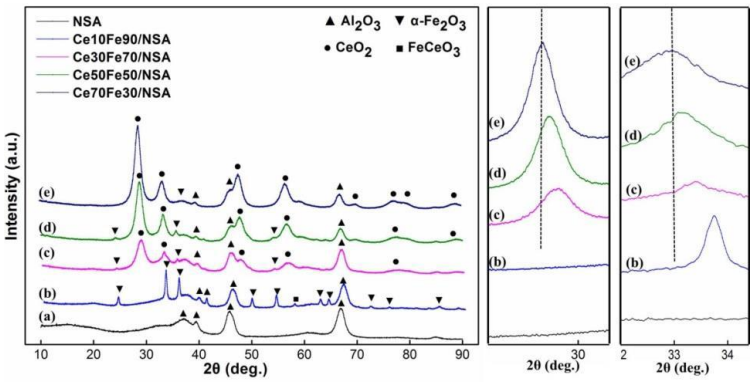

Fig. 1 XRD patterns of the (a) NSA, (b) Ce10Fe90/NSA, (c) Ce30Fe70/NSA, (d) Ce50Fe50/NSA, (e) Ce70Fe30/NSA.

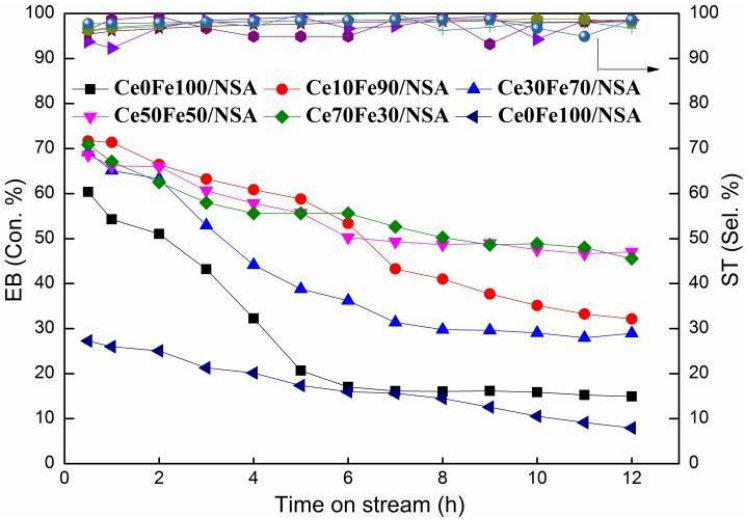

Fig. 2 Catalytic results Ce-Fe binary oxides for CO2-ODEB.

As shown in figure.1, the characteristic peak of CeO2 and Fe2O3 shifts towards higher 2θ position, indicating the formation of cubic CeO2 and α-Fe2O3 type solid solution. Furthermore, from figure.2, the activity and stability of Ce-Fe binary oxides in CO2-ODEB maintain a high level, after 10 h reaction, the conversion of ethylbenzene still above 30%.

SESSION 51
COAL SCIENCE - 11

51.1- Energy-Efficient and Wear Reduced Hydraulic Piston Press for Agglomeration of Coal, Waste and Renewable Resources

André Schmidt, Franz Fehse, Felix Stöhr, Thomas Müller, Hans-Werner Schröder, TU Bergakademie Freiberg, GERMANY.

Agglomeration of finely-dispersed materials is one of the major applications in process engineering. For a wide range of materials such as coal, renewable and mineral resources as well as waste and residual materials the appropriate agglomeration is an important process step for the following applications. An evaluation of technical opportunities for the production of high-quality agglomerates always depends on particular physical and chemical characteristics of the feedstock. Essentially a product distinction can be made between large (briquette) and small-sized agglomerates (pellet, granulate). Depending on the desired product shape different agglomeration technologies can be applied, e.g. Extrusion and Roller Presses for briquettes or Die Presses for pellets.

Through the technical limitations of certain press technologies, the applicable range of feedstock materials is restricted. This circumstance was the starting point for the development of a new agglomeration technology, which is characterized by a wide range of applicable feedstocks and which is suited to high quality briquette production. A major focus of the technical development was the task to find a briquetting process with a minimum specific power consumption. This can be achieved by performing a hydraulic driven two-stage-press-process, with an optimization of the length of hydraulic cylinder extension. Thus a significant reduction of operational expenses can be achieved, as well as an increase of the die profitability of industrial scale coal upgrading plants. This new operating principle opens the opportunity to reduce the relative movement between the emerging briquette and the forming tool at high pressure and results in a significant wear reduction of the forming tools. Hence a second major factor for the reduction of operational expenses can be derived. By extending the operating time of the forming tools the machine downtime for maintenance can be decreased and higher annual throughputs can be achieved. Furthermore, an easily maintainable machine design allows fast forming tool replacement and short maintenance periods.

Another major motivation for this new technology development was the situation at briquetting machine market for coal applications. Since decades the dominating briquetting technology in Germany is the Ram Extrusion Press. There are industrial coal processing plants where presses manufactured in the 1920's are still in operation. Hence to the operating principle of generating the counterforce for briquetting by friction and narrowing of the forming channel a massive wear occurs at the forming tools. Depending on feedstocks ash content, the operating time of a forming tool can go down to just some days. Thus the operational expenses and annual operating time of the single machine have a negative impact on plant profitability. Besides this technology is connected with huge capital expenses.

The only currently available substitution are Roller Presses for the production of egg and pillow-shaped briquettes, as well as coal scabs. The main disadvantage of these machines is a limited applicability for different coal types and fluctuations in feedstock quality. Huge briquette quality problems occurred when trying to adjust the Roller Press operation to feedstocks like soft-, subbituminous- and hard-lignite. It has been shown that an addition of binders such as starch; molasses or tar pitch is often inevitable for a stable briquetting process with high quality products.

By performing a two-stage press process with hydraulic cylinders it is easily possible to adjust the effective press force to the feedstock conditions. This enables the new universal High-Performance Press to adjust itself in operation and to generate a stable high quality product output. Coming from this considerations a team of young mechanical, process and electrical engineers started two years ago with the construction of a process demonstrator to verify the proof-of-concept. After finishing the assembly and initial commissioning first operating tests were made. The demonstrator with a throughput of about 50 kg/h was successfully tested with different feedstocks (soft lignite, wood chips, bagasse and dried sewage sludge) and briquettes were produced which are characterized by a high mechanical strength, good abrasion and drop resistance und a good thermostability. It was shown that an adjustment of the new High-Performance Press to soft and hard lignite feedstocks can easily produce briquettes which are suitable for coking processes, as well as for gasification in fixed and moving bed gasifiers. Currently the demonstrator is used for feasibility investigations in our technical center for a wide range of different feedstock materials.

With a publicly subsidized research transfer project the German state supports the developer's team on their way to the market launch with a total subsidy of 750,000 €. The current project stage takes place at the Institute of Thermal, Environmental and Natural Products Process Engineering of TU Bergakademie Freiberg and aims on the founding of a spin-off-company selling the new technology on an industrial scale. Therefore a pilot plant is under construction which should demonstrate the industrial scale briquetting of soft lignite with a total throughput of about 3.2 t/h. An initial commissioning of the pilot plant on workshop site is planned for November 2018. Within next year there will be a three-month industrial test period at the production site of an industrial partner with a 24/7 machine operation. Besides the mechanical development of the High-performance Press and its scale-up the project is focused on new technical measurement approaches. These will enable the machine to adjust its operating conditions fully automatically according to quality fluctuations of the feedstock. Furthermore a predictive maintenance concept will be integrated in the pilot plant. By measuring the change of material and surface characteristics of highly wear exposed components, such as the forming tools, an algorithm will extrapolate the wear impact up to the maximum allowed wear appearance and will enable the operator to schedule the downtime of a single machine in operation.

The project team will give a brief overview on state of the art briquetting technology and will derive the technology features of the new High-Performance Press. Furthermore, an overview of the current state of laboratory investigations and results of the agglomeration tests with different feedstocks at the two-stage-press-process will be given. Finally performance parameters of the new High-Performance Press such as power consumption and throughput may be discussed.

51.2- Effect of Additives on Semi-Coke Water Slurry Property and Quantum Chemistry Study

Meng Zhuoyue, Yang Zhiyuan, He Xiaoxiao, Xue Wenying, Xi'an University of Science and Technology, PR CHINA.

The proper molecular structure model of semi-coke and four kinds of additives of semi-coke water slurry (sodium humate, sodium lignin sulfonate, sodium dodecyl sulfonate, and (IA-PEG)-MAN-SMAS) were built by using the quantum chemistry calculations software-Material Studio (MS). Parameters of the structure such as geometric configuration, frontier molecular orbital and the adsorption energy between semi-coke and dispersants were calculated by the software, which were optimized by using the Density Functional Theory (DFT). The mechanism between the semi-coke and dispersants was revealed from the perspective of quantum chemistry, and the adsorption energy between semi-coke and dispersants were studied by MS. The higher the adsorption energy, the stronger the adsorption between semi-coke and dispersants, the adsorption energy order is (IA-PEG)-MAN-SMAS> sodium humate> sodium lignin sulfonate> sodium dodecyl sulfonate, which were in keeping with the results of experimental data. The comprehensive method of quantum chemical calculation combined with experimental data provides a novel research route of dispersants of semi-coke water slurry.

51.3- Adsorption and conversion of thiophene on the modified NaY zeolites in the atmospheres containing H_2, CH_4 and CO

Fanjing Wei, Junjie Liao, Xiaoqin Guo, Liping Chang, Weiren Bao, Taiyuan University of Technology, PR CHINA.

Coke oven gas, as one of the main by-product in the process of coal coking, is a very wide range of important industrial fuels and chemical synthetic materials. However, the ppm level sulfurs in coke oven gas, especially thiophene, can corrode pipes and poison the catalyst which restrict its subsquent utilization. H2, CH4 and CO, as three primary combustible components in the coal-based gases with complicated composition, undoubtly have different impacts on the adsorption and conversion of thiophene, and little effort has been spent on the mechanism of thiophene removal in coke oven gas by

using modified NaY zeolite which has been widely used in desulfuration of liquid fuel. A series of sorbents were prepared by Ag+ and Zn2+ modification of NaY zeolite in this paper. Adsorption and transformatin performances of thiophene in three kinds of atmospheres (55% H2, 25% CH4, 5% CO, Ar as the balanced gas) were evaluated by fixed bed at 100 oC with 200 ppm initial concentration of thiophene and Mass Spectrum was monitored to test online sulfur-containing compounds in the export of reactor. The fresh and spent sorbents were both characterized by X-ray diffraction, NH3 temperature programmed desorption, ICP and N2-adsorption specific area measurements. The results show that C4H4S can convert into H2S and COS at 100 oC on the surface of NaY, AgY and ZnY zeolite. AgY and ZnY have better desulfuration performance than NaY in the series of experiments. The order and amounts of generation of sulfur-containing compounds also differ because of the natural properties of medium gas, types of acids and active mental sites on Y zeolite. H2S is prefered to be generated in the atmospheres of H2 and CH4, where proton H can promote the cracking of thiophene. Compared to other two gases, the generation of COS is fiercer in CO gas. Tetrahydrothiophene, methanethiol and dimethyl sulfide were also analyzed to investigate the conversion mechanism of thiophene in the three atmopheres.

51.4- The Macromolecular Characteristics and Model Construction of Baode Coal by 13c-Nmr Analysis

Wenying Xue, Zhiyuan Yang, Zhuoyue Meng, Xiaoxiao He, Xiaoyu Song, Xi'an University of Science and Technology, PR CHINA.

The research of coal structure has been a core issue in the coal science, which plays a significant role in clean coal fields. In this paper, 13C-NMR and elemental analysis of Baode coal samples were carried out to obtain the structural distribution of carbon atoms and 12 structural parameters. The results indicate that naphthalene with condensation degrees of 2 is the main form of aromatic carbon in Baode coal, and benzene ring and aromatic heterocyclic ring is another existing form. Based on the results of structural parameters and elemental analysis, the macromolecular structure model of Baode coal was constructed, and the 13C chemical shift of Baode coal structure model was calculated. According to the calculation results, the macromolecular structure model of Baode coal was corrected, and finally the macromolecular structure model which can correspond well with the peak shape and peak intensity of the experimental spectrum was obtained.

51.5- The Humic Acid was prepared by Oxidation of Lignite and Study on the Flocculation of Humic Acid

Yan Zhao, Jun Guan, Demin He, Engineer, Dalian University of Technology; Xueqiang Li, Jianxuan Shang, Professorate Senior Engineer, Shanxi Coal and Chemical Industry Group Co. Ltd; Qiumin Zhang Professor, Dalian University of Technoloy; PR CHINA.

Coal, as a kind of conventional fossil fuels, plays an irreplaceable role in energy and chemical feed stocks supplies of China. Specifically, low rank coal and airslake-coal are in abundant reserves. But due to the high oxygen containing structures in these kinds of coal, direct combustion of them is not favorable for both economic and environmental concerns. On the other hand, lower degree of coalification or mild oxidation will be benefit for the extraction of humic acid (HA) from these coals, which are important and value-added chemicals with multiple uses.
In order to improve the yield of humic acid in lignite, the air oxidation pretreatment was adopted. It is investigated the effects of time (0-10 h), temperature (100℃-225℃), and oxygen content (20%-100%) on the yield and properties of humic acids by using a fixed bed reactor. The results indicate that the optimal condition for higher humic acid yield is with 0.1MPa, 150℃, 2h, and O2 20%. A maximum of 4.21% total humic acid was improved from that lignite by oxidation with fixed bed. The lignite is dissolved by a mixture of sodium pyrophosphate and sodium hydroxide, and the fulvic acid is obtained by extraction and separation. We can receive the functional groups, molecular weights and structures of fulvic acid by FT-IR、UV-Vis、Elemental analysis, then infer the oxidation mechanism of lignite. The preoxidation of lignite has improved the yield of humic acid, increased the utilization of fulvic acid, and enhanced the flocculation capacity of humic acid. In order to improve the application of humic acid in lignite, different oxidants (HNO3, H2SO4) and chelating agent (EDTA-2Na) were added to lignite to study the change of humic acid content and flocculation characteristics. Result suggested that flocculation ability had the enhancement in various degree, it is EDTA-2Na> HNO3>H2SO4. The use of humic acid in lignite is of great significance to the clean and efficient utilization of coal.

SESSION 52
COAL MINING AND BENEFICIATION - 3

52.1- Progress of Rock Burst Monitoring and Pre-warning in Underground Coal Mining in China

Anye Cao, China University of Mining and Technology, PR CHINA.

Rock burst is currently one of the severest threats to underground safe coal mining in China. Identification of precursory characteristics is a key issue for rock burst prevention. In this presentation, an investigation of microseismic multi-dimensional information for the identification and spatial-temporal pre-warning will be conducted. Firstly, by combining microseismic monitoring and tomographic imaging, seismic tomography technique for periodic spatial assessment of rock burst is introduced. Secondly, the bursting strain energy index is further shown for short-term spatial-temporal pre-warning of rock bursts. Through the intermediate and short-time quantitative predictions, it can guide the choice of measures implemented to control rock bursts in the field.

52.2- Influence of Temperature on Adsorption Selectivity: Coal-based Activated Carbon for CH_4 Enrichment from Coal Mine Methane

Yuannan Zheng, Qingzhao Li, Professor, Chuangchuang Yuan, Qinglin Tao, Yang Zhao, Guiyun Zhang, Junfeng Liu, China University of Mining and Technology, PR CHINA.

In order to study the effect of temperature on the adsorption separation characteristics of CH4/N2 mixtures, activated carbons (AC) were prepared from low-rank bituminous coal by KOH activation method, marked as DF-AC and SM-AC. The adsorption isotherms of pure CH4 and N2 on AC were described by Langmuir-Freundlich model based on the high-pressure adsorption experiments. The adsorption selectivity calculated by ideal adsorption solution theory (IAST) method was used to evaluate the adsorption and separation characteristics of CH4/N2 binary mixtures. The influence of temperature on adsorption selectivity from 273 K to 373 K (20 K interval) were systematically analyzed. Results show that the adsorption equilibrium states of pure CH4 and N2 on activated carbons are significantly different, and the CH4 is more sensitive to the variation of temperatures. The isosteric heat of adsorption of CH4 is always larger than that of N2 under experimental pressure condition. This indicates that the interaction between the CH4 molecules with activated carbons is stronger than that of N2 molecules. In the temperature range of 273 K to 313 K, the separation factor would increase firstly and then slightly decreases, while adsorption selectivity would decrease gradually with the increase of temperature. In the temperature range of 273-313 K, the adsorption selectivity would decrease sharply at low pressure and subsequently tended to increase. Conversely, the adsorption selectivity is increasing monotonically throughout the whole pressure range when the temperature higher than 313 K. Under present experimental condition, for CH4:N2 = 50:50 mixture, the maximum adsorption selectivity of DF-AC (S = 7.06) can be obtained at 273 K and low pressure, while the minimum adsorption selectivity of DF-AC (S = 2.82) is obtained at 373 K and low pressure. The influences of temperature on adsorption selectivity of CH4/N2 binary mixture on coal-based activated carbons indicate that the lower adsorption temperature is contributed to the CH4 enrichment from low-concentration coal mine methane. And the effect of temperature on adsorption selectivity is greater than that of pressure, which provides a certain guiding significance for the efficient separation of low concentration gas combined with PSA and TSA technologies.

52.3- Preparation of Activated Carbon @ MOFs Materials and Its Potential Application for Coal Mine Methane Enrichments

Qingzhao Li, Chuangchuang Yuan, Yuannan Zheng, Qinglin Tao, Yang Zhao, Guiyun Zhang, Junfeng Liu, China University of Mining and Technology, PR CHINA.

In present research work, three different types of activated carbon (including commercial coconut shell activated carbon-CoAC, Dafosi low-rank coal-based activated carbon-DfAC and Inner Mongolia mid-rank coal-based activated carbon-ImAC) were successfully loaded into MIL-101 (one kind of MOF material synthesized by Institute Lavoisier, which is named MIL-101). The aim of present study is to reduce the unutilized voids in MIL-101 by incorporating microporous activated carbon (AC) into MIL-101 materials (which is defined as AC@MIL-101) and thereby enhancing its volumetric methane adsorption capacity and CH4/N2 selectivity. Based on adsorption method, the pores structure of the AC @ MIL 101 materials had been analyzed systemically. Results show that the Brunauer-Emmett-Teller (BET) specific surface area of the composite material increased by 41.7% and the total pore volume increased by 10.1% compared with pure MIL-101 material. The most significant improvement is that the volume of micro pores in AC @ MIL 101 increase by 86.6%. Based on high-pressure adsorption experiments and Langmuir equations, the methane saturation adsorption (qs) increases by a maximum of 23.5% and the methane adsorption constant (b) increases by 2.67 times

of pure MIL-101. Electron Probe Micro analyzer (EPMA) shows that the supported activated carbon still maintains their complete crystal structure, but the homogeneity of the crystal surface is reduced. In addition, some fiber rod structures are formed on the surfaces of AC @ MIL 101 samples and proper amount of fiber rod interspersed structure can increase the crystal stability and adjust the pore structure. From the results of Fourier transform infrared spectroscopy (FTIR), it can be seen that the chemical structure of all AC @ MIL 101 materials are very similar, indicating that the original skeleton structure has not been destroyed by loading micro AC components. By Ideal Adsorbed Solution Theory (IAST) method, it shows that MIL-101@AC materials present higher selective adsorption properties for CH4/N2 binary mixtures. Especially for the MIL-101@ low-rank coal-based activated carbon, it has the largest saturated adsorption quantity qs, the highest adsorption constant b value, and the fastest increase in the CH4/N2 separation factor. Present results indicate that the coal-based activated carbon not only increases the saturated adsorption capacity of gas adsorption, but also increases the interaction between the adsorbent and methane gas, that provides favorable conditions for the separation of CH4/N2 and subsequent enrichment of coal mine gas.

52.4- A Feasibility Study On Magnetic-Field Treatment of Dust Suppressant for Economical Saving

Wufan Xuan, Hetang Wang, China University of Mining and Technology, Xuzhou, PR CHINA.

Dust control is very significant for mine safety, otherwise coal dust may cause explosion and pneumoconiosis. Magnetic field (MF) effects observed during and after the treatment on water and aqueous solutions has drawn the attention of scholars in recent decades. In previous studies, changes of water properties after MF treatment and the underlying mechanism have evoked heated discussions. This paper is aimed to figure out the feasibility of applying an external magnetic-field to dust suppressant and investigate the cooperative action of MF and surfactant on its dust removal ability. A self-developed magnetizer was used to provide MF treatment for 9 surfactant solutions (anionic and nonionic) based on the principle of a rotating magnetic induction line cutting fluid. The treatment was strengthened evenly through turbulence generated by automatic mechanical stirring. By changing the solvent concentration and exposure time to MF of dust suppressant in the invariant magnetic field, the properties of the dust suppressant before and after MF treatment were monitored and compared. Evaluation indexes of properties were selected in aspects of wetting ability and permeability. During the experiments, parameters like surface tension, contact angle and penetrating speed were measured. Experimental results show that wetting ability and permeability had the same trend of change, which was proved by formulas in the paper. And the fluctuation regularities can't be found quantitatively. Exposed to the same magnetic field, properties of nonionic surfactants compared with that of anionic ones tend to improve and fluctuate more generally. The most responsive surfactant is Tween-80 of a volume fraction as 0.05%, with a maximal improvement of 11.8 mN/m in surface tension, 16.3°in contact angle and higher penetrating speed than before. When the solvent concentration and magnetic field is the same, solutions with high surface tension and contact angle showed a relatively obvious improvement in properties, which can be utilized for the economical saving of surfactant use. Mechanism is proposed from a molecule and hydrogen bond point of view. The dynamic process of the formation and the fracture of hydrogen bonds in solutions is taken into consideration, which is affected by both MF and surfactant ionization. This research is of important guiding significance for the economic application of dust suppressants.

SESSION 53
GASIFICATION TECHNOLOGIES - 9

53.1- Effect of Lignite Support Precursor on Desulfurization Performance of Semicoke Supported Zinc Oxide Sorbent in Medium Temperature Coal Gas

Ting Li, LiuXu Bao, Jiao Kong, MeiJun Wang, XiuRong Ren, LiPing Chang, Taiyuan University of Technology, PR CHINA

In our preliminary work a semicoke supported zinc oxide sorbent is prepared through a simple method that impregnating the precursor solution of the active component directly onto the lignite followed by pyrolysis. In this method the effect of lignite characteristic as support precursor on desulfurization performances of the sorbents have not yet been studied. In the study four kinds of semi-coke supported zinc oxide sorbents were prepared by high-pressure impregnation followed by pyrolysis using four kinds of lignites (Zhaotong, Shengli, Huolinhe, and Xiaolongtan) as precursor of support and zinc nitrate as precursor of active component. The desulfurization performances of the sorbents were investigated in a fixed-bed reactor at 400 oC in simulated coal gas. And the physico-chemical properties of fresh and used sorbents were characterized by atomic absorption spectrometry (AAS), X-ray diffraction (XRD) and physical adsorption instrument. The results indicate that lignite support precursor influences the desulfurization performance of prepared sorbents through affecting the content of the active component and pore structure of sorbent. The higher content of active component and larger relative outer surface area result in a good desulfurization performance for the sorbent prepared by young Zhaotong lignite as precursor of support. The breakthrough time and sulfur capacity for the sorbent is 12 h and 3.22 g S/100 g sorbent respectively.

53.2- Solid Hydrogen in MGH2 for Hydrodesulfurization of Carbonyl Sulfide: A Density Functional Theory Study

Xinyuan Li, Ruiqian Jiang, Xiaojing Liu, Shixue Zhou, Shandong University of Science and Technology, PR CHINA.

Sulfur is widely found in various coal based syngas, of which carbonyl sulfide (COS) is the main form of organic sulfur. The presence of COS is very detrimental to catalysts used in several industrial processes, therefore, studying its removal technology and its theoretical problems is of great practical significance today in the rapid development of one carbon chemical industry, chemical fertilizer industry and coal gasification industry, and the increasing demand for environmental protection. To investigate the interaction mechanism between COS and the MgH2, the absorption properties of COS molecule on different surfaces of MgH2 is necessary. The calculations show that six state configuration of COS molecule on the MgH2 (001) surface, and all of the absolute values of absorption energy lower than 0.2 eV, which is typical of physisorption. In contrast with the MgH2 (001) surface, the absolute values of absorption energy of COS molecule on the MgH2 (110) surface that higher than 0.4eV and form stable chemisorption. Especially when COS molecule is perpendicular to the MgH2 (110) with the O atom closed to the Mg atom, the absolute values of absorption energy reached 3.57 eV. The migration of H from MgH2 to COS is the key for hydrodesulfurization (HDS). Two pathways for HDS reaction of COS with MgH2 surface are constructed, and the energy barrier and reaction energy of each step are calculated.

53.3- Highly-Efficiency Adsorption of Hexavalent Chromium on Low Rank Coals

Xing-Yun Zou, Lin Li, Xiao-Fang You, Peng Wang, Jun Qiu, Jun-Xiang Wang, Shandong University of Science and Technology; Xiao-Qiang Cao, Shandong University of Science and Technology and Peking University; Wei-ling Sun, Peking University; Qing-Jian Zhang, Shandong Entry-exit Inspection and Quarantine Bureau; Xian-jun Lyu, Shandong University of Science and Technology; PR CHINA.

In this study, low rank coals (LRCs) were evaluated as a potential lower-cost materials for the removal of Cr(VI) ions from aqueous solutions. The effect of initial solution concentration, adsorbent dosage, pH on the adsorption of Cr(VI) by LRCs were investigated by batch experiments. The results indicated that LRCs can adsorb Cr(VI) efficiently, and the maximum adsorption capacity of 43.066 mg/g can be obtained. The remove efficiency (RE) of Cr(VI) increases with an increase in LRCs dosage. In contrast, the remove efficiency (RE) decrease with an increase in the pH, and RE decreases sharply from 99% to 18% at pH >2. The adsorption of Cr(VI) on LRCs significant decrease with an increase in the Cl- ionic strength. The Freundlich isotherm model and pseudo-second-order kinetics can describe the isotherm and kinetics data, respectively. The results of the thermodynamics analysis showed that the adsorption is endothermic.

53.4- Turbulence Model Development and Validation for Gasification Applications

Omar M. Basha, North Carolina A&T State University; Nicholas Siefert, Isaac Gamwo, National Energy Technology Laboratory/U.S. Department of Energy; Badie I. Morsi, University of Pittsburgh; USA.

The use of advanced numerical models, namely Computational Fluid Dynamics (CFD) for the representation of multiphase units, such as gasifiers, has been widely attempted for design and optimization purposes. However, most CFD models over-rely on outdated, turbulence sub-models, most notably the k-epsilon turbulence models, which have been developed using primitive systems (such as rotating disks) and are theoretically unfeasible for multi-phase turbulent applications. This work will highlights the pitfalls of commonly used turbulence models, from both a theoretical and an experimental standpoint, and will propose corrections and experimental designs for the development of new turbulence models, with primary focus on gasifiers and slurry bubble column reactors.

SESSION 54
COAL SCIENCE - 9

54.1- Incidence Degree of the Operation and Structure Factors for the Performance of Three Products Hydrocyclone Screen (TPHS)

C. Wang, J. Chen, L. Shen, Y. Huang, Q. Nie, China University of Mining & Technology, PR CHINA.

A novel three products hydrocyclone screen (TPHS) has been designed at the Key Laboratory of Coal Processing and Efficient Utilization, China University of Mining and Technology, China for particle classification. The new device consists of a cylindrical screen embedded in a conventional hydrocyclone (CH), which combined both centrifugal classification and screening. The successful pilot-scale application in coal preparation plant indicated that the new hydrocyclone presented better performance in contrast to the CH by the removal fish-hook effect. In the present paper, a series of pilot-scale experimental studies using the Grey System theory were carried out to investigate the structural and operational effects on the performance evaluation (Hancock classification efficiency (HE), imperfection (I) and cut size (d50c)) of TPHS. The results show that the device performance of TPHS closely related to both operation and structure parameters. The order of grey incidence degree for the HE, I and d50c was that spigot diameter and aperture size the highest, followed by feed pressure and vortex finder diameter, feed concentration the lowest.

54.2- Effects of Hydrothermal Dewatering on Lignite Physico-Chemical Structures and Analysis of Moisture Removal Mechanism

Qiong Mo, Junjie Liao, Liping Chang, Weiren Bao, Taiyuan University of Technology, PR CHINA.

Lignite is featured with high moisture content, and thus being supposed to be dewatered before its large-scale utilization. Hydrothermal dewatering (HTD) is reported to be a relatively efficient way to upgrade the lignite. In this study, two lignite samples from Inner Mongolia and Yunnan province were hydrothermally dewatered at 200-300 °C. HTD samples were characterized using chemical titration and N2 adsorption to investigate the effects of HTD on physico-chemical structures of lignite. The pore volume and specific surface area of Inner Mongolia lignite increased first and then decreased with HTD temperature increasing, whereas those of Yunnan lignite decreased monotonously, which were caused by the development and collapse of meso- and macro-pores. During HTD process, carboxyl and phenolic hydroxyl groups in lignite would greatly decompose when HTD temperature was higher than 200 °C and 230 °C respectively, and their removal percentages increased with the rise of HTD temperature. Moreover, these samples were isothermally dried at 110 °C for 30 min to explore the moisture removal mechanism. The free water, capillary water and molecular water in lignite before and after HTD process were also quantified. The results show that the molecular water was reduced because of the removal of oxygen functional groups, and the removal of capillary water and free water was associated with the collapse of meso- and macro-pores respectively.

54.3- Study on the Coal Rock Microstructure Separation of Low-Rank Coal in Enhanced Gravity Field

Yushuai Xian, Youjun Tao, China University of Mining and Technology, PR CHINA.

Low-rank coal has large reserves in China, it has the characteristics of low ash, low sulfur, high volatile, highly hydrogen content and good chemical reactivity. So the low-rank coal is extremely suitable for liquefaction. The vitrinite group of coal is the active component for liquefaction. The larger the proportion of the vitrinite group, the higher the yield of the product oil after liquefaction. In this paper, vitrinite group content of concentrates can be significantly increased by using enhanced gravity. In this experiment, Shenhua low-rank coal was invoked as the raw coal and the enhanced gravity field was supported by Falcon centrifugal separator. After the enrichment of raw coal, the content of vitrinite in the vitrinite-rich concentrates was increased by 10-30% compared with the raw coal, and the content of the inertinite in the inertinite -rich concentrates was increased by 10-25% compared with the raw coal. The results of the experiments were fitted by Quadratic model, the vitrinite group recovery rate of concentrates was up to 71.30%, and the vitrinite group enrichment ratio could be 1.17.

54.4- Experimental Study of CO_2-Water-Mineral Interactions and Their Influence on the Pore Structure of High Rank Coal

Yi Du, Huazhong University of Science & Technology; Shuxun Sang, China University of Mining and Technology; Junying Zhang, Huazhong University of Science & Technology; Changqing Fu, Xi'an University of Science & Technology; PR CHINA.

Coal, as a kind of conventional fossil fuels, plays an irreplaceable role in energy and chemical feed stocks supplies of China. Specifically, low rank coal and airslake-coal are in abundant reserves. But due to the high oxygen containing structures in these kinds of coal, direct combustion of them is not favorable for both economic and environmental concerns. On the other hand, lower degree of coalification or mild oxidation will be benefit for the extraction of humic acid (HA) from these coals, which are important and value-added chemicals with multiple uses.
In order to improve the yield of humic acid in lignite, the air oxidation pretreatment was adopted. It is investigated the effects of time (0-10 h), temperature (100℃-225℃), and oxygen content (20%-100%) on the yield and properties of humic acids by using a fixed bed reactor. The results indicate that the optimal condition for higher humic acid yield is with 0.1MPa, 150℃, 2h, and O2 20%. A maximum of 4.21% total humic acid was improved from that lignite by oxidation with fixed bed. The lignite is dissolved by a mixture of sodium pyrophosphate and sodium hydroxide, and the fulvic acid is obtained by extraction and separation. We can receive the functional groups, molecular weights and structures of fulvic acid by FT-IR、UV-Vis、Elemental analysis, then infer the oxidation mechanism of lignite. The preoxidation of lignite has improved the yield of humic acid, increased the utilization of fulvic acid, and enhanced the flocculation capacity of humic acid. In order to improve the application of humic acid in lignite, different oxidants (HNO3, H2SO4) and chelating agent (EDTA-2Na) were added to lignite to study the change of humic acid content and flocculation characteristics. Result suggested that flocculation ability had the enhancement in various degree, it is EDTA-2Na> HNO3>H2SO4. The use of humic acid in lignite is of great significance to the clean and efficient utilization of coal.

54.5- The Cleanability Evaluation of No.3 Coal Seam in An'ping, Yitang and Xizhuang Exploration Area

Xiaoshuai Wang, Yuegang Tang, Chengwei Yang, Kai Ye, Qingshun Cao, Guohua Liu, China University of Mining & Technology (Beijing), PR CHINA.

Based on the drilling data of An'ping, Yitang and Xizhuang exploration area derived from through surveys, the cleanability of No.3 coal seam is calculated by the formula proposed by Tang Yuegang et al in 2017. According to the calculated cleanability value, the cleanability contour map is drawn by MAPGIS. The reserves of different cleanability coal resource are predicted through geological ore block method.
The cleanability range of No.3 coal seam in An'ping exploration area is between 6.41 and 10.17, which involves fair, good and proficient coal resources. Fair, good and proficient coal resources are accounted for 1.15%, 50.60% and 48.25%, respectively. Fair coal resources are distributed in northeast An'ping. Good coal resources are distributed in north, south and central An'ping. Proficient coal resources are distributed in middle part of An'ping. The No.3 coal seam belongs to Permian Cisuralian Shanxi formation. The depositional environment was mainly continental facies and magmatites were not developed. The distributions of different cleanability coal resources in two wings of fold are analogous, which may be affected by depositional environment. The cleanability range of No.3 coal seam in Xizhuang exploration area is between 2.25 and 9.32, which involves poor, fair, good and proficient coal resources. Fair, good and proficient coal resources are accounted for 5.14%, 58.22%, 26.61% and 10.03%, respectively. Fair coal resources are distributed in most parts of Xizhuang. Poor coal resources are distributed in north of central Xizhuang. Good coal resources are distributed in both north and south Xizhuang.proficient coal resources are distributed in north Xizhuang. The Shanxi formation in this area developed cross bedding and bioturbation structures, which may reflect the distributions of different cleanability coal resources is related to seawater effects. The cleanability range of No.3 coal seam in Yitang exploration area is between 3.36 and 10.47, which mainly involves fair, good and proficient coal resources. Fair, good and proficient coal resources are accounted for 50.93%, 47.11% and 1.80%, respectively. The different cleanability coal resources are distributed concentrically, which is not related to fold. Good and proficient coal resources are dominant.
In conclusion, the coal resources are mainly constituted of fair, good and proficient coal resources in the three exploration areas. The cleanability of coal may be related to depositional environment and seawater effects. The relationship between cleanability and magmatic activity is unknown.

POSTER SESSION 1
GASIFICATION TECHNOLOGIES

P.1.1- The Effect of Steam on Biomass Wastes Torrefaction, Shan Tong, Feng Wang, Huazhong University of Science and Technology

Xian Li, Huazhong University of Science and Technology and College of Chemistry and Chemical Engineering, Xinjiang University; Hong Yao, Huazhong University of Science and Technology; PR CHINA.

Torrefaction is an efficient way for the biomass waste dewatering and upgrading before its thermal conversion and utilization, such as gasification, pyrolysis. The traditional torrefaction is conducted in an inert atmosphere (such as N2) at a relatively low temperature range. However, in consideration of the cost the torrefaction in industry requires the flue gas as a heat source, in which steam presents. This study investigated the effect of the steam on the torrefaction of biomass waste. It was found that the steam promotes thermal decomposition of biomass during torrefaction. The torrefaction can be performed at relatively lower temperature and shorter time with the addition of steam. Furthermore, the steam improved the gasification and pyrolysis reactivity of the torrefied biomass, especially at high torrefaction temperature.

P.1.2- Study of Catalytic Steam Reforming of Toluene in Molten Salt

Quan Yuan, Taiyuan University of Technology, PR CHINA.

Coal gasification stand at the heart position of clean utilization of coal. Meanwhile, tar has always been the most critical issue for coal gasification technology. Tar accumulates in the pipeline, clogs the pipeline, corrodes the equipment, and wastes energy, which is difficult to reuse. At the same time, Tar has complex composition and it contains carcinogenic substance, which lead to environmental pollution. Steam reforming can remove the tar content and improve the gas production quality. It is generally considered as a tar treatment method with a good industrial application prospect. Considering the factor of cost, low-cost and high stability molten salts are more likely to be applied in practical gasification plants. The molten salt owning high temperature stability, high thermal capacity, low volatility, low viscosity, high ion migration and diffusion speed. These properties determine that the molten salt is a promising reaction medium for catalytic gasification.
In this subject, a set of catalytic reforming reactor for toluene was designed and developed. With toluene as the model compound of tar from coal gasification，the properties of molten salt were analyzed for its performance on the reactions of toluene cracking and toluene steam reforming in the fixed bed reactor. Catalytic effects of different cracking conditions on toluene pyrolysis rate, gas products generation rate were investigated. The result shows that: The fixed bed reactor for catalytic cracking of tar was successfully was built，and the stability of the reactor device was also carried out. The detection method and calculation method of catalytic cracking of toluene were constructed．When the reaction temperature was 700℃，the toluene feed rate was 0.2ml/min，S/C was 2.0，the conversion of toluene reached 93%, the toluene cracking rates are sutantial increased, respectively, compared with only steam reforming. And the molten salts showed good stability and good catalytic effect.

P.1.3- Modelling of Hot Flow Field in an Entrained-Flow Gasifier with Single or Flat Flame Burner

Feng Ziyang, National Institute of Clean and Low-Carbon Energy; Liu Zhen, Guan Qingliang, Liu Bing, Peng Baozai, Fang Xinhui, An Haiquan, Suo Ya, Li Wenhua National Institute of Clean and Low-Carbon Energy; PR CHINA.

Computational fluid dynamics was used to study the hot-flow characteristics of an entrained-flow gasifier with downdraft flat-flame burners based on the EDC method. The flow field, backflow rate, temperature distribution, solid particle distribution, and the residence time were investigated using the design process parameters. The simulation results were validated using measured gas component fractions, carbon conversion efficiencies, and gasifier outlet temperatures. The difference between the flat flame burner gasifier and the single burner gasifier was also discussed.
It is found that the flat flame burner leads to more appreciable hot gas backflows. These gas backflows account for the max temperature reduction near the burner and more uniform temperature field along the gasifier. The coal particles are also dispersed more uniformly resulting in longer averaged particle residence time and fewer transient particles than that of the single burner gasifier. Further study shows that the flat flame burner structure intensifies the mass transfer near the impinging stream zones. Therefore, the carbon conversion with flat flame burners is higher than that of the single burner which implies that the reaction volume of the flat flame burner gasifier can be designed smaller than that of the single burner for the same production capacities.

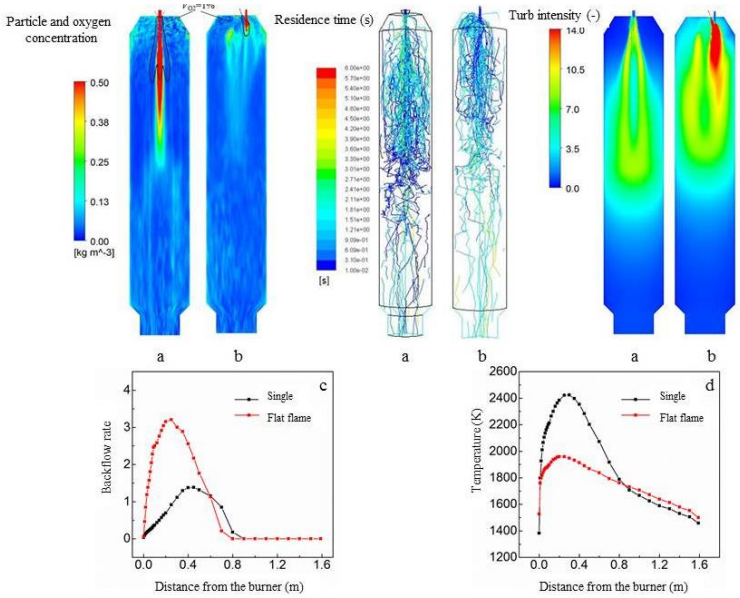

Figure 1: Simulation results of the EDC model with single and flat flame burner a) Single burner; b) Flat flame burner; c) Backflow rate along the distance from the burner; d) Temperature along the distance from the burner

P.1.4- Using Inexpensive Sodium/Iron Bimetallic Catalyst in Steam Gasification of Coal Char

Yiwei Jiang, Haibo Yan, Jie WANG, East China University of Science and Technology, PR CHINA.

Coal gasification is an important technology for clean utilization of coal, which is widely applied in industry on a large scale. However, common coal gasification without catalyst requires a higher temperature leading to a higher energy consumption. Catalytic gasification has an advantage of low-temperature operation and higher efficiency. There is no doubt that to use an effective and low-cost catalyst brings great benefit to gasification process. In the present work, we tried to use sodium- and iron-based compounds as a cheaper catalyst for gasification. The main aim of this work is to investigate the synergistic catalysis of Na and Fe towards the gasification rate. Gasification experiment was carried out in a horizontal boat reactor at 700–850 ° C under atmospheric pressure, using steam as gasifying agent. Result showed that sodium carbonate had a strong catalytic effect, and an ash-free lignite char with 10% loading (mixture basis) could lead to a complete gasification at a low temperature of 750 ° C within 45 min, whereas the catalytic effect of sole iron-based additive was insignificant. An interesting finding was that the Na/Fe bimetallic catalytic exhibited a distinctly higher effect than the sole sodium catalyst. A better Fe/Na atomic ratio was 1:2 for the bimetallic catalyst. The catalytic char gasification produced a hydrogen-rich gas but the CO fraction was higher than that obtained with potassium carbonate as a catalyst. In order to reveal the synergistic mechanism of the Fe/Na catalyst, thermogravimetry and differential scanning calorimetry coupled with mass spectrometry (TG/DSC-MS) was used to investigate the interactions between coal char and catalyst in the process of char formation. X-ray diffraction (XRD) was used to identify the crystalline transformations of Na/Fe catalyst during gasification. Moreover, inductively coupled plasma optical emission spectrometer (ICP-OES) was employed to investigate the active Na loss during the gasification. Some mechanisms were revealed. The first was that the addition of Fe to Na catalyst promoted the dispersion of sodium carbonate on the surface of char in an amorphous form. The second was that the addition of Fe facilitated the interaction between sodium and char around 750 ° C, forming an active complex intermediate. The third was that the addition of Fe suppressed the vaporization of Na during the gasification.

POSTER SESSION 2
CLEAN COAL DEMONSTRATION AND COMMERCIAL PROJECTS

P.2.1- Novel Nanocomposite Surface Treatment for High Efficiency Low Emission Coal Power

Vinod Veedu, Matthew Nakatsuka, Erika Brown, Ganesh Arumugam, Oceanit, USA.

Fouling of heat transfer surfaces plays a significant role in the efficiency and greenhouse gas emissions of a coal-fired utility, particularly in those plants utilizing nearby bodies of unprocessed water such as rivers or oceans for cooling. Buildup of either biofilms or scale deposition can significantly increase the effective thermal resistance within the condenser unit, turbine backpressure, fuel consumption, and greenhouse gas emissions. In order to mitigate these factors, every plant must adopt some form of cleaning and mitigation strategy, all of which require significant operational expense and/or regular required offline time.

This paper details the adaptation of a novel, fouling resistant surface treatment to improve the heat transfer performance of a prototypical shell-and-tube exchanger unit. The surface treatment, unlike most conventional epoxy coatings, was applied at a thickness of less than 100µm, and was shown to have a negligible effect on thermal energy transfer in a liquid-liquid model system. Characterization of biofilm growth and attachment on the treated surface was shown to be significantly reduced, both in static and dynamically controlled testing conditions. Additionally, despite the extremely thin application, the surface treatment showed excellent abrasion and erosion resistance, even when applied to a previously worn/cleaned substrate, indicating its potential for refurbishment of existing, in-service units.

The surface treatment was applied both on a laboratory coupon scale as well as on a pilot basis, in order to demonstrate both suitability at the micro- and macro-scale. This paper will detail the changes in exchanger performance and behavior after application, along with outlining the expected improvement both in operational efficiency. Additionally, initial trials on applying the coating on the vacuum-side of a condenser unit in order to promote more efficient drop-wise condensation shall be discussed, and an estimate on the overall effect on plant operations and estimated backpressure penalty shall be determined.

POSTER SESSION 3
COMBUSTION TECHNOLOGIES

P.3.1- Mechanism Analysis and Experimental Study of Ammonia Denitrification Technology in High Temperature Reduction Zone of Coal-Fired Boiler

Bo Zhang, Xiangyu Zhang, Ning Gao, Xu Lu, Xiaofeng Xiang, Hongjie Xu, Xi'an Thermal Power Research Institute Co., Ltd., PR CHINA.

Under the condition of graded combustion, the injection of amino reducing agent into the high temperature region of the cyclone furnace and the pulverized coal boiler burner can reduce the production of NOx in the high temperature zone. Through reaction mechanism analysis and experimental research, the factors that affect the amount of NOx generated under the condition of adding amino reductant were quantitatively studied, and the kinetic parameters of reaction were obtained.

P.3.2- Study on Removal of Hg from Flue Gas by Modified Activated Carbon

Yang Li, Xiangyang Li, Pang Huang, Lijun Jin, Haoquan Hu, School of Chemical Engineering, Dalian University of Technology, PR CHINA.

Mercury is considered as one of the most toxic heavy metals because of its persistence and bioaccumulation around the world. Release of mercury and some toxic trace metals/metalloids into the environment have an adverse effect to human health and throughout the ecosystem. Among all the anthropogenic mercury emission sources, coal combustion is the major one. In the face of increasingly serious problems of mercury pollution, it has been an urgent issue to reduce mercury emission from coal fired power plants. Activated carbon injection is one of the mercury removal approaches that can remove mercury effectively from flue gas using conventional particulate matter controller. However, application of activated carbon sorbents is limited by lack of products for low rank fuels. Therefore, it is important to develop alternative sorbents and chemical treatments to promote mercury removal capacity of carbonaceous sorbents.

In this study, ammonium iodide (NH4I)-impregnated activated carbon was synthesized to investigate its capacity to elemental mercury (Hg0) removal in simulated coal combustion flue gas. Potassium hydroxide (KOH) was used as activating agent to obtain activated carbon derived from a Guizhou anthracite by chemical activation. The adsorption experiments of vapor-phase elemental mercury were carried out in a laboratory-scale fixed-bed reactor. Specifically, the effects of loading values of NH4I, sorption temperature (100 - 200 oC) and individual flue gas components (O2, SO2, NO, HCl) on Hg0 removal efficiency were investigated. In addition, thermal stabilities of mercury compounds were studied by using temperature-programmed desorption (TPD). Proximate and ultimate analyses, BET surface area analysis and scanning electron microscope (SEM) analysis were carried out to determine pore structure and surface chemistry of sorbents. It was observed that impregnation of ammonium iodide (NH4I) significantly improved the performance of activated carbon to Hg0 capture. The optimum loading of NH4I was found to be 7 wt.%. Hg0 removal efficiency decreases with the rising temperature in a range of 100-200℃. The existence of O2, HCl and NO promote the removal of Hg0, while the presence of SO2 could inhibit Hg0 capture. The X-ray photoelectron spectroscopy results indicated that the functional groups of C=O and C-I in the sorbent participate in mercury removal process. The regeneration performance of sorbent was investigated by thermal regeneration. The results showed that the used sorbent could successfully be regenerated and reused for Hg0 removal, and the Hg0 removal efficiency of used sorbent is 95.8 % after regeneration at a temperature of 400℃.

POSTER SESSION 4
CLEAN COAL AND GAS TO FUELS

P.4.1- Effect of Precursors on the Active Site Formation of Cu/Zn/Al Methanol Synthesis Catalyst

Yulong Zhang, Fan Zhang, Xiaoying Xu, National Institute of Clean and-low-Carbon Energy, PR CHINA.

Subcarbonates and hydrotalcite-like (HTl) compounds are two typical kinds of precursors in the preparation of Cu/Zn/Al methanol synthesis catalyst by co-precipitation method. The objective of this work is to investigate the effect of these precursors on the formation of active sites for methanol synthesis. Two kinds of catalysts with mainly subcarbonates or HTl compounds as precursor were synthesized by co-precipitation method and fractional precipitation method, respectively. The catalyst samples were characterized with various methods including XRD, TG-MS, XRF, XPS, TPR, SEM, TEM/EDS, and N2 physisorption. Results show that the formation of HTl compounds was detrimental to the BET surface area and the surface Cu contents of the prepared catalyst. Subcarbonates in the precursors included malachite, zinc malachite and aurichalcite [1]. Zinc malachite phase can be obtained from malachite crystal structure by substituting part of the Cu2+ ions with Zn2+ [2]. The XRD and TG-MS results show that higher Cu-Zn substitution in the subcarbonates was achieved by using fractional precipitation methods. TEM results show that the formation of HTl compounds consumed high proportion of Zn2+ in the co-precipitation process, and thus the obtained subcarbonates performed lower Cu-Zn substitution compared to their counterparts from fractional precipitation. Evaluation results show that the catalysts with mainly subcarbonates in precursor demonstrated better catalytic performance than the HTl-derived catalysts. Although distributed evenly in the HTl structure, CuO derived from HTl compounds had unfavorable effect on the active site formation for methanol synthesis. CuO originated from the co-produced subcarbonates performed large particle sizes because of the low Cu-Zn substituion. On the other hand, fractional precipitation benefits to the formation of zinc malachite and/or aurithclate. The porous CuO-ZnO structure derived from zinc malachite and/or aurichalcite facilitates the intimate contact of Cu and ZnO, and was beneficial to the formation of active sites during the reaction. As such, fractional precipitation, which restrains the formation of HTl compounds, can be a promising method for preparing the Cu/Zn/Al methanol synthesis catalyst.

P.4.2- Fe-modified Nickel-Based Catalyst for CO_2 Reforming of Methane

Peipei Wang, Lijun Jin, Haoquan Hu, Dalian University of Technology, PR CHINA.

More attention has been paid to the comprehensive utilization of CH4, main component of natural gas, and CO2, main greenhouse gas, with the aim for syngas production. The nickel-based catalysts have been widely used in carbon dioxide reforming of methane because of low cost and comparable catalytic activity to noble metal catalysts, but easy deactivation from carbon deposition limits its industrial application. To improve the catalytic performances, in this paper, Fe-modified Ni-based catalyst (Fe-Ni/LDO) with different Fe loading was prepared by microwave-assisted impregnation of [Ni,Mg,Al]-double layer hydroxide (Ni-LDH) with the solution of Fe(NO3)3. Their catalytic performances towards carbon dioxide reforming of methane were evaluated. The results showed that the addition of iron and the presence of oxygen in the reaction system significantly improve the catalytic activity, stability and carbon deposition resistance of the nickel-based catalysts. The specific surface first increases and then decreases with increasing the iron amount. When the Fe loading is 1wt%, the catalyst has larger specific surface area being 135 m2/g, and higher activity and better stability in the carbon dioxide reforming of methane. About 75% conversions of CH4 and CO2 can be obtained after 570 min at 750 °C.

P.4.3- Cleaning of Bitumen Streams by Hydrothermal Treatment and In-Situ Hot Filtration

Qiang Chen, China University of Mining and Technology, PR CHINA.

The intimate association between hydrocarbon oil and mineral matrix is an important feature of unconventional petroleum resources, such as bitumen-bearing oil sands. In bitumen extraction from oil sands ore (both water-based extraction and non-aqueous extraction), contamination of bitumen oil by mineral solids is a nuisance. In the present work, a new bitumen cleaning approach is proposed, which combines the hydrothermal treatment of bitumen-water or bitumen-solvent product, water/solvent separation by venting, and solids removal by in-situ hot filtration. A small-scale laboratory hydrothermal treatment using 500-mL Parr reactors was conducted at 300–420°C for 0–180 min. The filterability of fine solids was quantitatively characterized by room-temperature filtration using 0.22-μm pore size filter membrane and hot filtration using 0.5-μm pore size stainless steel filter medium. The results show that hydrothermal treatment followed by venting and filtration is an effective way to remove water and fine solids from bitumen froth: the water content was reduced from 14 wt% to 0.03 wt%, and the fine solids content was reduced from 8 wt% to 0.08 wt% by hot filtration. After the hydrothermal upgrading, the viscosity of bitumen was reduced, and the filterability of fine solids was improved.

P.4.4- Synthesis and Characterization of Carbon Microspheres and Their Performance as Catalyst Carriers in Sulfur-Containing Model Compound

Xiongchao Lin, Meng Luo, Jianan Yin, Xiongwen Ding, Yunhe Bai, Xiaojia Li, China University of Mining and Technology (Beijing), PR China.

Iron-based catalysts are widely accepted for the coal direct liquefaction. The catalyst carriers were carbon microspheres which prepared from glucose by hydrothermal method and Fe(NO3)3·9H2O serve as precursor. Besides that, nano ferric oxides' phase composition, microstructure and pore structure were analyzed by XRD, SEM, BET, etc.; and their performances were evaluated through a high pressure reactor. In order to investigate the effect of the catalyst on the sulfur-containing model compound, thiophene, benzothiophene and phenyl sulfide were separately used as raw materials. The aim of this work is to explore the influence of heteroatom migration on sulfur was investigated.

POSTER SESSION 5
CARBON MANAGEMENT

P.5.1- A Viable Path Forward to Carbon Capture and Storage in Wyoming, USA

Erin H. Phillips, Kipp Coddington, Scott Quillinan, J. Fred McLaughlin, University of Wyoming; Nick Bosshart, Energy and Environmental Research Center; Anne Oudinot, Advanced Resources International, Inc.; Yuri Ganshin, Heng Wang, Matthew Johnson, Zunsheng Jiao, Tom Moore, Davin Bagdonas, Charles Nye, University of Wyoming; USA.

The State of Wyoming, USA, benefits from favorable geologic, regulatory, and infrastructure attributes that promote efficient and sustainable carbon capture and storage (CCS). Two research sites in Wyoming exhibit high potential for the underground geologic storage of greater than 50 million metric tons of carbon dioxide (CO2) over 25 years. Funded by the U.S. Department of Energy's (DOE) Carbon Storage Assurance and Facility Enterprise (DOE CarbonSAFE) Phase I prefeasibility initiative, studies of both sites indicate promising capture, transport, utilization, and storage characteristics.

The Dry Fork site is located near Gillette, in northeast Wyoming. Four storage reservoir/seal pairs have been identified at the Dry Fork site that provide excellent prospects for stacked storage of CO2. All four reservoirs lie at sufficient depths to maintain supercritical CO2 and all four seals exhibit favorable characteristics for stratigraphic confinement. The reservoir with the highest expected significance is the Pennsylvanian/Permian Minnelusa Formation, which consists of near-shore dunes and shoreline sands, as well as shale and carbonate layers. The Minnelusa resides at a depth of ~2,900 m below the land surface and is ~45 m thick in the study area. Average porosity for samples from core within 10 km of the study area is 9%, with permeability values as high as 169 mD (n=6). The Permian Opeche Formation seals the Minnelusa and consists of redbed shales with minor fine-grained siltstones and evaporite deposits. Entry pressures as high as ~4700 psia were measured by mercury injection capillary pressure (MICP) analysis on core samples from the Opeche. A CarbonSAFE Phase II feasibility proposal at the Dry Fork site has recently been selected for award by the DOE. The second proposed site is located at the Rock Springs Uplift (RSU) in southwest Wyoming. Four reservoir/seal pairs have been studied at the RSU, all of which present promising geologic attributes for the stacked storage of CO2. The two deepest reservoirs (Mississippian Madison Limestone and Pennsylvanian/Permian Weber Formation) and their seals were studied previously under the auspices of the Wyoming Carbon Underground Storage Project (WY-CUSP), which was funded by DOE and the State of Wyoming. For the more recent CarbonSAFE initiative, two shallower reservoir/seal pairs were studied in detail. The highest priority of these reservoirs is the Triassic/Jurassic Nugget Formation, which consists of eolian sands and minor fluvial and interdune deposits. The Nugget lies at a depth of ~2,800 m and is ~140 m thick in the study area. Average measured porosity for samples from core within 40 km of the study site is 9%, with permeability values as high as 91 mD (n=10). The Nugget is sealed by the overlying Jurassic Gypsum Spring and Morrison Formations, as well as a thick (~1,700 m) regional Upper Cretaceous seal that includes shales from multiple geologic units. Entry pressures as high as 1120 psia were measured by MICP for shales within this regional confining unit.

Overall, the State of Wyoming provides an advantageous climate to develop sustainable integrated CCS projects based on the following considerations: (1) well-characterized and favorable geology; (2) some of the largest deposits of economically recoverable coal in the USA; (3) an existing CO2-enhanced oil recovery industry, including CO2 pipeline infrastructure; (4) supportive commercial enterprises, including utilities and the oil and gas industry; (5) supportive policymakers; (6) a favorable legal and regulatory environment; (7) proximity to carbon-constrained markets such as the State of California; (8) large CO2 emission sources, including coal-fired power plants; and (9) backing for carbon capture, storage, and management related research and development, specifically implementation of the Integrated Test Center at Dry Fork Station, which is hosting the coal-track of the NRG/COSIA Carbon XPrizeÒ competition.

POSTER SESSION 6
COAL SCIENCE

P.6.1- Drying and Stabilization of Powder River Basin Coal Using Heat from a NuScale Nuclear Reactor

Ying Wang, Dr., William C. Schaffers, David A. Bell, University of Wyoming; Jong Suk Kim, Richard D. Boardman, Idaho National Laboratory; USA.

Low rank coals, such as Powder River Basin coal, tend to have high moisture levels and drying these coals has long been recognized as a means of increasing power plant efficiency. Low rank coals, however, are prone to low temperature oxidation when dried, and this can lead to spontaneous combustion. This tendency to low temperature oxidation can be eliminated by lightly oxidizing the coal in air. The heat for drying and partial oxidation can be provided by a nuclear reactor, such as the small, modular, nuclear reactor under development by NuScale Power, which produces steam at 280 to 300 ºC.

We investigated coal drying at 100 to 350 ºC, which roughly corresponds to the heat available from a NuScale reactor. We also studied the stabilization of the dried coal via controlled exposure to air at 150 to 250 ºC. A quadrupole mass spectrometer was used for real-time analysis of vapor production. Heavier volatile materials were condensed and analyzed by GC-MS. Oxidation reactions in a tubular reactor and a differential scanning calorimeter were used to analyze gas production and heat generation. The passivation of coal was clearly observed during oxidation. We investigated the mechanism of low temperature oxidation of the surface using ultimate and approximate analysis, surface area measurement, Fourier transform infrared spectroscopy (FTIR), and scanning electron microscopy (SEM, JEOL 5800LV) equipped with energy dispersive spectroscopy (EDS).

The dried and lightly oxidized coals tend to re-absorb moisture from humid air. The moisture re-absorbed by passivated coal was less than the original coal moisture content, particularly at lower humidity levels.

P.6.2- Petrological Characteristics of the Lopingian Coals from the Yueliangtian Coalfield, Guizhou, Southwestern China, with Particular Emphasis on Brecciation

Panpan Xie, China University of Mining and Technology (Beijing), PR CHINA; James C. Hower, University of Kentucky, USA; Shifeng Dai, China University of Mining and Technology (Beijing), PR CHINA.

Petrological characteristics of the Lopingian coals from some coalfields of southwestern Guizhou, China, have been described by a number of researchers. However, previous studies paid more attention to the abundance and occurrence of macerals but less to the plant precursor and formation process of them, especially macerals in the inertinite group. In this paper we reported the petrological characteristics of the Lopingian coals from the Yueliangtian coalfield, southwestern Guizhou, China, with particular emphasis on brecciation.

The coals from the Yueliangtian coalfields are high-volatile A bituminous coal. The maceral assemblage of the studied coals is dominated by collodetrinite, fusinite, and

semifusinite, and to a lesser extent, telinite, collotelinite, micrinite, and sporinite. Barkinite, reminiscent of cutinite and sporinite, are also observed in some coal samples. Poorly consolidated collodetrinite, fecal pellet-derived macrinite, and funginite observed in the present coals suggest fungal and/or bacterial degradation of the peat. Fusinite and semifusinite exhibit thickened and tattered cell walls in some cases, indicating microbial degradation of the plant precursors, followed by wildfire combustion. Coals from the No. 12 coal seam of the Yueliangtian coalfield, especially the lower portion, show some signs of brecciation and mineralization. Vitrinite, particularly collotelinite, displays uneven surface, deformation, and crumbling (fig.1) as a result of differential tectonic movements; detrital fusinite and/or semifusinite are either dispersed in vitrinite (fig.1) or cemented by exudatinite; clay-sulfide-maceral assemblage brecciation occurred in the base bench. The mineralization is predominated by carbonate assemblages (e.g., calcite and siderite) cemented by minor sulfides. The Panxian fault and other synsedimentary tectonic movements are responsible for the brecciation and mineralization happened in the Yueliangtian coals.

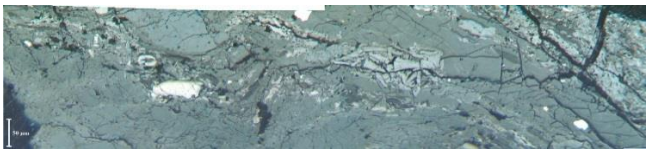

Fig. 1. Optical microscope images for brecciation in the Yueliangtian coal sample, reflected light, oil immersion.

P.6.3- Study on Temperature, Spectral Emissivity and Soot Loading of Single Burning Coal Particle Using Hyper-Spectral Imaging Technique

Mengting Si, Qiang Cheng, Zixue Luo, Qi Zhang, Dongxu Wang, Huazhong University of Science and Technology, PR CHINA.

A hyper-spectral imaging device that simultaneously carries three-dimensional data information of spectral, space and time is employed to experimentally investigate the combustion behavior of single coal particle. Three kinds of pulverized single coal particles are injected and burned on a Hencken flat-flame burner. An advanced high-speed camera is firstly used to observe the single burning coal particle envelope flame. It is observed that the three kinds of pulverized single coal particles form elongated tail-like flames. The image of the burning coal particle taken by the hyper-spectral imaging device records the spectral and spatial history of the combustion. From the spectral radiative intensity taken by the hyper-spectral imaging device, the temperature and spectral emissivity of the burning char particles at different times are calculated. The spectral emissivity of the three char particles at different combustion times all rises sharply in the shorter wavelength range (419-565 nm) and then levels off in the longer wavelength range (570-1036 nm). The spectral emissivity fits well by a second order polynomial in the shorter wavelength range, and by a linear polynomial in the longer wavelength range. Finally, the temperature and volume fraction in the volatile flame of single burning particle is obtained to investigate the formation of soot during combustion. The soot yield peaks in the area behind the char particle for the DT and SH coal, but peaks in the area ahead the char particle for the IL coal.

P.6.4- Qualitative and Quantitative Analysis of Coal-based Crude Oil Fractions by GC-MS/FID

Wei Wang, Cui-ping Ye, Hai Mu, Wen-ying Li, Jie Feng, Taiyuan University of Technology, PR CHINA.

Fractions of coal tar and coal direct liquefaction oil were selected as the research objectives, and they were analyzed by GC-MS/FID (Gas Chromatography-Mass Spectrometer/Flame Ionization Detector), where MS was used for qualitative analysis and FID for quantitative analysis. At the same time, due to the complexity of coal-based crude oil composition, it is necessary to introduce material balance as a constraint to ensure the credibility of the analysis results. Results showed that the amount of the most of coal direct liquefaction oil fractions which can be balanced is 85 wt% or above, but the amount of coal tar fractions can be balanced varying from 49 wt% to 102 wt%. Furthermore, the molecular weight distribution analysis by gel permeation chromatography gives the reason why the insufficient material balance is that the obtained samples still contain a large amount of large molecular weight substances that are difficult to vaporize.

P.6.5- Evolusion of Physical and Chemical Structures of Lignite during Dewatering Process and Their Effects on Combustion Reactivity

Yankun Yang, Junjie Liao, Liping Chang, Weiren Bao, Taiyuan University of Technology, PR CHINA.

In this study, the effects of upgrading methods on evolution of physical and chemical structures and combustion reactivity were investigated. For this purpose, hydrothermal upgrading, fixed bed upgrading and microwave upgrading were conducted to dry and upgrade Inner Mongolia lignite. The physical and chemical structures of parent and upgraded coals were characterized by nitrogen adsorption instrument, FT-IR technique and chemical titration method, and their results elucidated that different drying methods had different effects on characteristic evolution of physical and chemical structures. Thermogravimetry was employed for analyzing the combustion behavior of the coals, and their apparent activation energies were obtained according to the Non-isothermal single heating rate method. The results of thermal analysis illuminated that upgraded coals has low spontaneous combustion tendency and high burn-out property. The results of the apparent activation energy show that the ignition temperature of parent coal and upgraded coal samples were mainly affected by the intrinsic chemical reactivity; the maximum combustion reaction rates of parent coal and hydrothermal upgraded coal sample were affected by intrinsic chemical reactivity and pore diffusion, and the temperature corresponding to the maximum combustion reaction rates was mainly affected by the chemical reaction activity; the burn-out temperature of the parent coal was affected by the diffusion rate. The fixed bed and microwave upgraded coal samples were mainly affected by the chemical reaction activity during the combustion process.

P.6.6- Study on the Co-Combustion Characteristic and Pollutant Emission of Coal Gangue and Coal Slime in O_2/CO_2 Atmosphere

Baofeng Wang, Wenxiu Li, Shaolong Gao, Fengling Yang, Fangqin Cheng, Shanxi University, PR CHINA.

The combustion characteristics and emission of SO_2 and NOX during the combustion of coal gangue and coal slime have been studied by Thermogravimetry (TG) and flue gas analyzer (Testo350), and the influences of temperature, mixing ratio, heating rate and oxygen concentration on combustion characteristics and emission of SO2 and NOX were also investigated. The results showed that the combustion performance of coal gangue can be optimized by the addition of coal slime in the air and O2/CO2 atmosphere, while there is no synergism between them. In the atmosphere of O2/CO2, with the increase of the heating rate, the weight loss curve moved to the high temperature region. The increase of oxygen concentration can effectively reduce the ignition temperature and promote combustion. The results also showed that the emission content of SO2 is significantly reduced with the increase of the blending ratio of coal slime. During co-combustion of coal gangue and coal slime, with the increase of temperature, the SO2 content increased, and two release peaks of SO2 appeared above 800 ℃; In the range of oxygen concentration selected in the experiment, with the increase of oxygen concentration, the release peak of SO2 in gas increased, and the amount of SO2 and the conversion rate also increased. During co-combustion in O2/CO2, NO emission is lower; with the increase of coal slime blending ratio, NO peak concentration was gradually increasing, which may be caused by the relatively high content of volatile N. With the increase of temperature, the concentration of NO gradually increased; with the increase of O2 concentration, the concentration of NO also gradually increased.

P.6.7- Aliphatic Species in Mobile Phase of a High-Volatile Bituminous Coal and Its Thermal Decomposition Behavior

Bin Tian, Northwest University; Yi-Liang Tian, Bachelor, China University of Petroleum-Beijing at Karamay; Long Xu, Xiao-Xun Ma, Northwest University; PR CHINA.

Aliphatic species in mobile phase of the coals are the important fraction that can be separated by the solvents and affect the thermal decomposition behavior and volatile composition during raw coal pyrolysis. The aliphatic species in a high-volatile bituminous coal was separated combined with thorough extraction followed by column chromatography and then its composition was deeply identified by the GC/TOF-MS. Subsequently, mass loss behavior and thermal decomposition kinetics of the aliphatic species were investigated using thermogravimetric analyzer under different heating rates with maximum up to 1000 oC/min. The results showed that the aliphatic species were mainly composed of straight alkanes, branched alkanes, alkyl ketone, and biomarkers. Carbon numbers of the alkanes ranged from 11 to 40 and their contents showed normal distribution. Decomposition of the aliphatic moiety showed one mass loss stage. Initial decomposition temperature (Tin), temperature of maximum decomposition rate (Tmax), and terminal decomposition temperature (Tf) were 247.1, 311.5, and 363.8 oC, respectively at heating rate of 5 oC/min. At the same heating conditions, the values of maximum decomposition rate (Tmax) and volatile release index (Di) achieved 3.5 and 44.5, respectively. Tin, Tf, and Tmax presented lognormal distribution, while Rmax and Di exhibited linear relation with heating rate increased from 5 up to 1000 oC/min. As reaction proceeded, the activation energy during decomposition of the aliphatic species increased from 63.6 to 169.3 kJ/mol at heating rate of 5 oC/min using Friedman model. Furthermore, heating rate had no influence on the activation energy during thermal decomposition of the aliphatic species, while it could alter the reaction order of the compounds with different bond energies in the aliphatic species.

P.6.8- Removal of Toxic Elements from High-Uranium Coals of Rongyang Mine by Stepped Release Flotation

Piaopiao Duan, Wenfeng Wang, Shuxun Sang, China University of Mining and Technology, PR CHINA.

Many coals in southwestern China are characterized by a high sulfur (S) content, and uranium (U) is usually enriched in these high-S coals. Uranium is a naturally radioactive element, and the ultra-fine particles released from U-rich coals during combustion can have potentially adverse effects on human health. Coal preparation is one effective approach to reducing environmental pollution from toxic elements. Rongyang Mine is located in Xingren County, southwestern Guizhou Province. Samples were collected from the coal-bearing Upper Permian Longtan Formation, which was formed in the tidal flat environment of an open carbonate platform. The Rongyang coals are significantly enriched with U and other toxic elements, such as cobalt (Co), copper (Cu), and selenium (Se). Therefore, it is necessary to remove these toxic elements from high-U coals before combustion. Previous studies have shown that U cannot be effectively removed by flotation and gravity separation. In this study, the stepped release flotation and acid leaching tests were conducted for coals of the Longtan Formation from the Rongyang Mine.

Stepped release analyses revealed that the contents of molybdenum (Mo) and U in cleaned coals are higher than in flotation products, and the elements beryllium (Be), fluorine (F), vanadium (V), chromium (Cr), cadmium (Cd), barium (Ba), tungsten (W), cesium (Cs), and thallium (Tl) that existed in the flotation products exhibited a similar trend to ash yield. With an increased number of cleaning stages, the content of these elements in tailings decreased, which indicates that a multi-stage cleaning process can help to separate lithophile elements from cleaned coals. However, with an increased number of cleaning stages, the content of the sulfophile and siderophile elements scandium (Sc), Co, nickel (Ni), Cu, arsenic (As), Se, antimony (Sb), bismuth (Bi), and mercury (Hg) in the tailings increased.

Through stepped release flotation, the removability of V, Cr, and Mo in cleaned coals was negative, indicating that V, Cr, and Mo cannot be remove by stepped release flotation. Uranium had a removability of 25.67%. The removability of U by stepped release flotation was higher than that by gravity and flotation separation, but the removal effect of gravity separation for thiophilic elements was greater than that of flotation.

Since stepped release flotation cannot effectively remove some elements (such as V, Cr, Mo, U), and part of these elements are adsorbed in clay minerals and organic matter, acid leaching was conducted on cleaned coals to remove the adsorbed state of V, Cr, Mo and U, and the results revealed that the adsorbed state of the thiophilic and siderophile elements Co, Ni, Cu, Zn, As, Cd and lead (Pb) was higher than that of the lithophile elements Sc, Rb, Ba and Tl. Small amounts of Cr, Mo and U existed in the adsorbed state, and the adsorbed state of V was only ~2%.

POSTER SESSION 8
COAL BED AND SHALE GAS

P.8.1- Study On the Coalbed Methane Enrichment Law and Its Influencing Factors in Hancheng Mining Area, China

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Based on the analysis of logging, cores, and samples test from the Hancheng mining area, this paper believes that the Carboniferous-Permian in the Hancheng mining area is formed under various sedimentary environmental conditions. The Taiyuan formation is formed in the coastal environment, which is mainly a lagoon-tidal flat-barrier island sedimentary system. Three kinds of marine peat-plated coal accumulating environments are developed in this formation namely; barrier island peatland, tidal flat peat floor, and carbonate platform peat-plate. The Shanxi formation is a river-controlled delta sedimentary system with two kinds of coal-forming environments: delta plain peat swamps and river-diver peat swamps. The coal ranks are mainly meagre coal and lean coal, which have reached their late stages of mature gas generation and high maturation, have strong gas-generating capabilities and large overall hydrocarbon generating potentials. The adsorption capacity of coal-rock is strong, the langmuir volume ranges from 3.83 to 32.02 m3/t, and the average value is 28.20 m3/t. The structure of the mining area is simple, the coal seam distribution is stable, and the sealing conditions are good. The roof and bottom plates of 3# and 11# coal seams are mudstone, which are impervious capping layers and are very favorable for the storage of coalbed methane. There is a large area of sandstone capping on the 5# coal roof, but its porosity is poor, which is also conducive for the storage of coalbed methane. The mining area is in a hydraulic stagnant area which is also beneficial for the storage of coalbed methane. The study considers that the depositional environment controls the spatial distribution of coal seams, and tectonic movement is the main factor for the differential enrichment of coalbed methane. Lastly, through the optimization of evaluation indicators, a multi-level gray evaluation theories and methods were adopted to divide the entire mining area into 474 evaluation units, and quantitative evaluations were carried out. Three sets of the most favorable areas, favorable areas and general areas of coalbed methane development distribution scopes were proposed.

P.8.2- Comparison of Pore Size Distributions On Crushed and Whole-Rock Coal Samples Using Nuclear Magnetic Resonance

Yanhai Chang, Yanbin Yao, Dameng Liu, Yong Liu, Sijian Zheng, Lutong Cao, Xing Wen, China University of Geosciences, PR CHINA.

The core data plays a very important role in coal reservoir evaluation and coal bed methane development. However, coring is time consuming and sometimes it is difficult to retrieve whole cores. Drill cuttings, which are typically collected in millimeter scale, are brought to the ground during the drilling through the circulation of the drilling fluid. Drill cuttings show strong potential to represent all the formations encountered during the drilling process. In this study, nuclear magnetic resonance (NMR) and mercury intrusion porosimetry (MIP) have been used to determine the pore size distributions and porosity of coals from cuttings and the whole core. The cuttings are obtained from crushed and screened cores into three different sizes: A (6700-4750μm), B(3350-2360μm), C (1700-1000μm). Our results show that estimating the porosity and pore size distribution from cuttings by using the NMR is effective and reasonable. Especially in the adsorption pore range (<0.1μm), the RSD (relative standard deviation) is less than 5%. In addition, it has been found that the high pressure in the MIP measurement may deform or destroy the original pore structure and low pressure may measure interparticle pores result in an invalid result of pore size distributions. Based on a comparative analysis of the measurement results, NMR is an effective method for quantifying the pore size distributions and porosity of coal from both cuttings and core.

P.8.3- Shale Gas Enrichment of Wufeng-Longmaxi Formation Shale in Southeast Chongqing

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In the current research, the evolution characteristics of pores in the organic-rich shale samples from Wufeng-Longmaxi Formation in Southeast Chongqing and the accumulation process of shale gas are analyzed, revealing the controlling factors of shale gas enrichment and picking out the "dessert zone" for shale gas development. On the basis of microstructure observation, the rock structure analysis and the fracture development characteristics, dividing the tectonic evolution of the studied area into four stages: the uplift into land during the early period of the Indosinian movement, the strong compression in SE-NW direction between the later period of the Indosinian Movement and the early period of the Yanshan Movement, the formation of a trough-like deformation band between the later period of the Yanshan Movement and the early period of the Himalayan Movement and the tectonic superposition during the later period of the Himalayan Movement. The field investigation work and comprehensively studying the reservoir characteristics of shale gas as well as the "three histories" of shale, namely, construction - burial - hydrocarbon generation are carried out. The results show that shale gas accumulation in the studied area can be divided into four stages: the deposition period of source rock, the initial accumulation period, the main accumulation period and the preservation period, and the periods after the middle and later period of the Yanshan Movement is critical for the migration, dissipation and accumulation of shale gas. The evolution law of shale pore structure is studied and an evolution model of shale pores is established. Basing on the analysis of main factors controlling shale gas enrichment in the studied area, the laws of shale gas enrichment in southeast Chongqing are as follows: the material basis for the accumulation of shale gas is the organic-rich shale controlled by the deep-water shelf depositional environment; the decisive condition for the enrichment is the occurrence of shale gas under the control of reservoir physical properties; and the key guarantee for the enrichment is shale gas preservation under the combined effect of multiple factors. These laws reveal that the enrichment of shale gas is jointly affected by multiple factors among which depositional environment, reservoir characteristics and preservation conditions are the main controlling factors. Ten "Dessert zones" with a total area of 2100.14 km2 can be selected from Wufeng-Longmaxi Formation in the studied area on the basis of the above laws, auxiliary evaluation parameters, superposition of multiple factors and comprehensive analysis. The reservoir characteristics and the shale gas enrichment laws of Wufeng-Longmaxi Formation in southeast Chongqing revealed in this paper are of great significance for guiding the high efficiency exploration of shale gas in this area.

P.8.4- Numerical Simulation for Enhanced Coalbed Methane Recovery by CO_2 Gas Injection

Ning Zheng, Jianwei Li, Xi'an University of Science and Technology, PR CHINA.

Enhanced coal bed methane recovery by injecting CO2 gas is a new technology attracting more and more attention for the potential ability both in increasing coal bed methane production and reducing the greenhouse effect by storing CO2 gas into the coal

seam, which can bring the economic and environmental benefits at the same time. In this article, the adsorption equilibrium and competitiveness is analyzed by experiment, and the permeability parameters are calculated. Based Maxwell-Stefan equations, a dynamic multi-coupling model for the CO2 gas injection displacing process is established and numerically simulated using finite elementary mothed. The simulation can predict different gas composition changing with time both in the well pipe or coal matrix. The influence of CO2 injecting pressure and temperature is also considered in the simulation. The result shows the higher temperature or higher CO2 injecting pressure can result in the increase of CH4 output rate.

POSTER SESSION 9
POWER PLANTS

P.9.1- Research for Long Period Maintenance Technology of Double-Inlet Double-Outlet Coal Mill

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To master the law of steel balls abrasion, optimize the unit electric consumption and characteristics of pulverized coal, and implement a reasonable long period maintenance for double-inlet double-outlet coal mills, we sampled and tested the pulverized coal for a long period, sieved the steel balls and supplemented some steel balls on a supercritical W-flame boiler. The technique of optimized supplement improved the situation that the pulverized coal is too fine, increased pulverized coal uniformity index from 0.58 to 0.82, and reduced the unit electric consumption of the mill by 2.54kWh/t. Therefore, it is feasible that we can obtain the real-time distribution of steel balls and reasonable signal of supplement for double-inlet double-outlet coal pulverizing system meanwhile maintain the unit electric consumption of pulverized coal and the characteristics of pulverized coal in a high-level.

P.9.2- Large Eddy Simulation of a 660 MW Double-Reheat Ultra-Supercritical Boiler

Haoshu Shen, Yuxin Wu, Hai Zhang, Guangxi Yue, Tsinghua University, PR CHINA.

Computational fluid dynamics has been widely applied to the research and development activities of boilers. In recent years, LES has become a promising simulation tool when compared to RANS and DNS. LES directly solves the Navier-Stokes equation of large eddies and models small eddies which are less important for the main flow. Previous studies have showed that LES can well predict the pulverized coal jet flames. Due to the growth of renewable energy and frequent grid peak shaving, the low-load operation is required for the next-generation boilers such as double-reheat ultra-supercritical boilers. The turbulent and chemical processes in the boilers should be further investigated under a wide operating conditions. In this paper, a set of models used in LES was validated by a lab-scale burner. Then this simulation method was applied to a 660 MW double-reheat ultra-supercritical boiler. The results showed that LES could provide a deep understanding of flame ignition behaviors and pollutant formation mechanisms.

P.9.3- Combustion and Control Optimization of 30% Rated Load of a 300 MW Condensing Power Plant

Xiang He, Yingguan Cheng, Dafu Ma, Shanghai Power Equipment Research Institute Co., Ltd, PR CHINA.

A 300MW subcritical power plant, which can operate at 30% rated load. But the reheat steam temperature is below 500℃and the main steam temperature is more than 540℃. In order to raise the reheat steam temperature and control the main steam temperature, tcombustionandthermotechnical logicofboilerare optimized. Firstly, Atthe high loadof the unit, tpressureof primary air at outlet of air preheated is reduced 8%, and the second air volume of boiler is enhancedabout 10%. Secondly, under low loadof the unit, the primary air and second air volumesare both reduced.In terms of theNOxvolume at a reasonable level, the combustion isstrengthened to raisethe furnace temperature to improve the reheat steam temperature. Thirdly, the heat deviationof A/B side is reduced by means of adjust thevelocity of four tubesofpulverized coal out of mills, and the offset islevelledless than 5%.Moreover, thevalve baffle of the secondair are adjustedin detail.Forthly, the thermotechnical logicoptimization is also carried out, the partial logicconfiguration is modified, and theprotection parameters are optimized.After above steps, the 30%rated loadworking condition is completed by two millsoperationwhich depends ontheadjacent B and C mills. Results shows that the combustion stabilization is well, moreover the temperature of main steam is more than 530℃and that of reheat steam is raised to 515~520℃.

P.9.4- Efficiency and Water Consumption Comparison of IGCC Power Plants Using Different Unit Technologies

Xin Zheng, Bo Wang, Lifeng Zhao, Yuan Lu, Yunhan Xiao; Institute of Engineering Thermophysics; Chinese Academy of Sciences; University of Chinese Academy of Sciences, PR CHINA.

Due to high efficiency, low environmental emissions and low cost for carbon capture, Integrated Gasification Combined Cycle (IGCC) power plant has been recognized as an attractive option for coal-based power production. Besides, the water consumption of IGCC power plant is much less than the pulverized coal (PC) power plant. The goal of this study is to evaluate the effects of different units or processes in an IGCC power plant on the thermodynamic performance and water consumption. Those units and processes include gasifier, the method of thermal NOx control, the integration degree of gas turbine (GT) and air separation unit (ASU), and GT. Five different IGCC configurations were analyzed in this study which uses consistent design requirements for all technologies examined, as well as up-to-date performance. As a result, the IGCC based on air-blown gasifier has a higher net efficiency by 0.52 percentage points and less water consumption by 42.7 kg/MWh than the oxygen-blown gasifier based IGCC. When steam injection is replaced by N2 injection, the system net efficiency is increased by 0.66 percentage points and water consumption is decreased by 25.5 kg/MWh. The IGCC with 100% integration between GT and ASU has a higher net efficiency by 1.57 percentage points and less water consumption by 86.8 kg/MWh. Because of higher thermal efficiency, the 9HA.02 GT case can achieve net efficiency of 49.60%, which is 3.37 percentage points higher than that of the FA class GT case, while 129.8 kg/MWh of water consumption can be reduced. The net efficiency of the 9HA.02 case is 9.6 percentage points higher than the average net efficiency of nominal 600MW PC power plants, and the water consumption is 980.9 kg/MWh less than the average water consumption of nominal 600MW PC power plants with water cooling tower, which means a reduction of about 50%.

POSTER SESSION 10
SUSTAINABILITY AND ENVIRONMENT

P.10.1- Is Zero Solid Waste For Fly Ash Possible?

Jinder Jow, Yang Dong, Department Manager, Shuqiang Ding, National Institute of Clean-and-Low-Carbon Energy, PR CHINA.

Coal has organic and inorganic components. The organic components are used for generating heat through combustion or producing chemicals through gasification, liquefaction or coking. The inorganic components become solid wastes, since not the target products, in these utilization processes. Fly ash is one of largest industrial solid wastes from the coal combustion process. The total production volume in 2015 for global, China and USA are 1.143 billion tons, 566 million tons, and 44 million tons with utilization rates of 60%, 70%, and 52%, respectively. Most current fly ash utilizations are in the low-end low-value building and construction applications which are extremely location-dependent and seasonal. Most coal-fired power plants, particularly located in remote areas, have not reached 100% utilization due to local market needs lower than its production quantity.

All fly ashes have three fundamental materials properties: particle size distribution and particle morphology, chemical compositions, and mineral compositions. Not every fly ash has the same values in these properties and due to its significant variations, resulting in low-end low value applications. Particle size distribution and its morphology depend on the coal pretreatment, combustion processes, and ash collection system. Chemical compositions primarily depend on coal type, but also extent of combustion and environmental control system, such as incomplete combusted carbon, sulfur and calcium from the furnace desulfurization, as well as ammonia from abnormal denitrification catalytic process. Mineral compositions depend on coal type, fly ash particle size, boiler temperature, and ash cooling and collection systems. The variations in coal fired power plant operation can make fly ashes with significant differences in properties.

Zero fly ash solid waste is possible only if new mind-sets and approaches are adapted by each coal-fired power plant. Below are the important partnership between each power plant and scientific community to achieve zero fly ash solid waste and achieve its full utilization for each coal fired power plant:

Each power plant needs to establish quality-control operational procedure to constantly produce fly ash with consistent quality as raw materials,

Scientific community needs to fully utilize this fly ash with consistent quality to develop high-value and low-value marketable products, meeting the industrial product standards, to achieve the positive economic benefit to achieve zero fly ash solid waste.

This paper reviews the current solid waste policies in China and USA, promotes mind-set changes, champion standardization, and presents innovative product technologies developed at NICE with one example to achieve zero solid waste for fly ash at a given coal fired power plant in a remote area.

P.10.2- Measurements of Toxic Heavy Metals Contamination in Drinking Water of Islamabad, Lahore, Jung, Multan and Khushab and Their Damages to Human Health

Muhammad Sarfraz, Yang Li, Dalian University of Technology, PR CHINA; Zahid Gulfraz, Bahria University, PAKISTAN; Javeed AAwan, University of the Punjab, PAKISTAN; Waseem Raza, Haoquan Hu, Dalian University of Technology, PR CHINA.

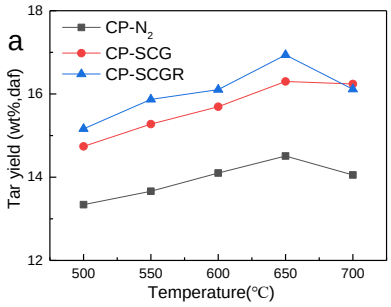
In this paper, toxic heavy metals contamination in drinking water of Pakistani cities: Islamabad, Lahore, Jung, Multan and Khushab, was studied. Damages caused by polluted drinking water to human health were also discussed. Heavy metals concentration (Lead, Chromium, Cobalt, Cadmium, Zinc, and Nickel) in 18 drinking water samples through Atomic Absorption Spectrophotometer (AAS) was investigated. Concentration of Lead and Chromium are above the Standard Permissible Limits (SPL) of WHO, U.S., and Pakistan Standard Quality Control Authority (PSQCA), in water sample # 8 and 17, respectively. Concentration of Cobalt and Zinc are within SPL in all the water samples. Concentration of Cadmium is within SPL in all samples except in sample obtained from Home tube well G-13/3, Islamabad and Home Boring G-13/3, Islamabad. Concentration of Nickel is also within SPL in all water samples except in sample obtained from Home tube well G-13/3 Islamabad, F-11 Water plant Islamabad, G-11 Water plant Islamabad and Walton Cant Lahore.

POSTER SESSION 13
VALUE-ADDED PRODUCTS FROM COAL

P.13.1- Integrated Process of Coal Pyrolysis with Simulated Coal Gas Reforming for Tar Production

Haibin Zhao, Lijun Jin, He Yang, Yang Li, Mingyi Wang, Haoquan Hu, Dalian University of Technology, PR CHINA.

Owing to low molar ratio of hydrogen to carbon in coal, tar yield from traditional coal pyrolysis technology is limited. Coal gas, especially coke-oven gas, a by-product from coking plants, contains a lot of hydrogen-rich gases, such as hydrogen and methane, which provides a potential H2 source. To improve the yield and quality of tar, in this study, the integrated process of coal pyrolysis with simulated coal gas reforming over Ni/Al2O3 (CP-SCGR) was put forward. As shown in Figure 1a, the tar yield of pyrolysis in simulated coal gas (CP-SCG) is significantly higher than that in N2 at the same temperature, however, the integrated process CP-SCGR can further improve the tar yield, which is attributed to the radicals, like •H and •CHx, generated from the reforming of SCG over Ni/Al2O3 catalyst. These small molecular radicals combine with coal pyrolysis radicals to retard the polymerization reaction among large radicals from coal cracking. The compositions of SCG influence the tar yield during coal pyrolysis (shown in Figure 1b). H2 and CO in SCG will inhibit the reforming reaction of CH4 and CO2, the improvement of tar yield in SCG is not as obvious as CH4+CO2, but this can be compensated by optimizing the proportion of each gases in SCG. Simulated distillation and GC/MS analysis showed that the pitch content of the integrated process was reduced and the light tar content was improved, such as benzenes and phenols. Pyrolysis tar from CP-SCG and CP-SCGR has higher aromatic proton ratio and lower aromatic carbon ratio compared with that from CP-N2.



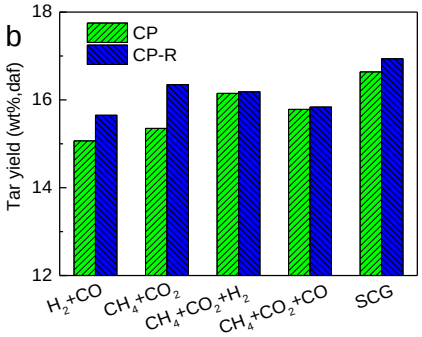


Figure 1. Effect of different temperature (a) and atmosphere (b) on tar yield

P.13.2- Analysis of Coal Tar Derived from In-Situ Catalytic Upgrading Over Nickel Loaded Activated Carbon

Mingyi Wang, Haoquan Hu, Lijun Jin, Dalian University of Technology, PR CHINA.

A tar upgrading process, which integrated in-situ catalytic cracking of coal pyrolysis tar with CO2 reforming of methane (CRM), can improve light tar yield. In this study, tars from pyrolysis of three kinds of low rank coal (BLG, NMH and YL) were catalytically upgraded over nickel loaded activated carbon (Ni/AC). The results show that the content of light tar fractions (boiling point < 360 °C) and light tar yield increase after upgrading. Compared with that without upgrading catalyst, light tar contents increase to more than 95% and corresponding light tar yields increase by about 50% over Ni/AC catalyst at 650 oC. The results also show that Ni/AC can catalyze coal tar cracking and CRM simultaneously, and some radicals, like •H and •CHx, produced in CRM over Ni/AC could combine with the radicals from catalytic cracking of tar to avoid excessive cracking of tar. BLG coal was chosen to further analyze the composition and structural change of coal pyrolysis tar in the upgrading process. Compared with non-upgrading tar, the upgrading tar has high contents of light oil, phenol oil, naphthalene oil and wash oil, which remarkably increases by 224%, 283%, 132% and 36%, respectively. The average molecular weight of the upgrading tar over Ni/AC decreases from 279 to 160 amu, and the light components, such as benzenes, phenols and naphthalenes, are all improved significantly. What's more, the tar has higher uncondensed aromatic hydrogen ratio and lower aromatic carbon rate after upgrading over Ni/AC.

ANNOUNCING

THIRTY-SIXTH ANNUAL INTERNATIONAL PITTSBURGH COAL CONFERENCE

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