

**International  
Collaborative Centre  
for Carbon Futures**



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University of Newcastle  
Newcastle, Australia

Host: International Collaborative Center for Carbon Future (ICCCF),  
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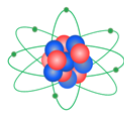
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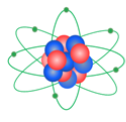
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# Plenary Lectures

## Gas quality control for carbon capture and storage: Experiments at the Callide Oxyfuel Project

Terry Wall, Rohan Stanger, Tim Ting, Dunyu Liu, and Lawrence Belo

*Chemical Engineering, University of Newcastle, Callaghan, NSW 2308, Australia*

The paper quantifies the extent of potential removal and the impact of impurity levels in the CO<sub>2</sub> rich flue gas with laboratory experiments on ‘synthetic’ oxyfuel gas and several trials at the coal-fired 30MW Callide Oxyfuel Project (COP) in Biloela, Queensland, to test the impact of ‘real’ oxyfuel gas. The COP tests included experiments over the fabric filter, samples taken directly from the CO<sub>2</sub> processing (compression) unit (CPU) as well as compressed sampled (slip stream) gases and resulting liquids from an apparatus developed for compression of oxyfuel flue gas using a piston compressor.

The research provides unique data, and is based on the need to reduce cost of cleaning and risk associated with CO<sub>2</sub> gas quality in the technology for CCS. In particular, the removal of mercury species prior to CO<sub>2</sub> liquefaction is critical in avoiding the cost and risk of corrosion in brazed aluminum cryogenic heat exchangers of the CPU. The CO<sub>2</sub> impurities from oxy-fuel technology for CCS differ greatly from pre- and post-combustion technologies for CCS in quality and quantity, having higher levels of gas impurities which impact efficiency and operation such as sulfur oxides (SO<sub>2</sub>, SO<sub>3</sub>), nitrogen oxides, (NO, NO<sub>2</sub>), and mercury gases (as atomic or oxidised form, Hg<sup>0</sup> or Hg<sup>++</sup>).

The results confirm that for C-in-ash>5%, mercury capture by a fabric filter operating at atmospheric pressure is high (>80%) with little impact on ash quality. The results indicate that competition between mercury and SO<sub>3</sub> capture by ash can be neglected for C-in-ash >2%. In the CPU, SO<sub>x</sub> and NO<sub>x</sub> can be removed as liquid acids in the condensates created by reaction with the water vapour formed during compression of the flue gases, to removal levels of ~100% SO<sub>x</sub> and 80% NO<sub>x</sub> during compression to 30 bar. Also in the CPU, mercury can be removed from the CO<sub>2</sub> rich gas, partially in the acidic liquids and partially retained in the compressor, to result in levels of less than the 0.01 µg/m<sup>3</sup> set by the natural gas industry to avoid attack of the aluminium units integral to the CPU. But the form of the removal product is unknown.

## Directional catalytic hydroconversion of coals based on the coal structural features

Xian-Yong Wei\*, Zhi-Min Zong, Wei Zhao, Zhong-Hai Ni, Zi-Wu Liu, Jing-Pei Cao, Xing Fan,  
Yun-Peng Zhao, Xiao-Yan Zhao, Xiao-Min Yue

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The main species of organic matter in coals are macromolecular condensed aromatics. Most of the aromatic rings in organic matter of coals except anthracites and high-rank bituminous coals are connected by bridged linkages and there are alkyl and heteroatom-containing groups on a number of the aromatic rings. With the increase of coal rank, the bridged linkages become shorter and the alkyl and heteroatom-containing groups tend to decrease, while the aromatic rings tend to be more condensed.

Relatively mobile  $H^+$  and  $H^-$  can be produced by heterolytically splitting  $H_2$  over highly active supported superacids and superbases, respectively. The bridged linkages can be cleaved and some alkyl and heteroatom-containing groups on a number of the aromatic rings can be removed by directional catalytic hydroconversion with the relatively mobile  $H^+$  and/or  $H^-$  under mild conditions so that organic matter in coals can be converted to soluble organic small molecules mainly consisting of condensed aromatics with relatively simple composition. A series of value-added pure organic chemicals can be obtained by separating the soluble organic small molecules. On the other hand, both biatomic active hydrogen ( $H\cdots H$ ) and relatively mobile  $H^+$  (or  $H^-$ ) can be generated by activating and heterolytically splitting  $H_2$  over highly active Ni-loading supported superacids and superbases. Over such catalysts, aromatic rings in the soluble organic small molecules can be saturated and heteroatoms in the soluble organic small molecules can be effectively removed to produce high-quality liquid fuels, especially high-density liquid fuels.

# Fundamental advancements in thermal conversion of heavy organic resources

Zhenyu Liu

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Thermal conversion of organic resources or matters, such as coal, biomass, heavy oil, oil shale and waste organics, plays an important role in fuel and chemical production. The conversion generally involves two types of reactions, the bond cleavage of a feed to generate free radical fragments and the reaction of the radical fragments to yield products. While most of the past publications treated these reactions indiscriminately as a whole, some publications did try to decouple these reactions and study them separately, although these literatures focused mainly on the effects individual steps on products' yield instead of the radical mechanism.

This presentation shows the authors' recent researches on radical behavior in thermal reaction of coal, biomass, heavy oil and oil shale, including quantification of feed-structure dependent radicals' generation, reaction of free radical fragments especially the reactions with the feed, the relations between the active radicals and stable radicals (measurable by electron spin resonance, ESR), as well as coking of free radical fragments in the volatile state and on the catalyst surface.

It is found that thermal reaction of the organic feeds can be decoupled into three types of reactions, bond cleavage of the feed to generate free radical fragments, the reaction between the free radical fragments, and the reaction between the free radical fragments with the feed. Radicals associated in these steps can be quantified. The conversion of the feed is greatly promoted by the reaction between the free radical fragments with the feed (termed induced conversion). The products distribution is governed by manipulating the active free radicals. The coke formation in the volatile state and on the catalysts surface can be analyzed by the changes in stable radical concentration.

**Keywords:** organic resources, thermal reaction, radicals, radical induced reaction, coking.

## A Study on biomass torrefaction process to achieve HELE thermal power system in Korea

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Biomass is a renewable energy source that can be used as a base load energy resource for electricity supply. Additionally, it is expected to be used in various ways to fulfill government policy (greenhouse gas and particulate matter). Korea South-East Power Co. Ltd (KOEN), a Korean power generation company, is producing 125MW of energy through Yeongdong #1 using only biomass, and in coal-fired power plant, biomass such as a wood pellet is also used to reduce carbon dioxide. In order to apply biomass in existing coal-fired power plants, physical and chemical properties of the fuel must be analyzed. As these properties are indispensable, as it can bring about changes in the whole boiler system. However, if the fuel properties are similar to those of existing fuels, it is possible to apply the fuel only with relatively minor changes. For this reason, using the torrefaction technology of biomass, focus on optimizing the energy density with grindability and moisture contents for utilize more completely than unsophisticated application (raw biomass). Pusan Clean Coal Center (PCCC) at Pusan National University, actively carries out various biomass fuel researches. For the analysis of torrefaction process, solid-state <sup>13</sup>C NMR was used to determine the optimum conditions such as chemical characteristics and torrefaction temperature. Pyrolysis characteristics of the torrefied biomass were analyzed by TGA-IR. As the conventional model in relation to the surface expansion is unlikely to apply for the the high-rank carbonaceous fuel, the Flexibility-Enhanced Random Pore Model (FERPM) was proposed. The process of biomass boiler and hydrogen production technology (fuel cell and bio-fuel generation system) can be prepared through High-Efficiency Low-Emission (HELE) poly-generation system technology in ICCCF. In addition, a comprehensive analysis of biomass fuels was carried out through computational dynamics analysis of the biomass power plant.

**Keywords:** Korea power plant, biomass boiler, torrefaction, High-Efficiency Low-Emission (HELE).



# **A State-of-the-Art Report on Chemical Looping Based LET Options for Coal**

Behdad Moghtaderi

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The drive to develop cleaner and more efficient energy systems has stimulated an extraordinary array of research and development activities on chemical-looping-based process concepts over the past 15 years. An overview of these technology options, particularly those proposed/developed at the University of Newcastle (Australia), is presented in this talk. The focus, however, would be primarily on process-related aspects of such advanced chemical looping concepts for novel energy and fuels applications rather than aspects such as oxygen carriers, redox properties, and solid circulation/transport, which have been adequately covered in the literature.

## New understanding and evaluation of coking coal and coke properties

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Evaluation of coking coal properties in coking industry depends on several independent indicators tested in different test conditions for a long time, for example, Gieseler fluidity, Arnu-Audibert's dilatometer, plastometer indice, Roga index, and volatile content. On the other hand, evaluation of coke thermal properties depends on Coke Reactive Index (CRI) and Coke Strength after Reaction (CSR) tested in 1100[U+2103] and lasted in two hours. In view of the fact that there are some shortages of evaluation coking coal properties and coke thermal properties, the evaluation methods for "the related properties during carbonization of coking coal" and "the comprehensive thermal performance of coke" were developed. The former one was used to measure the relevance between the volatile matter escaping, plastic layer forming, and swelling pressure during single and blending coking coal carbonization process; the latter one was used to detect the initial temperature of coke reaction, the average coke reaction rate and the coke strength after reaction at the coke weight loss up to 25%, the dependence of the coke strength after reaction on the reaction temperature, the coke polycondensation index and coke strength after polycondensation for the coke weight loss up to 25%. These two methods can be used to further identify the performances of coking coal and coke, and establish some new evaluation methods of coking coal and coke quality.

**Keywords:** coking coal; coke; related properties during carbonization; comprehensive thermal properties.

## Effects of pressure on pyrolysis of biomass: enhanced production of hydrogen and nitrogen-containing compounds

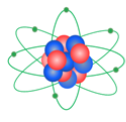
Jianglong Yu<sup>a,b,\*</sup>, Kristina Maliutina<sup>a</sup>, Arash Tahmasebi<sup>a,b</sup>

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Pressurized entrained-flow pyrolysis of *Chlorella vulgaris* microalgae was investigated. The impact of pressure on the yields and composition of pyrolysis products were studied using various analytical instruments. The results showed that the yield of H<sub>2</sub> in bio-gas increased sharply with increasing pyrolysis pressure. The hydrogen concentration reached 88.01 vol.% in bio-gas at 900 °C and 4 MPa. Increasing pyrolysis pressure significantly promoted the formation of nitrogen-containing compounds such as indole, quinoline, isoquinoline and phenanthridine. The nitrogen retention in bio-char and its content in bio-oil reached a maximum value at 1.0 MPa. The highest conversion of nitrogen (50.25 wt.%) into bio-oil was achieved at 1.0 MPa and 800 °C, which was about 7 wt.% higher than that at atmospheric pressure. Pressures promoted the formation of pyrrolic-N (N-5) and quaternary-N (N-Q) compounds in bio-oil in expense of nitrile-N and pyridinic-N (N-6) compounds. Higher pyrolysis pressures led to increased sphericity, enhanced swelling, and higher carbon order of bio-chars. Pressurized pyrolysis of microalgal biomass has a great potential for poly-generation of H<sub>2</sub>, nitrogen containing compounds and bio-char.

**Keywords:** Microalgae; Pressurized-entrained-flow pyrolysis; Hydrogen yield; Nitrogen-containing compound.



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# Oral Sessions

# Rapid Synthesis of Magnetic Zeolite Materials from Fly Ash and Iron-containing Waste by the Supercritical Hydrothermal Method for Mercury Removal Application

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In this work, the novelty of the process is related to the use of a mixture within industrial waste materials (fly ash, FA) and iron-containing waste (Red Mud, RM), Steel Slag, SS) as precursors and little amount NaOH as an the activator for the one-step synthesis of zeolites. The preparation of magnetic zeolite was completed in a high-pressure reaction kettle. Some magnetic zeolites were modified by hydrochloric acid steam for the evaluation of mercury removal activity. The magnetic zeolites were used to remove elemental mercury from flue gas. At the same time, the effect of HCl gas on remove mercury activity of sorbents was discussed. The evaluation test of Hg<sup>0</sup> removal was carried out using a fixed-bed quartz reactor. The simulated flue gas consisted of 6vol% O<sub>2</sub>, 12vol% CO<sub>2</sub>, 0-100ppm HCl, 40±3 μg/m<sup>3</sup> mercury vapor and balance gas (N<sub>2</sub>). The mechanism of mercury removal over sorbents was explored using the results of XRD, BET, XPS. According to the XRD results, the major crystalline phase turns out to be cancrinite in the samples. As the amount of iron oxide in the raw material was increased, the synthetic samples had the characteristic peak of magnetite. The synthesized samples can be easily separated by an external magnetic field. 4FA5RM1SS can remove 35-50% Hg at the temperature of 200 °C. Hg removal efficiency of the other zeolites were low, which were around 10%. The samples of 8RM2SS, 4FA4RM2SS and 8FA2SS were modified by hydrochloric acid steam can improve the capacity of removal Hg from 5% to above 95% at temperature of 200 °C and maintains over 4h. The removal efficiency of the 8FA2SS at 10 ppm HCl increased to 100% after 5h. The content of iron oxide in raw materials has an effect on the magnetic properties of zeolite and the mercury removal efficiency of modified samples. Iron oxide proportion of the magnetic zeolites were between 12%~15%, its Hg removal efficiency was best after modified by hydrochloric acid steam. Hg<sup>0</sup> oxidation on the modified magnetic zeolites probably occurred through the Eley-Rideal mechanism, physically or chemically adsorbed Hg<sup>0</sup> reacted with reactive chlorine species on the modified magnetic zeolites surface to form Hg<sup>2+</sup>.

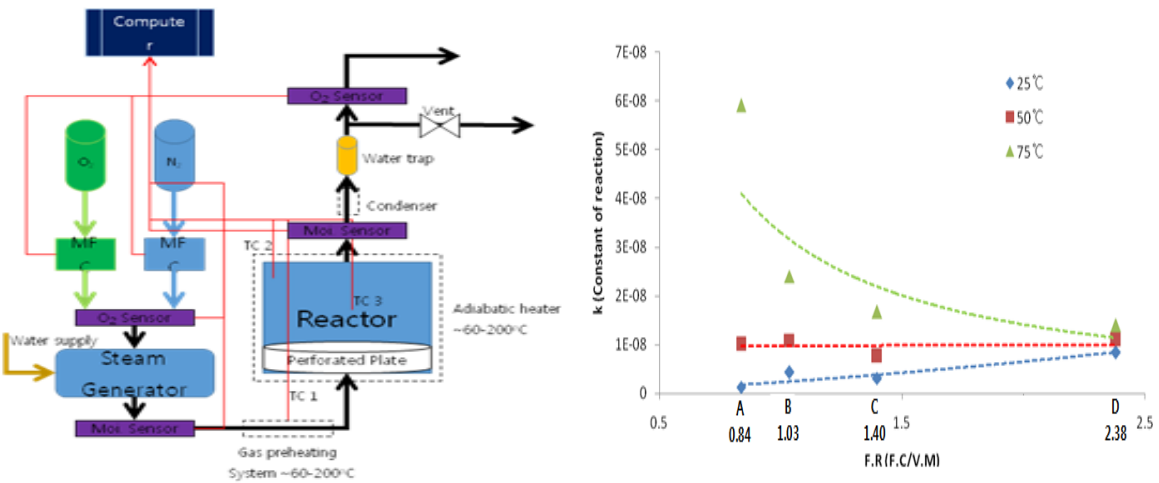
**Keywords:** Fly ash, Red mud, Magnetic zeolite, Supercritical hydrothermal synthesis, Mercury removal.

# A Study on Spontaneous Combustion between Low temperature oxidation and petrographic characteristics of coals

Dae-Gyun Lee<sup>1</sup>, Yanuar Yudhi Isworo<sup>1</sup>, Kyeong-Hoon Park<sup>1</sup>, Chung-Hwan Jeon<sup>1\*</sup>

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This study is to investigate the correlation between low temperature oxidation and petrographic characteristics of coals. Using the Low Temperature Oxidation Experiment, this research has been done like real coal piled. And being extracted at this experiment, coals are analyzed in case of petrographic characteristics. Petrographic analysis has been done by using a Coal petrographic Microscope Spectrophotometer, which can calculate vitrinite reflectance and morphology. The proximate analysis and ultimate analysis of coals used in this experiment is analyzed with TGA and Calorimeter. Four different types of coal were used to determine the oxygen consumption, which is the concentration of oxygen discharged into the reactor, and the reactivity and kinetics according to the basic properties such as proximate analysis and ultimate analysis were derived. With comparing the oxidation rates of coals and petrographic analysis, it is possible to deduce the cause of spontaneous combustion and predict which coal is easy to be burned in low temperature.



**Fig.1** Schematic diagram of Low temperature Oxidation experiment and Diagram of  $k$ (constant of reaction)

**Keywords:** Low temperature oxidation, Petrographic analysis, Spontaneous combustion, kinetics.

## **Pore structure and integrity of a bio-coke under simulated blast furnace conditions**

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Australia*

A pilot oven produced coke with the addition of 7.5 wt% charcoal (bio-coke) and the similarly produced base blend coke were subjected to gasification and annealing under the simulated blast furnace conditions. The effect of charcoal addition on the coke properties after gasification and annealing was characterised using Raman spectroscopy, ultra-micro indentation, tensile testing and image analysis. The addition of charcoal significantly increased the coke reactivity with CO<sub>2</sub> as a result of its increased surface area by charcoal. The addition of charcoal made no further contribution to the devolatilisation or mineral reactions of coke during annealing. The charcoal particles were well preserved after annealing at 2273 K, but preferentially consumed in the gasification. Annealing temperature had less effect on the graphitisation of the charcoal component compared to the coexisting inert maceral derived component (IMDC) and reactive maceral derived component (RMDC). The charcoal addition had no effect on the microstructure and microstrength of coexisting microtextural types during annealing and gasification. The charcoal presented a higher resistance to fracture than IMDC and RMDC under annealing conditions. The addition of charcoal did not deteriorate the coke resistance to strength degradation under the thermal load of blast furnace. However, charcoal addition caused more severe degradation by gasification as demonstrated by more reduction in the tensile strength of the bio-coke. This was attributed to the preferential solution loss reaction of the charcoal particles leaving voids which caused a considerable change in coke pore structure, thereby increasing the defects that cause stress concentration under loading.

## **An Investigation of the Molecular Changes in Coal Maceral Concentrates Prepared under Dimensional Heating Condition**

Quang Anh Tran<sup>1,\*</sup>, Rohan Stanger<sup>1</sup>, Wei Xie<sup>1</sup>, Nathan Smith<sup>2</sup>, John Lucas<sup>1</sup>, Terry Wall<sup>1</sup>

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Three maceral samples with vitrinite content of 88, 77 and 66 vol.% (mmf) obtained from an Australian coking coal were investigated to understand the difference in their thermoplastic development on a molecular level. Each maceral concentrate was packed vertically in a quartz tube which was heated solely from the bottom by a refractory heating plate. A thermocouple was inserted at 55 mm from the tube base to monitor the temperature change at this position as heat is transferred naturally through the packed column via conduction. To simulate the great thermal gradient existed in a coke oven between the oven side-walls and the centre of the coal charge, the experiment stopped when the temperature of the heating plate reached 900 °C. The thermocouple measured temperatures at 469, 486 and 495 °C for the three maceral samples, suggesting a greater thermal gradient existed in maceral samples with higher vitrinite concentration.

The sample quartz tube after cooling under inert atmosphere was filled with resin and sectioned axially to produce samples suitable for laser desorption/ionisation time of flight imaging mass spectrometry (LDI-TOF-IMS) investigation. Significant intensity of ionisable species was recorded at plastic regions close to the thermocouple position with samples of lower vitrinite concentration exhibiting higher intensity than samples with higher vitrinite content. The most abundant species in vitrinite-rich samples, on the contrary, showed a greater molecular weight discrepancy ( $\Delta m/z$ ) in the plastic region compared to that in samples with lower vitrinite content. In specific, the 88 vol.% sample possessed a  $\Delta m/z$  value of 2900 Da with molecular weight of most abundant molecules spanning between 1100 and 4000 Da. By comparison,  $\Delta m/z$  values of the 77 vol.% and 66 vol.% samples were only 2000 and 800 Da, respectively. These results suggested that a greater molecular change occurred during the pyrolysis of samples with higher vitrinite concentration and might be an indication of a more rigorous chemical change taken place in these samples.



## Poisoning effects of quinoline on the hydrodesulfurization of active and refractory sulfur species in light cycle oil

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Quinoline was used as a model nitrogen compound to simulate the poisoning effects of high nitrogen content compounds on the hydrodesulfurization of active and refractory sulfur species in light cycle oil (LCO). BET, XRD, Raman, TEM and XPS analysis was used to monitor changes to the structure, morphology and metal composition of NiMoS phases. These results revealed that low and high quinoline content had a distinct influence on both the hydrogenation and direct desulfurization pathways, which in turn altered the amount and ratio of active and refractory sulfur species present in the hydrotreated products of LCO. The amount of refractory sulfur species present in hydrogenated products at high reaction temperature was dependent on the steric hindrance of specific refractory sulfur species and not related to the initial sulfur content of the LCO. Low pressures of H<sub>2</sub> increase the poisoning effect of quinoline and significantly decrease the conversion rate of both active and refractory sulfur species. Low quinoline content favoured the formation of uniformly stacked NiMoS clusters, however, these stacked NiMoS clusters were disrupted when high contents of nitrogen compounds were present, resulting in formation of more easily-poisoned shorter (2-4 nm) monolayer NiMoS clusters.

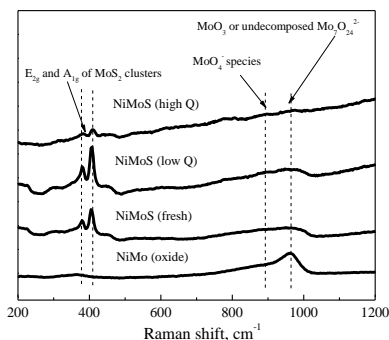


FIG. 1. Raman spectra of oxide and sulfided NiMo/Al<sub>2</sub>O<sub>3</sub> catalyst

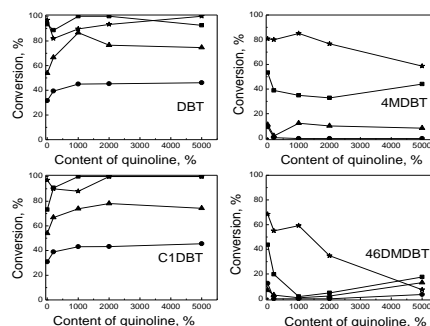


FIG.2. Selectivity and conversion of sulfur species in hydrotreated products obtained at 310 °C in the presence of quinoline.

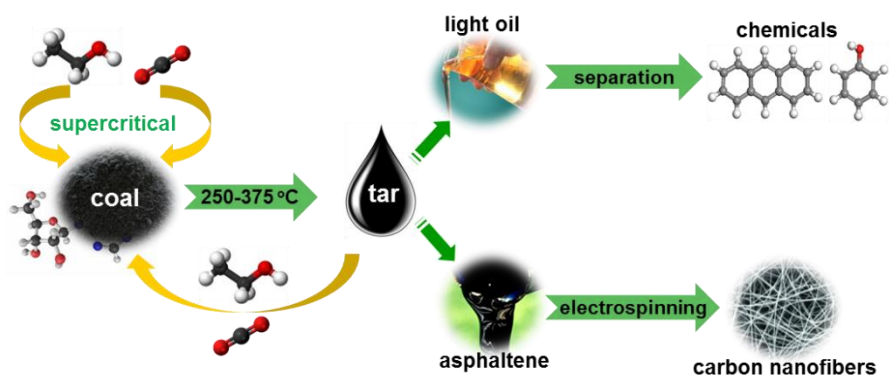
## Valuable liquid tar produced from Powder River Basin coal through degradation in supercritical CO<sub>2</sub>-ethanol system and its application

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A novel and environmentally benign supercritical CO<sub>2</sub> and ethanol (SCCO<sub>2</sub>-ethanol) system, was employed to convert Powder River Basin (PRB) coal into high-value liquid tar which can be used as the feedstock for the production of fuels/chemicals and carbon fibers. The results show that the yield of liquid tar is about 45 wt% at 350 °C and 500 psi initial CO<sub>2</sub> pressure. The SCCO<sub>2</sub> can promote the liquid tar yield by ca. 7 wt% compared to that using pure supercritical ethanol due to the synergistic effect between ethanol and SCCO<sub>2</sub>. The liquid tars are better candidates as clean fuels than the raw coal or even bituminous coal due to their higher heating values and almost free from ash. The liquid tar can be separated into light oil and asphaltene fractions by ultrasonic extraction with *n*-heptane. Both light oil and asphaltene fractions were characterized with elemental analysis, FTIR, GC-MS, and NMR to evaluate their properties. The light oil fraction is promising feedstock for producing small-molecular valuable chemicals. The asphaltene fraction has potential to be used as the precursor for fabricating carbon nanofibers via electrospinning.



**Keyword:** coal; supercritical CO<sub>2</sub>; ethanol; degradation; liquid tar.

## Effects of substrate and carbon source on the growth of CNTs by microwave-CVD

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Microwave-assisted CVD method was applied for synthesis of carbon nanotubes (CNTs) on different substrates of pine nut shell chars, activated carbon and graphite, respectively. Methane and ethylene were used as a carbon source and nickel as a catalyst. A series of experiments were carried out to investigate the effects of catalyst, carbon source, and carbon substrate on the synthesis of the CNTs. The morphologies and structures of the samples were evaluated by the scanning electron microscopy (SEM), High resolution transmission electron microscope (HRTEM), Raman spectroscopy, X-ray diffraction (XRD) and Thermogravimetric analyser (TGA). Microwave irradiation, carbon source and catalyst were found to be the governing factors during the formation and growth of CNTs on different substrates at low temperatures for 600 °C. SEM analysis showed that the largest amount of CNTs were formed in presence of nickel catalyst on different substrates, suggesting that nickel had a critical role in the formation and growth of CNTs. HRTEM analysis results indicated that the CNTs growth on pine nut shell chars and graphite substrates had multiwalled structure, however, the solid structure of CNTs on the surface of activated carbon was obtained. The d-spacing of graphite sheets in the CNTs walls was 0.34 nm using the pine nut shell chars as a carbon substrate. The diameter of CNTs growth on pine nut shell chars, activated carbon and graphite was  $59\pm 6$  nm,  $30\pm 4$  nm and  $37\pm 5$  nm, respectively. The X-ray diffraction (XRD) analysis of the CNTs on different substrates showed a typical and strong carbon peak at around  $2\theta=26.3^\circ$ . Raman spectroscopy analysis revealed that the high degree of carbon order was achieved due to the formation of CNTs on the surface of on different substrates. The formation and growth mechanism of CNTs on different substrates under microwave irradiation was proposed and discussed.

# Evaluation of denitrogenation and deoxygenation on molecules in coal during catalytic treatments by ion-source collision-activated dissociation

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In 2018, National Natural Science Foundation of China has setup a new research area, basic chemistry in coal conversion, to resolve scientific problems in coal chemistry for industry. Currently, most analytic methods aim to evaluate total heteroatom release which is the main goal of most catalytic processes. However, productions of value-added chemicals from complex mixtures like coals are technically more demanding which inevitably need more detailed evaluation of the coal treatment processes. Therefore, a method for rapid evaluation of heteroatom release on aromatic cores will be valuable for further optimization of current coal upgrading processes. In this study, ion-source collision-activated dissociation (ISCAD) was used for dealkylation of ions from coal-derived liquids, which allows the observation of ionized aromatic cores via mass spectrometry (MS). ISCAD-MS was used to evaluate catalytic treatments of a low-rank coal in four solvents. Cyclohexane and methanol demonstrated the lowest deoxygenation and denitrogenation efficiency on aromatic cores, respectively. In addition, catalytic preference index was introduced to provide a preliminary description of the heteroatom release preference of catalyst on aromatic cores. Methanol was observed with the lowest denitrogenation and deoxygenation preference index among the four solvents. Overall, ISCAD-MS not only provided new insights in catalytic heteroatom release processes but also is a promising evaluation method for coal conversion.

**Keywords:** Heteroatom release; Ion-source collision-activated dissociation; Low-rank coal; Mass spectrometry

## Facile preparation of coal-based porous graphene as high-performance anode materials for lithium-ion batteries

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The excessive utilization of fossil fuels has increased the risks of global energy crisis and environmental issues, which has led to a great demand for sustainable energy sources and reliable technologies for energy conversion and storage. Lithium-ion batteries (LIBs), as a promising candidate in portable electronics, smart grids and electric vehicle, have attracted tremendous attention in recent years because of their high energy density, long cycling life, flexible lightweight design and excellent environmental compatibility. However, conventional LIBs based on graphite as anode materials suffer low theoretical capacity of 372 mAh·g<sup>-1</sup> and poor rate performance, which cannot meet the current urgent demands for high energy storage systems (the rapid development of practical applications). Therefore, it is highly important to develop high performance anode materials with high capacity and excellent rate capability to improve the performance of LIBs. Most recently, porous graphene is recognized as the most promising anode materials for LIBs due to its high specific surface area with hierarchical porous structure, excellent electrical conductivity and superb electrochemical stability.

In this work, we report a graphitization coupled with liquid oxidation-thermal reduction strategy to prepare porous graphene for anode materials in LIBs using anthracite as starting materials. The earth-abundant anthracite was firstly graphitized at a high temperature of 2800 °C under argon atmosphere, where the macromolecular structure enriched aromatic units in the precursor experienced a graphitization step to form highly ordered layered structure of graphite-like carbon. The resultant graphitized coal was converted into graphene oxide through modified Hummers method followed by further thermal reduction to prepare porous graphene. The morphology characteristics, porous structure and surface chemical property of obtained porous graphene were

systematically investigated by various characterization techniques. The electrochemical performances of coal-based porous graphene applied as anode materials for LIBs were also evaluated through galvanostatic cycling, cyclic voltammetry and electrochemical impedance spectroscopy.

The results show that the obtained porous graphene possesses highly continuous corrugated nanosheets with micro-meso-macro hierarchical porous structure, plenty nanopores and structural defects with high specific surface area ( $640 \text{ m}^2 \cdot \text{g}^{-1}$ ) and large pore volume ( $3.792 \text{ cm}^3 \cdot \text{g}^{-1}$ ) as well as appropriate oxygen-containing functional groups located in graphene framework. Such unique microstructure features of porous graphene are favorable to be applied as high-performance anode materials for LIBs. The corresponding anode materials presents a maximum reversible capacity of  $943 \text{ mAh} \cdot \text{g}^{-1}$  at current rate of 0.1C and still remains as high as  $223 \text{ mAh} \cdot \text{g}^{-1}$  at current rate of 20C. Moreover, the porous graphene also exhibits superior rate capability and outstanding cycling performance with over 96.7% initial capacity retention after 100 cycles. The excellent electrochemical behavior of the obtained porous for anode materials in LIBs are attributed its unique microstructure characteristics. Large specific surface area with interconnected pore structure in porous graphene can shorten the diffusion distance of electrolyte to enhance the rate capability, whereas the nanopores and defects can provide sufficient active sites for lithium ions insertion to achieve high capacity. Besides, the integrated porous nanostructure skeleton with high conductivity can facilitate electron transfer and relieve the volume expansion effects during lithium ions insertion-extraction process. This study demonstrates a promising feasibility for large-scale production of porous graphene from earth-abundant coal for high performance lithium-ion batteries.

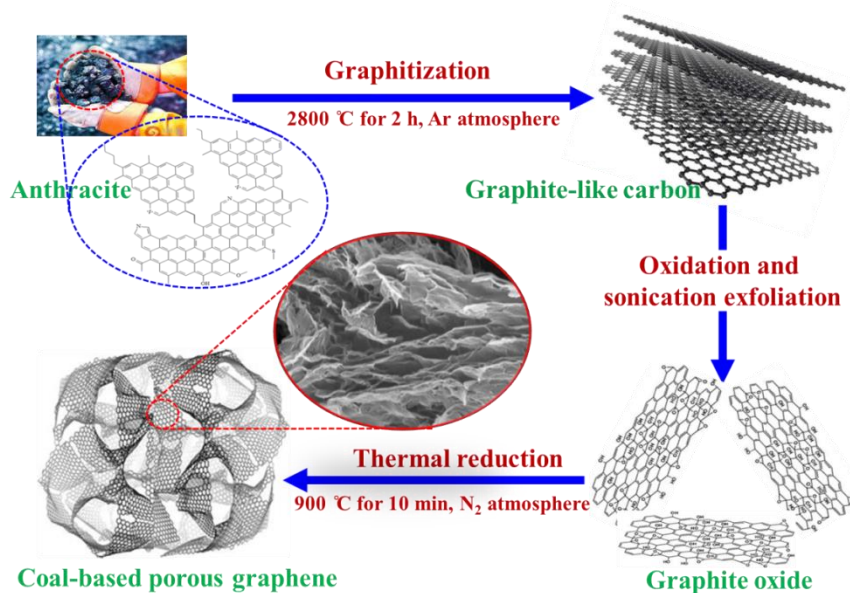
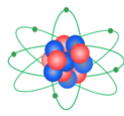


Fig. 1. Schematic illustration of the procedure for preparation of coal-based porous graphene



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## **Environmental Retrofit of 500 MW level's thermal power Plant**

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## Denitrification performance of simulated flue gas using Fe(II)TBAB-EG DES

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The selective absorption of NO from simulated flue gas has been investigated using a series of deep eutectic solvents (DESs) as novel denitrifying agents. Using deep eutectic solvent (DES) for removing NO without secondary pollution, which can also achieve good results. Ethylene glycol (EG) and tetrabutylammonium bromide (TBAB) (molar ratio 50:1) were prepared by Fe(II)TBAB-EG DES in this paper. Effect of reaction temperature, gas velocity, oxygen partial pressure and amount of additive FeCl<sub>2</sub> on the removal of NO in the flue gas were investigated. The kinetics of NO absorption reaction by Fe(II)TBAB-EG DES was also systematically studied. The inlet and outlet concentration of NO by using Flue gas analyzer (Testo 350) to characterized denitrification performance of Fe(II)TBAB-EG DES. Functional groups of Fe(II)TBAB-EG DES before and after denitrification were characterized by Fourier transform infrared spectroscopy (FT-IR) analysis. The experimental results showed that the temperature of 50 oC, the flow rate of 50ml/min, the oxygen partial pressure of 5%, Fe(II) concentration of 1mol/l, DES showed the best denitrification performance. After several adsorption and desorption recycling, Fe(II)TBAB-EG DES shows good denitrification stability. FTIR results showed that the Fe(II)TBAB-EG DES removed NO by physical adsorption. The absorption reaction is in according with the first-order reaction, the reaction equilibrium constant of denitrification reaction was 100.



## **A Mechanistic Study on the Characteristics of the Plastic Layer during the Heating of Australian Coking Coals**

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Coke is formed in industrial coke ovens when a coking coal undergoes a plastic transformation during pyrolysis. During heating some components of the coal (vitrinite macerals) melt to form a viscous zone called the plastic layer. The plastic layer has crucial influences on coke quality, and the formation of the plastic layer would seem to involve the generation of internal gas pressure (IGP) and coking pressure, which subsequently affect the operation of the coke oven. Even though the mechanisms involved during this plastic layer are well accepted concepts, its underlying science, which is largely based on significant empiricism, has yet to be fundamentally understood. Therefore, this study aims to achieve the understanding of the characteristics of the plastic layer and its relevant phenomena by means of a 4kg dual-heated wall coke oven (4kg coke oven). The 4kg coke oven enabled in-situ measurements of a range of parameters, such as temperature history and internal gas pressure and plastic layer sampling under the heating condition which is similar to that of pilot scale coke oven. A micro CT at Australian Synchrotron was used to examine the macro structure of the plastic layer with non-destructive way. Subsequently, samples extracted from the plastic layer samples were analyzed by an Attenuated Total Reflectance-Fourier Transform Infrared (ATR-FTIR) and a Thermo-Gravimetric Analyzer coupled with a Fourier Transform Infrared Spectrometer (TGA-FTIR) to investigate the change in the chemical structure of the plastic layer from different phases of the process, such as the initial soften layer, intermediate plastic layer and solidified semi coke. Additionally, it was possible to investigate mechanism of the IGP by means of the analysis of the in-situ measurement data linked to the characteristics of the plastic layer discussed. Combination of findings from this study provided a fundamental understating of natures of the plastic layer. In addition, this identified sample properties that affect the formation of the plastic layer and its relevant phenomena.

## CO<sub>2</sub> sequestration by direct aqueous mineralization of fly ash: Ash screening and kinetic investigation

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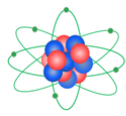
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CO<sub>2</sub> mineralisation by industrial wastes is a promising option for mitigating CO<sub>2</sub> emissions safely and permanently with low material cost. But there is still absence of detailed understanding on the fly ash properties affecting the kinetics of carbonation reactions. To deal with this problem, five fly ashes from China and Australia (BJ, YA, LY, WH and HW ash) were selected for carbonation in this study. The experiments were performed in a batch reactor at 40 and 140°C with 20 bar initial CO<sub>2</sub> pressure, 200 g/L solid to liquid ratio, 450 rpm stirring rate for 2 h to compare the carbonation characteristics of the five fly ashes and the effect of fly ash properties on carbonation reactions. Then BJ, YA and HW ashes were selected for further kinetic study at various temperature (20–220°C). Rietveld quantitative X-ray diffraction (XRD) was used to characterize the crystalline and amorphous phases present in the fresh and carbonated fly ashes qualitatively and quantitatively. Scanning electron microscope (SEM) and energy dispersive spectroscopy (EDS) were used to characterise the morphological properties of fresh and carbonated fly ash samples. Compared to LY and WH ashes, BJ, YA and HW ashes displayed much higher CO<sub>2</sub> sequestration capacity due to the higher fraction of reactive Ca/Mg-bearing crystalline phases including lime and portlandite in BJ ash, periclase and srebrodolskite in YA ash, and periclase and brucite in HW ash. Compared to YA and WH ashes, BJ ash displayed faster kinetic of carbonation reactions because the reactant phases of BJ ash were mainly Ca-bearing phases which has higher reactivity with CO<sub>2</sub> than Mg-bearing phases. Also, the particle size analysis and the morphological investigation indicate that the reacted particles displayed a lower porosity, tortuosity, and pore area than the fresh sample due to the newly formed precipitation not only deposited on the active surface, but also filled the pores of the fly ash particles, which was responsible for the reduced kinetic with time.



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# **Operational Improvement and Optimize Management of Samcheok CFB Boiler**

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## **Poly-generation of hydrogen-rich gas and fine chemicals during pressurized entrained-flow pyrolysis of lignite**

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Pressurized entrained-flow pyrolysis of Chinese lignite was investigated. The impact of pressure on the yield and composition of pyrolysis products were studied in detail. The results showed that higher pressures hindered the volatile release, leading to higher char yields. The concentration of H<sub>2</sub> in bio-gas increased sharply with pyrolysis pressure, while those of CO, CO<sub>2</sub>, CH<sub>4</sub>, and C<sub>2</sub>H<sub>6</sub> were dramatically decreased. The concentration of H<sub>2</sub> in pyrolysis gas reached 91.7 vol.% at 900 °C and 4 MPa. The GC-MS analysis of tars derived from pressurized pyrolysis of lignite indicated that the complexity of tar was decreased at elevated pressures. The tar samples were predominantly composed of PAHs at temperatures higher than 800 °C and pressures of higher than 1 MPa. The highest concentration of PAHs in pyrolysis tars (90.4 area%) was achieved at 900 °C and 4 MPa. The major PAHs detected in pyrolysis tars were naphthalene, biphenylene, fluorine, phenanthrene, and Pyrene. The formation of hydrogen and PAHs via Hydrogen Abstraction-Acetylene Addition (HACA) and Diels-Alder mechanisms were proposed and discussed. Different from atmospheric pressure, pyrolysis at elevated pressures showed a great potential for poly-generation of H<sub>2</sub>, fine chemicals and bio-char.

## **A study on the formation of carbon nanotubes from microwave pyrolysis of cellulose component isolated from palm kernel shell**

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As a result of developing environmental concern and increase in the demand of carbon nanomaterials, renewable and eco-friendly materials are being used to produce carbon nanomaterials such as carbon nanotubes (CNTs). There has been recent progress in the production of CNTs from lignocellulosic biomass, serving as available alternative of fossil resource, because it is renewable, relatively available in nature and low cost. However, the controlling process and better understanding of CNTs formation in biochar is yet to be clarified. For this purpose, palm kernel shell (PKS) biocomponents were separated by chemical pretreatment methods. Microwave pyrolysis was carried out on the isolated biocomponents at different temperatures. The bio-chars of each biocomponent were collected and analyzed. Scanning electron microscope (SEM) results revealed the formation of carbon nanotubes (CNTs) only on the isolated cellulose char and none was found in isolated lignin char, making cellulose the biocomponent responsible for CNT formation. Further analysis carried out on the formed CNTs revealed distinct X-ray diffraction (XRD) carbon peaks at  $2\theta = 26.2^\circ$  and  $43.2^\circ$  indicating a good graphitic structure compared to the untreated PKS bio-char. Raman spectroscopy results also revealed a decrease in the  $I_D/I_G$  ratio to 0.85 compared to the untreated PKS CNT coated bio-char of 0.91 indicating a higher order of the carbon layers of CNTs. Building on the previous study novel method of direct conversion of biomass to CNTs via microwave pyrolysis, microwave irradiation is the key factor responsible for the direct conversion of isolated cellulose to CNT as well as the pretreatment method and the structure of the cellulose biocomponent. CNT formation is strongly dependent on the interaction or exposure of the cellulose biocomponent particle to the microwave electric arc.

## **SO<sub>x</sub>/NO<sub>x</sub> co-removal and N<sub>2</sub>O formation during compression of oxy-fuel flue gas**

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The co-removal of SO<sub>x</sub> and NO<sub>x</sub> during CO<sub>2</sub> compression is an option in oxyfuel CO<sub>2</sub> compression based on an Air Products patent on sour gas cleaning. This would potentially reduce the capital and operating cost of oxyfuel CCS by avoiding the common inclusion of a SO<sub>2</sub> scrubbing unit operation prior to compression.

In order to clarify three critical aspects of the possibility of co-removal, controlled laboratory experiments on a small pressure vessel and bench scale compression unit were conducted to improve our understanding regarding;

- a. The extent of the reactions of SO<sub>x</sub> and NO<sub>x</sub> associated with their absorption when in contact with water vapour known and liquid water in CO<sub>2</sub> compression and also with representative liquids representing the condensates, being water, HNO<sub>3</sub>(l) and H<sub>2</sub>SO<sub>4</sub>(l);
- b. The conditions and liquids where N<sub>2</sub>O is formed, this being known as a strong greenhouse gas;

Experiments were conducted in a small pressure vessel at conditions representative of typical gas compression from oxy-fuel combustion without SO<sub>2</sub> removal involving the gases SO<sub>2</sub>, NO (at 1000ppm inlet levels) and O<sub>2</sub> (at 5% v/v inlet), with water vapour, liquid water, nitric and sulphuric acids at pressures of 5 and 25 bar. The results indicate that in the standard oxy-fuel CO<sub>2</sub> compression system - with several stages of compression at increasing pressures - in the initial low pressure stages, soluble SO<sub>2</sub> will be readily removed; and the partial oxidation of insoluble NO to soluble NO<sub>2</sub> will occur in higher pressures stages. At 25 bar, complete removal of SO<sub>x</sub> and 90% removal of NO<sub>x</sub> (as NO<sub>2</sub>) was achieved. The N<sub>2</sub>O measurements reported appear to be the first experimental confirmation of N<sub>2</sub>O formation with simultaneous SO<sub>2</sub> and NO<sub>x</sub> removal at pressure. These have indicated that N<sub>2</sub>O formation requires gas/liquid contact (ie two phase) and simultaneous capture of NO<sub>x</sub> and SO<sub>2</sub>. Partial but substantial release of the absorbed SO<sub>2</sub> and NO from the liquids after depressurisation was measured. Some desorption of N<sub>2</sub>O was also measured. The results indicated that N<sub>2</sub>O formation was a maximum of 30ppm concentration which was equivalent to <1% CO<sub>2</sub> for GHG impact. The N<sub>2</sub>O formation was found to be related to SO<sub>2</sub> capture with ~4-6% of SO<sub>2</sub> feed utilised to form N<sub>2</sub>O. Interactive effects between SO<sub>x</sub> and NO<sub>x</sub> were measured but found to be relatively insignificant.

Overall, the compression of oxy-fuel flue gases containing acid gases, may prove to be a cost effective alternative for impurity control. The control of released gases on depressurisation and formation of N<sub>2</sub>O must be evaluated as part of the CPU design.

## Post-combustion capture of CO<sub>2</sub> by diamines bearing one primary and one tertiary amino group: reaction kinetics and mechanism

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Amine scrubbing remains the most mature technology available for large-scale CO<sub>2</sub> capture in the short term, but suffers from high energy consumption and high capital costs and thus requires improvement of CO<sub>2</sub> absorption capacity and kinetics of amines. In this regard, diamines bearing one primary and one tertiary amine group (1°/3° diamines) were proposed to be ideal liquid absorbents for CO<sub>2</sub> absorption which could exhibit the fast CO<sub>2</sub> absorption kinetics of primary amines while retaining the intrinsic high absorption capacity of diamines. Here, we presented a detailed kinetic study of five 1°/3° diamines for CO<sub>2</sub> absorption using a bubble column and a wetted wall column. Then, we further investigated the relationship between the structure of various 1°/3° diamines and their CO<sub>2</sub> absorption kinetics. Results showed that increasing alkyl spacer between two amine groups within 1°/3° diamines promoted the CO<sub>2</sub> absorption kinetics, while a large decrease in their reactivity with CO<sub>2</sub> was observed when the tertiary amine group exists in the cyclic structure. Among these studied 1°/3° diamines, 3-(Dimethylamino)-1-propylamine (DMAPA) displayed the highest absorption kinetics under relevant conditions, also exhibited higher overall mass transfer coefficients than that of MEA over the entire range of CO<sub>2</sub> loadings. To determine the reaction mechanism between CO<sub>2</sub> and DMAPA, the Fourier transform infrared (FT-IR) spectroscopy and <sup>13</sup>C nuclear magnetic resonance (<sup>13</sup>C-NMR) were used to elucidate the mechanism involved in the reaction of MAPA with CO<sub>2</sub>. Finally, the main reaction routes for CO<sub>2</sub> absorption into DMAPA solution via formation of the protonated DMAPA-carbamate were proposed.

**Keywords:** wetted wall column, absorption, Fourier transform infrared, nuclear magnetic resonance, protonation.

## A study of the coal volatile gas related with its chemical structure

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Among the various processes of coal combustion, which is a typical solid fuel, focus on the devolatilization process, the gas components releasing is not just determined by the phase changes due to the temperature increment. The origin of the devolatilization gas should be approached in the chemical structural aspects of the coal because coal is not only consisted with simple crystal structure but also complex organic chemical structure. At present, furthermore, applications of coal are not only as a simple heat source moreover as gasification, liquefaction and reductant. Therefore, we have to attention about the coal devolatile gas composition. In this study, we select different ranks of coal (A to E) according to volatile matter content for investigate devolatile gas composition variation in pyrolysis process. Using FT-IR (Fourier Transform InfraRed), NMR (nuclear magnetic resonance) for chemical structure analysis and TGA-IR/GC for gas composition analysis during pyrolysis process. As the result, the side chain of coal chemical structure affects volatile matter contents and the aromatic, aliphatic stretches and oxygen containing structure control the devolatile gas composition.

**Keywords:** coal pyrolysis, coal chemical structure, coal volatile composition.

Table 1. Proximate analysis of the coals

Coal Name	Moisture	Volatile Matter	Fixed Carbon	Ash
A	1.1%	14.51%	73.4%	10.99%
B	1.5%	12.33%	76.7%	9.47%
C	1.4%	18.6%	70.11%	9.89%
D	2.35%	23.05%	61.06%	13.54%
E	18.37%	34.75%	35.20%	11.68%

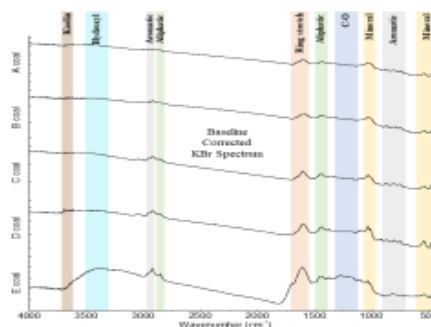


Fig. 1 FT-IR absorbance curves of the coal samples in 4000-400cm<sup>-1</sup> range and domains of chemical structure pick ranges



## Low-temperature microwave graphitization of activated carbon as renewable carbon material

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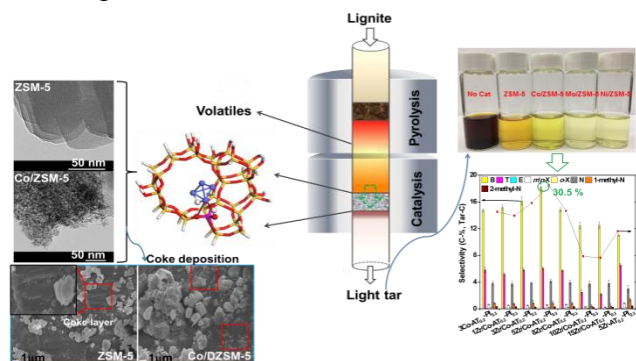
In recent years demand for graphite increased rapidly due to its vast application. Conventional method used for graphitization involves high temperature and extended periods of time. Here, we investigate the effect of temperature, catalyst type, catalyst percentage and processing time on the graphitization of activated carbon. The graphitized activated carbon samples were characterized using X-ray diffraction, Raman spectroscopy and transmission electron microscopy. The degree of graphitization was determined by X-ray diffraction using Rietveld refinement. Temperature had the greatest influence on the graphitization degree. Complete graphitization of amorphous carbon was achieved at 1300 °C with 10% nickel. Raman spectroscopy analysis showed that the maximum of G-band to D-band increased from 0.91 to 3.27 as the temperature increased to 1300 °C. Transmission electron microscopy analysis showed that the order of the carbon layer in the activated carbon transformed into graphite-like structure. The Graphitization process with the increase in the temperature improved the electrochemical properties in terms of both specific capacity and cycle stability.

## Channel Control of ZSM-5 Zeolite and its Application in Lignite Pyrolysis Volatiles Reforming for Light Aromatics Production

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ZSM-5 zeolite is widely used in lignite pyrolysis and in-situ upgrading pyrolysis tar for producing light aromatics. However, the single active center and the smaller pore size (0.5 nm) of traditional ZSM-5 zeolite limited the mass transfer of macromolecules, resulting in a sharp decline in catalytic activity and the tendency to induce the formation of coke deposition. In this work, hierarchical ZSM-5 zeolite was prepared by piperidine-assisted desilication method using the traditional ZSM-5 as support, and further synthesized bifunctional zeolite by impregnating monometal and/or bimetal to improve mass transfer and catalytic performance. The catalytic performance of the modified zeolite on the catalytic reforming reaction of lignite was studied in a drop tube reactor under mild conditions to achieve the light compounds of tar. Bimetallic hierarchical ZSM-5 composed of Zr-Co metal particles dispersed on the zeolite was developed for catalytic reforming reaction of pyrolysis volatiles to light aromatics (BTEXN) with high selectivity. BTEXN with 30.5% selectivity based on the tar-C was achieved over 5Zr/Co-AT<sub>0.2</sub>-PI<sub>0.3</sub>. The metal sites can facilitate the removal of hydrogen species formed on zeolite, and the controllable channel can be conducive to diffusion of volatiles towards internal pore. In addition, the formation of coke deposition in zeolite pores during catalysis leads temporary deactivation of catalyst, resulting in partial permanent loss of catalytic efficiency. A series of approaches were adopted to investigate catalytic deactivation due to hydrocarbon coking or poisoning of zeolites.



**Fig. 1.** Upgrading pyrolysis tar over metal-modified hierarchical ZSM-5

## **Impact of large inertinite particles on thermo-swelling and coke strength of coking coals**

Wei Xie\*, Rohan Stanger, Quang Anh Tran, Merrick Mahoney, Terry Wall, John Lucas,  
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A suite of large size inertinite particles (1.6-2.0 mm) were concentrated on the water based reflux classifier from two different ranked inertinite rich coking coals. The impact of these inertinite particles on thermo-swelling of other coking coals was investigated at a heating rate of 5 °C/min from room temperature (25 °C) to 900 °C. Coke samples of the blends composed of large size inertinite particles (1.6-2.0 mm) and other coking coals were prepared on a Sole Heated Oven. Coke strength was estimated by Drop Shatter tests. The results indicated that the reflux classifier is able to generate high concentrated inertinite particles with varying inertinite contents from 58% to 74% while the reflux classifier feeding sample contains only 31% inertinite. When blended, these inertinite-rich particles could decrease the swelling of other coking coals, and may promote the swelling to higher temperatures. These inertinite concentrates could also significantly improve the strength of coke made from their blends with other coking coals, depending on the property of the coal.

## Theoretical and experimental study on molecular structure and coking properties of the vitrinite in coking coal

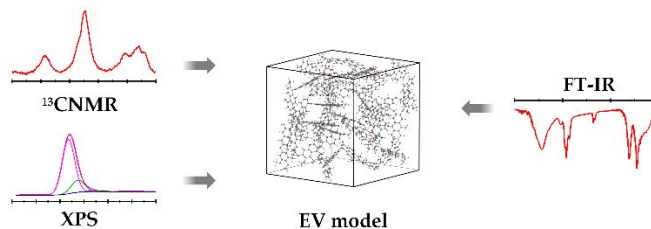
Jieping Wang<sup>1,2</sup>, Guangyue Li<sup>2</sup>, Lu Tian<sup>1</sup>, Yi Chen<sup>1</sup>, Jianglong Yu<sup>1,3\*</sup>

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Vitrinite is the main maceral in coking coal. The molecular structure of vitrinite is intimately connected to the coking properties of the corresponding coal. Ewirgol coking coal, from Xinjiang province of China, is selected as the sample in this work. We have isolated the pure vitrinite from Ewirgol coal (> 95%, EV) is by zinc chloride solutions, and obtained its characteristics of coal petrology by measuring the percentage composition and reflectance. The molecular structure of EV is then investigated by elemental and proximate analyses, X-ray photoelectron spectroscopy, infrared spectroscopy, <sup>13</sup>C nuclear magnetic resonance. Based on the characterization results, we have constructed the three-dimensional structure model. The spectra of the model, calculated by ab initio calculations, agree well with the experimental spectra. To confirm the relationship between coking properties and molecular structure, we have simulated the heating process of EV model by molecular dynamics method with the reactive force field and the isothermal-isobaric ensemble. The van der Waals energy and Coulomb energy are calculated to represent the weak interactions between hydrocarbon moieties and the hydrogen-bond interactions between oxygen-containing moieties, respectively. The simulation trajectories show that cleavage reactions of bridge bonds and alkyl chains destroy the weak interactions in the model, which is responsible for the high fluidity of EV. Abundant oxygen-containing moieties in EV are not beneficial to cross-linking reactions of carbon-carbon bonds, and then weaken the interactions between graphite layers in the produced coke. It could explain the low coke strength after reaction of EV coke.



**Keywords:** vitrinite, molecular structure, coking properties, reactive force field

## An in-situ study the effect of coal blend on the plastic layer formation in coking coals using a lab-scale test furnace

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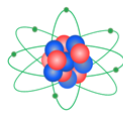
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Understanding the plastic layer formation during coking coal carbonisation are one of the most rapidly declining groups of insects in coke quality and coke making process. In addition, coking coal blends is at the heart of the understanding of coke making industry. It is critical to gain an understanding of how the coking coal blends effect the plastic layer formation during this process.

The thermoplastic property of coking coal contributes to the formation of plastic layer during the coking processes. Fluidity and maceral content are critical properties of coking coal, which is used to identify thermoplastic and coke quality. This study try to use the different fluidity, vitrinite reflectance and vitrinite content blends to analyse the influence for the plastic layer formation during coking process. The plastic layer sampling is used the UON double-side heat 4kg lab-scale coke oven, which is simulated the 400kg coke oven in Australia and the coke produce process all followed the 400 kg coke oven Australia test standard (AS 2267-1997). The UON 4kg coke oven allows in-situ measurements of a range of parameters, such as temperature history and internal gas pressure. An Attenuated Total Reflectance-Fourier Transform Infrared (ATR-FTIR) and <sup>13</sup>C Nuclear Magnetic Resonance (<sup>13</sup>C NMR) are used to investigate the chemical structure change of plastic layer formation and the transform of the density of different functional group from the different phase of the plastic layer. The Micro-CT imaging of plastic layer samples were performed at the Imaging and Medical Beamline (IMBL) in the Australian Synchrotron facility located in Melbourne. The influence of different coking coal particle can be identify clearly under the high resolution (9.81 micron) micro-CT image.

This study aim to find out the influence of different coking coal blends for the plastic layer formation during coking process. To improving a deep understanding about the mechanism of plastic layer formation of coking coal blends. The analysis of chemical structure and physical structure transform is critica significant. The micro-CT is used to analysis the physical structure influence and ATR-FTIR and <sup>13</sup>C NMR are used to study the chemical structure effect. Overall, this study outline a critical role for the quantitatively linking the chemistry of coking coal blends to the characteristic parameters of plastic layers in the industry coking process.

**Keywords:** Coking coal blends; Plastic layer; Micro-CT; ATR-FTIR; <sup>13</sup>C NMR.



## Three-dimensional simulation of gas-solid flow in a CFB boiler

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Numerical analysis using CPFD Barracuda was performed to investigate the flow characteristics of a 500 MW circulating fluidized bed (CFB) boiler. CFB boiler modeling can be divided into three fields: hydrodynamics, heat balance and chemistry. The heat balance and chemistry are sensitive to hydrodynamics. Thus, the simulations of gas-solid flow were carried out under an isothermal state of 1143 K, and the heat transfer and chemical reactions were excluded from this work. The bed material is assumed to sand of which size distribution was set to design distribution. To begin with, the grid sensitivity test without computational particles was performed to select the optimal grid. Also, the pressure obtained from the simulation was compared with the data measured in the industrial CFB boiler to select the most suitable drag model. As a result, the energy-minimization multiscale (EMMS) model predicted the pressure at the furnace bottom better than other models. The calculations were conducted during 200s of computational time, and the results were averaged from 100s. Despite to the transient phenomena of fluidized bed system, the averaged values were often reached at quasi-steady state. The flow analysis was mainly performed in terms of solid fraction, velocity and circulation. The particles were suspended by the upward gas flow, and exit to the cyclone or fall at wall. The falling particles has major influence on heat transfer, therefore, the characteristics such as solid mass flux and wall layer thickness were also predicted. The gas and solid flow inside the furnace basically followed plug flow and core-annulus structure, respectively. In the lower part of furnace, however, the gas flow was uneven due to high velocity of secondary air (SA), which affected the solid flow characteristics.

**Keywords:** Circulating fluidized bed (CFB), simulation, flow characteristics.

## **Advanced absorbent design and kinetic insights of CO<sub>2</sub> absorption into aqueous Ammonia (NH<sub>3</sub>) solvent with a new cyclic amine additive - 4-aminomethyltetrahydropyran (4-AMTHP)**

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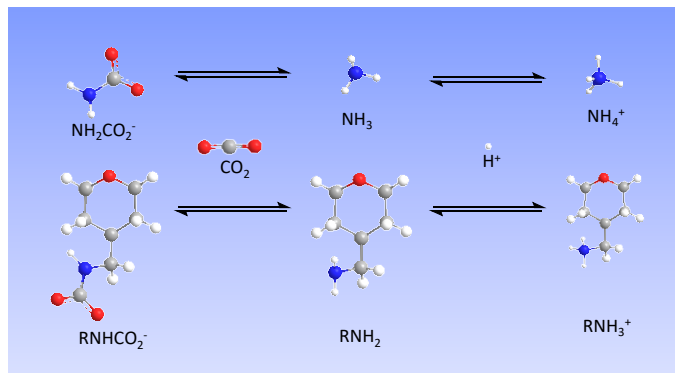
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Post combustion capture is the most mature and well-deployed technology for the removal of CO<sub>2</sub> from exiting fossil fuel-fired power plants and other industrial sources. Compared with the traditional and most widely employed amine, monoethanolamine (MEA), the application of aqueous ammonia based solvent has many advantages such as inexpensive chemical cost, high CO<sub>2</sub> absorption capacity, no oxidative or thermal degradation issues, and the potential for the combined removal of all acid gases present in the flue gases. However, the low CO<sub>2</sub> absorption rate and high evaporation loss are the major issue that aqueous ammonia based CO<sub>2</sub> capture process. Research on the improvement of CO<sub>2</sub> absorption rate for the ammonia-based solvent via addition of fast reactive primary/secondary amines are of great interest. Herein the mass transfer of CO<sub>2</sub> absorption into a mixture of ammonia and a new heterocyclic amine 4-aminomethyltetrahydropyran (4-AMTHP) solutions were tested on wetted-wall column apparatus. Results showed that 4-AMTHP can effectively enhance on the CO<sub>2</sub> absorption mass transfer and absorption into aqueous ammonia solutions. The performance were compared with other previously published primary/secondary amine additives as well. Furthermore, the detailed reaction mechanism of dissolved CO<sub>2</sub> reacting with mixed 4-AMTHP/NH<sub>3</sub> solutions have been investigated on a Stopped-flow spectrophotometry at 25.0 °C. Furthermore, a comprehensive model describing the blended 4-AMTHP-NH<sub>3</sub>-CO<sub>2</sub>-H<sub>2</sub>O system, which involves in total 11 reactions and 15 species, has been evaluated to rationalise the experimental kinetic and mass transfer results. Figure 1 shows the dominant reactions between 4-AMTHP/NH<sub>3</sub> solutions and CO<sub>2</sub>/H<sup>+</sup>.

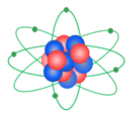
From the mechanism, the main reason of the additional of 4-AMTHP can enhance the CO<sub>2</sub> absorption into aqueous ammonia solution is that 4-AMTHP offer another fast reaction path for CO<sub>2</sub> absorption. For the mixed 4-AMTHP/NH<sub>3</sub> solutions, both NH<sub>3</sub> and 4-AMTHP can react with CO<sub>2</sub> but also to accept the proton that released from formation of carbamate species. As there are essentially less 4-AMTHP (~0.3 M) than NH<sub>3</sub> (~3M) in solution, NH<sub>3</sub> act as the dominant proton acceptor and therefore buffers the pH and resulting in more 4-AMTHP and enhanced CO<sub>2</sub> absorption rate. Furthermore, the reaction mechanism have been further extended and some

suggestions towards the design of blended amine solutions for CO<sub>2</sub> capture have been provided in this study.



**Figure 1.** Reaction mechanism between 4-AMTHP/NH<sub>3</sub> solutions and CO<sub>2</sub>/H<sup>+</sup>.





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# Poster Session

## Catalytic Oxidation of NO from Coal Fired Flue Gas over Mn-Co-TiO<sub>2</sub>

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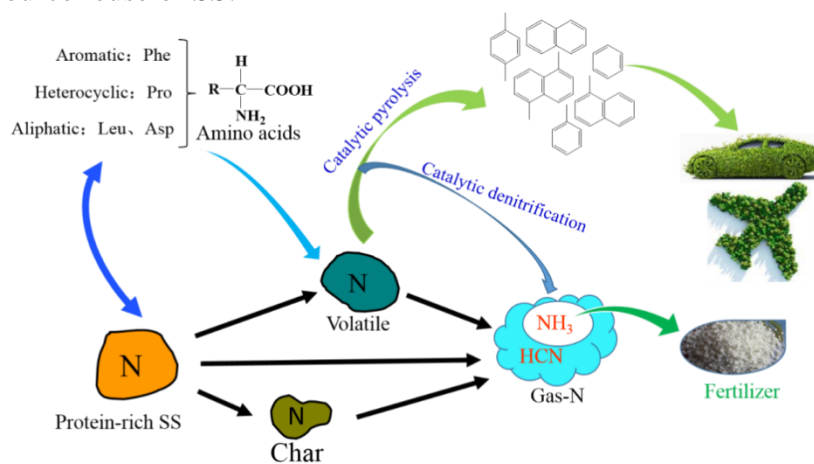
The aim of this research was to advance a viable and environmental-affable catalyst for NO catalytic oxidation. A series of Mn-Co-TiO<sub>2</sub> were prepared using sol gel method and tested for low temperature catalytic oxidation of NO with O<sub>2</sub>. The catalytic performance of this catalyst was measured on a fixed-bed reactor. The characterization techniques of Scanning Electron Microscope (SEM), Transmission Electron Microscopy (TEM), Brumauer-Emmett-Teller (BET), X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FTIR) were performed to investigate the morphology, surface area, crystal structure, of the catalyst samples. As comparison, single oxides were also investigated, and their activities were slower than those of Mn-Co-TiO<sub>2</sub> catalyst.

## Simulation of sewage sludge catalytic pyrolysis: Comparison of amino acids with different chemical structures

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The green environmental-friendly disposal of sewage sludge (SS), the by-product of sewage treatment, has become severe challenges today. Catalytic fast pyrolysis (CFP) is a potential approach for reforming the properties of pyrolysis bio-oil over HZSM-5. However, the complex intrinsic characteristics and multi-components of protein-rich SS limited the reuse of SS. To elucidate the catalytic mechanism and nitrogen transfer behavior of SS during CFP, product distributions and nitrogen transformation from SS and amino acids were investigated on a drop tube quartz reactor over HZSM-5. During CFP of SS, the maximum aromatics yield of 16.4% was obtained over HZSM-5 with Si/Al ratio of 25 at 500 °C, and increasing temperature promoted the conversion of nitrogen to NH<sub>3</sub>. Amino acids with aromatic ring or saturated hydrocarbon side chain favored the formation of aromatics and NH<sub>3</sub>. Amino acids of N-ring structure promoted the formation of N-containing heterocyclic compounds, which were prone to coke on catalyst and inhibited the catalytic cracking of SS to produce more aromatics and NH<sub>3</sub>. Excessive Asp of short chain dibasic acid structure was not conducive to the complete thermal decomposition of SS under the optimum pyrolysis condition. A general catalytic mechanism of SS was proposed to provide support for the resource reuse of SS.



**Fig. 1** Design route schematic of SS fast pyrolysis

**Keywords:** Sewage sludge, Amino acids, Catalytic pyrolysis, Aromatics, Nitrogen transformation.

## **SnO<sub>2</sub> decorated graphene nanoplatelet composites: Synthesized by one-step solid-state method and enhanced ethanol gas-sensing property**

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N-type semi-conductive SnO<sub>2</sub> decorated graphene nanoplatelet composites (SnO<sub>2</sub>/GNP) were successfully synthesized via one-step solid-state reaction method. The procedure is convenient and environment-friendly, and can be used for industrial production. X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), transmission electron microscopy (TEM), Thermal gravity and differential scanning calorimeter (TG–DSC), and N<sub>2</sub> adsorption-desorption were used to confirm the structure and morphology of the as-prepared materials. The as-prepared SnO<sub>2</sub>/GNP composites possess the two-dimensional (2D) structure, and the 2D GNP accelerating the preferential growth and preventing the agglomeration of the SnO<sub>2</sub> nanoparticles. In comparison to pure SnO<sub>2</sub> nanoparticles, the SnO<sub>2</sub>/GNP composite-based gas sensors exhibited a better selectivity and stability, shorter response and recovery time, and lower work temperature toward ethanol. The improved ethanol gas sensing properties are proposed to relate to the good conductivity of graphene nanoplatelet, and interactions between SnO<sub>2</sub> and graphene nanoplatelet. And, the as-prepared SnO<sub>2</sub>/GNP composites will be an ideal candidate for ethanol gas sensor application.

# The effect of Torrefaction Process on the structure and combustion of Biomass Fuel

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Torrefaction is one of the methods to improve biomass combustion calorific value and hydrophobicity. In this study, the effects of devolatilization and char kinetics on reactivity and biomass structure were analyzed. EFB and Kenaf were selected to see the differences between woody biomass and herbaceous biomass. Those biomass were used as fuels to be torrefied in the N<sub>2</sub> environment at 200, 250 and 290 °C. Devolatilization and char kinetics were analyzed by using TGA and biomass structure was investigated through petrography image. The reactivity showed different trends depending on the torrefaction temperature and biomass structure. The herbaceous biomass, Kenaf, was shown as high reactivity and thin wall structure. On the contrary, the woody biomass, EFB, had relatively low reactivity and thick wall structure.

**Keywords:** Torrefaction, Biomass, Kinetics, Devolatilization, Biomass structure.

# Numerical Simulations of Low NO<sub>x</sub> Combustion Emissions in a Shaft Furnace

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In a special ceramics factory, shaft furnace is important process equipment that usually has high NO<sub>x</sub> emissions because of special working conditions. This work addresses the computational fluid dynamics (CFD) simulation for a shaft furnace combustion to determine the effect of combustion system retrofit on reducing NO<sub>x</sub> emissions. Based on NO<sub>x</sub> emission mechanism, staged combustion (SC), flue gas recirculation (FGR) and hybrid SC/FGR schemes are taken into account separately to evaluate the combustion model and predict NO<sub>x</sub> emissions. The simulation results show that three retrofit strategies all can reduce the NO<sub>x</sub> emissions effectively. Only considering SC retrofit, six additional fuel nozzles are set up above the original burner and the natural gas amounts increase by 50%. Then the NO<sub>x</sub> emissions can decrease to about 3000 mg/m<sup>3</sup>. In addition, the optimal location of additional fuel nozzles is 0.6 meter above the original burner for mitigating the negative influence of furnace temperature distribution. With regard to FGR, part of flue gas at 400 K is sent back to the furnace for replacing auxiliary air. Four working conditions ( $V_{O_2}=20\%$ ,  $V_{O_2}=15\%$ ,  $V_{O_2}=10\%$ ,  $V_{O_2}=5\%$ ) are studied. The results show that the peak temperature of furnace flame and NO<sub>x</sub> emissions both decrease as the O<sub>2</sub> content in flue gas decreases. NO<sub>x</sub> emissions can decrease to 4500 mg/m<sup>3</sup> when the O<sub>2</sub> content is controlled at 15% for satisfying the process requirement. Finally, SC and FGR are simultaneously adopted in the combustion system retrofit and NO<sub>x</sub> emissions can decrease substantially to 900 mg/m<sup>3</sup>. Therefore, according to simulation conclusion, the hybrid SC/FGR retrofit is best choice of reducing NO<sub>x</sub> emission while the combustion performance is satisfied.

**Keywords:** Numerical simulation; Low NO<sub>x</sub>; Combustion characteristic.

## Synthesis of magnetic chitosan nanocomposite and its adsorption property

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Nowadays, the adsorption of contaminants from wastewater by nanomaterials has drawn enormous interest. Among various nano adsorbents that have been applied for dye adsorption, magnetic nanoparticles have attracted great attention. Here magnetic Fe<sub>3</sub>O<sub>4</sub> coated with amino-functionalized magnetic chitosan composite was synthesized simply by one-pot and characterized. The feasibility of MCS-NH<sub>2</sub> composite for the removal of anionic dye ORII from an aqueous solution was investigated systematically. At the optimal conditions: pH 7.07, initial ORII concentration 100 mg L<sup>-1</sup>, adsorbent dose 3 g L<sup>-1</sup>, room temperature (293 K) at 30 min, the highest ORII removal of 94.3 % was obtained. The kinetic adsorption isotherms and thermodynamics were studied and the experimental data fitted better with the pseudo-second-order kinetic and the Freundlich model, with spontaneous and exothermic characteristics. Based on its excellent adsorption performance, it can be concluded that MCS-NH<sub>2</sub> could be used as a low-cost and efficient adsorbent for removal of anionic dye from wastewater.

**Keywords:** Magnetic; Chitosan; Ethylenediamine; OR II; Adsorption

## Nitrogen transformations during in situ upgrading of sewage sludge pyrolysis vapors over metal-loaded HZSM-5

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This study investigated catalytic fast pyrolysis (CFP) of sewage sludge (SS) for bio-oil production over metal loaded HZSM-5 (HZ). The effects of metal species (Ni, Co) and metal loading on carbon and nitrogen distribution in the products were studied. The results show that the presence of metals significantly improved total carbon yield and selectivity of light aromatics (BTEXN) in the bio-oil. The maximum BTEXN selectivity in the bio-oil of 47.42% was obtained over 0.5 wt% Ni-HZ. Furthermore, the NH<sub>3</sub> yield increased with increasing metal loading amount while the yield of HCN decreased. Metal loaded promoted the cracking reactions during CFP to generate more H radicals and these H radicals have advantages to the ring-opening of N-containing heterocycles in SS to produce aromatics and NH<sub>3</sub>. With the addition of metals, the nitrogen trend to released as NH<sub>3</sub> or fixed in the solid product instead of bio-oil.

**Keywords:** Sewage sludge; Catalytic pyrolysis; Metal-loaded HZSM-5; Aromatics; Nitrogen.



## Microwave-assisted catalytic pyrolysis of lignite and biomass for single-ring aromatic compounds production in a two-stage reactor

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Due to the lower coalification degree of lignite, the structure has its own unique characteristics. In lignite structure, the single ring structure is major component connected by the bridge bonds, while the fused ring structure is few. Thus, the cracking reaction of lignite is easy to produce single ring compounds during the heating process. Biomass has been popularly regarded as renewable and clean because of the concerns for high demand for energy and global climate change in recent years. Lignin as the main component in the structure of woody biomass, which the major building blocks were p-coumaryl, coniferyl and sinapyl alcohol units and both could called the single-ring aromatic structure. Microwave pyrolysis was considered as a prospective pathway for converting lignite and woody biomass into single-ring aromatic compounds. This study has been focused on single-ring aromatic compounds production during microwave catalytic pyrolysis of Hailar lignite and palm kernel shell biomass with HL char, PKS char, Co-loaded PKS char, Fe<sub>3</sub>O<sub>4</sub>, and AC as catalysts in a two-stage reactor. The results showed that high concentration of single-ring aromatic compounds in tar obtained from microwave catalytic pyrolysis of HL and PKS by using a two-stage reactor. Compared to the non-catalytic pyrolysis, PKS char, Co-loaded PKS char, Fe<sub>3</sub>O<sub>4</sub>, and AC were used as catalyst placed on the upper bed in two-stage pyrolysis, a significant increase in selectivity of single-ring aromatic compounds (mainly phenolic compounds) significantly in tars. The highest concentration of single-ring aromatic compounds and phenol in tar reached 84.25 area% and 67.44 area%, respectively, when PKS was loaded to the bottom bed and the upper bed contained AC.

## Effects of thermal treatment on the chemical structure of Chinese bituminous coals

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In this paper, Four Chinese bituminous coals (Coal A, Coal B, Coal C, Coal D) used were 90-150  $\mu\text{m}$  and they were different ranks. The behavior of thermal pretreated coking coals pyrolysis under different temperatures (300-500  $^{\circ}\text{C}$ ) were studied by using Fourier transform infrared (FTIR) spectroscopy in order to study the properties of the plastic layer. The chemical structure parameters were analyzed by FTIR curve-fitting and they showed better fluidity and thermoplasticity around 400 and 450  $^{\circ}\text{C}$ . After that the main trend was decreased gradually because of the plastic layer became into char stably. Coal C decreased was concerned with aliphatic chain lengthen and the better thermoplasticity among these coals.  $H_{\text{ar}}/H_{\text{al}}$  and the aromaticity indexes increased caused of the coal structure became more aromaticity and compactness as pretreated. The aliphatic hydrocarbon was related with the structure plastic layer directly. The functional groups of the pretreated coal samples were analyzed to correlate the chemical structure changes during thermal treatment to the volatile composition because of the aliphatic structures breakdown and condensation. This was due to the thermal treatment leading to the changes the length of aliphatic chains and chemical structure.

**Keywords:** bituminous coal, pyrolysis, thermal treatment, chemical structure.

## A new way to produce Semi-coke using Microwave pyrolysis

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The research target was to produce semi-coke from coking coal and coke dust using microwave energy. A Lili Li series of batch experiments were carried out using a 2000 W power microwave to heat 200 g of an Australian different ranking and vitrinite coking coal, sample sized at < 3 mm at different power i.e. 500 W and 1000 W and temperature i.e. 350°C, 400°C, 450°C, 500°C, 550°C and 1000°C. The power and temperature were maintained to prolong the coking process. The collected products were Semi-coke sample and Tar sample. Each product characterization was investigated using a variety of instruments such as ATRFTIR, TG-FTIR, SEM-EDS, BET, XRD and GC-MS, and delivers a comparison with Semicoke sample produced using Electric Furnace. The measured characteristics of microwave produced Semi-coke sample became gradually similar to electric furnace produced sample. The treatment time was increased in Electric furnace.

# Lotus Leaf-based Porous Carbons for High Performance Supercapacitor

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Porous carbons were directly prepared via one-pot KOH activation from dried lotus leaf. The morphology and microstructure of the as-obtained porous carbons were characterized by Field emission scanning electron microscopy (FESEM), Transmission electron microscope (TEM), Nitrogen adsorption-desorption isotherms, Powder X-ray diffraction (XRD) patterns, Raman spectra and X-ray photoelectron spectroscopy (XPS). The electrochemical performance of symmetric supercapacitor was evaluated by galvanostatic charge-discharge (GCD), cyclic voltammetry (CV), rate capability, electrochemical impedance spectroscopy (EIS) and cyclic stability in 3 M KOH aqueous solution. Porous carbon obtained at 700 °C with the KOH/precursor mass ratio of 1 (denoted as AC-1-700) exhibits a wormhole-like morphology with interconnected carbon frameworks, which is favorable for rapid ion diffusion inside the porous carbon. It also presents a high specific surface area (1229 m<sup>2</sup>/g), high total pore volume (0.550 cm<sup>3</sup>/g), moderate mesoporous porosity (18.7%), rich nitrogen (3.68%) and oxygen (12.35%) doping. With the synergistic effects of these features, the electrode in AC-1-700//AC-1-700 supercapacitor delivers high specific capacitance (240 F/g at 0.25 A/g), good rate performance (208 F/g at 5 A/g) and remarkable cycling stability (98.2% capacitance retention after 5000 cycles at 2.5 A/g). Lotus leaf-derived porous carbon has been demonstrated to be a promising candidate as electrode active material for supercapacitor.

**Keywords:** lotus leaf; one-pot activation; porous carbons; electrode active material; supercapacitor.

## The production of hydrogen-rich bio-gas during pressurized entrained-flow pyrolysis

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Pressurized entrained-flow pyrolysis of palm kernel shell (PKS) was investigated in the temperature range of 700-900°C and at 0.1, 1, 2 and 4MPa. The effect of pressure and temperature on the yield of bio-gas and the composition of bio-oil was investigated. The highest H<sub>2</sub> gas concentration was 79.14% at 900°C 1MPa. The concentration of CH<sub>4</sub> gas increased with increasing pressure at all temperatures investigated. At 800°C and 900°C the concentration of CO<sub>2</sub> increased by increasing the pressure. The concentration of CO decreased the most at 4MPa at all temperatures studied. The total concentration of phenolics at 700°C was 39.59%, 54.85% and 41.43% at 1, 2 and 4 MPa respectively. Pressurized entrained-flow pyrolysis of PKS at 700°C increased the selective production of phenols, the %area of pure phenols at 700°C were 34.61%, 46.83% and 36.96% at 1, 2 and 4 MPa respectively, this was due to the decomposition of lignin. Increasing the temperature resulted in the increase of polyaromatic hydrocarbons (PAH) to 95.29% at 900°C 4MPa. The increase in PAH at high temperature and pressure was due to the secondary gas phase reactions as a result of direct combination of aromatic rings. The main PAH compounds present in bio-oil were naphthalene, phenathrene, fluoranthene and pyrene. The selective production of pure naphthalene, phenathrene, fluoranthene and pyrene was enhanced at 900°C 4MPa. The total PAH %area at 900°C 4MPa was 95.29% out of which 25.38%, 20.63%, 13.19% and 12.59% was attributed to pure naphthalene, phenathrene, fluoranthene and pyrene respectively.

**Keywords:** Entrained-flow pyrolysis, PKS, bio-oil, bio-gas, phenols, PAH.

## A study on co-combustion characteristics of coal and pre-treated biomass blends by TG-FTIR analysis

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Fuel pre-treatment technique is one of the most effective ways of using biomass fuel to solve the problem from disadvantage of it. Biomass fuel can gain high calorific value and lower ash content by torrefaction and ash removal technology respectively. In this study, thermogravimetric analysis and FTIR spectra of chemical structure and gas emission characteristics of coal and pre-treated biomass blends have been investigated by analysis of TG-FTIR to evaluate the combustibility and environmental influence. In FTIR analysis, structural parameter was studied as the blending ratio increases (10, 20, 30%) to show that the quantities of various functional groups. Also, the activation energy (E) and frequency factor (A) calculated by first-order reaction can be explained with structural parameters. The gas emissions (CO, CO<sub>2</sub>, CH<sub>4</sub> etc.) were investigated during combustion process (N<sub>2</sub> 21%, O<sub>2</sub> 79%) to demonstrate the impact on the carboxyl groups and aliphatic chains. These can indicate that co-combustion of using the pretreatment biomass fuel is relatively better than those of the untreated biomass fuel about combustibility and environmental effect.

**Keywords:** Ash removal technology, Torrefaction, TG-FTIR, gas emissions, kinetics.

## Experimental study on the formation of single-ring aromatic compounds via catalytic pyrolysis of water hyacinth

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Water hyacinth as a floating organism has caused problems such as reduced fish production, channel blocking, and water pollution. Efficient conversion of water hyacinth to value added products is an efficient method of utilization of this biomass while solving environmental pollution. This study focused on microwave-induced thermal decomposition of water hyacinth in the temperature range of 200-700 °C. The properties of pyrolysis products were studied by using of FTIR, GC-MS, and GC. The effects of Fe<sub>3</sub>O<sub>4</sub> and AC as microwave receptors on the pyrolysis behavior of water hyacinth were studied in detail and were compared with SiC as an inert receptor. The results showed that pyrolysis at low temperatures of 200-300 °C favored the formation of char, while the yield of bio-oil reached highest values at 400-500 °C. The bio-oil had a high calorific value and was mainly composed of oxygen-containing aromatics, aromatic hydrocarbons, linear hydrocarbons, and heterocyclic hydrocarbons. Pyrolysis at high temperatures of 600-700 °C promoted the formation of H<sub>2</sub> and CO in the gas phase, where the mixture of H<sub>2</sub> and CO accounts for nearly 80% of the gas products. The type of microwave receptor had a great influence on the yield and composition of pyrolysis products. The presence of Fe<sub>3</sub>O<sub>4</sub> led to an increase in the concentration of alcohol in the bio-oil, while AC significantly promoted the formation of long-chain hydrocarbons. These results indicated that catalytic pyrolysis of water hyacinth in the presence of AC is a promising way of production of liquid fuels and gaseous fuels.

## Catalytic upgrading of gaseous tar from coal microwave-assisted pyrolysis over Co and Ni-modified lignite char

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The utilization of catalysts in coal pyrolysis is essential to obtain a high yield of BTEXN (Benzene, toluene, ethylbenzene, xylene, and naphthalene) and improve the quality of coal tar, which can be achieved either by catalytic conversion of coal over catalysts added directly to coal, or catalytic conversion of coal volatiles over catalysts placed separately from coal. Lignite microwave pyrolysis can improve the selectivity of micromolecular compounds which may become an important technology for high value and efficient conversion of lignite. In this study, Co and Ni loaded lignite char was used as catalyst during dual-bed microwave pyrolysis of lignite to establish the reaction mechanism formation of aromatic hydrocarbons such as BTEXN at different temperatures by GC-MS. The results showed that when Ni was added to lignite char, the tar yield increased from 7.13% to 8.5%, respectively at 700 °C and the metal content of 10%. The GC-MS results showed a significant increase in the yield of BTEXN compounds from 49.17 area% to 79.17 area% when 10% Ni was used (5/1 ratio) at 600 °C and 700 °C. Furthermore, the content of benzene also increased by 60 area% at 700 °C using 10% Ni (5/1 ratio). The experimental results suggested that during secondary pyrolysis reactions, the PAHs decompose to form monocyclic compounds, particularly BTEXN compounds. Brown coal is a kind of solid carbon material which has free moving  $\pi$ -electrons. With the addition of Co and Ni to lignite char as catalyst and at higher temperatures, the intensity of microwave pyrolysis increased. This resulted in higher total tar yield and an increase in selectivity of BTEXN compounds and aliphatic hydrocarbons in expense of PAHs compounds.



## **In situ reforming of cellulose pyrolysis volatiles over HF and Ni/HF modified HZSM-5 for light aromatics formation**

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Catalytic fast pyrolysis (CFP) of cellulose over modified HZSM-5 (Z5) was studied in a drop tube quartz reactor. To increase the yield of light aromatics (LAs), Z5 was treated with different concentrations of leaching agent HF and Ni loading. The pore structure, acidity, and morphology of the catalysts were investigated by N<sub>2</sub>-adsorption and desorption, NH<sub>3</sub>-TPD, XRD and SEM. Z5 modified with 0.5 mol/L HF (0.5F-Z5) showed better LAs yield during cellulose CFP, which can be attributed to the enhancement in the middle pore (5.5-10 nm) and mild reduction in the acidity. Simultaneously, the loading of a suitable amount of Ni produced more LAs than 0.5F-Z5, due to the improvement of deoxidation/hydrogenation reactions. In addition, careful analyses are conducted on the reaction routes over different metal active centers and acid-catalyzed reactions, based upon the composition of the bio-oils and catalyst characterization.

**Keywords:** Cellulose, Catalytic fast pyrolysis, modified HZSM-5, BTEXN, Coke.

## Selective cleavage of C-O bond in benzyl phenyl ether over Pd/C at room temperature

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Selective cleavage of C-O bonds in benzyl phenyl ether (BPE) as a typical lignin  $\alpha$ -O-4 ether to produce aromatics is a challenging and attractive topic. Herein, the Pd catalyst was applied to the catalytic cleavage of C-O bond in benzyl phenyl ether to aromatics. For comparison, Ni/C and Ru/C catalysts were also investigated. Although Ru/C catalyst showed the high conversion of BPE, the selectivity for aromatics was low due to saturation of aromatic ring. Ni/C catalyst showed lower conversion and higher selectivity of BPE than Ru/C. Among these catalysts, Pd/C exhibits highest activity for cleavage of C-O bond. The reaction with BPE was carried out at pretty mild condition of 25 °C and 0.1 MPa H<sub>2</sub>, which is highly selective afforded toluene and phenol as the products with the yields of 100%.

**Keywords:** Selective Cleavage; Benzyl Phenyl Ether; Room Temperature; Aromatics; Pd/C.

## Synthesis and characterization of glass-fiber/silica aerogel composites using coal fly ash

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Silica aero-gel is a novel light mesoporous material with low density, high porosity, high surface area and low thermal conductivity which may find wide applications. However, the current methods of synthesis use toxic and expensive feedstock and the processes are of high cost. Utilization of cheaper and abundant feedstock and cost effective process for silica aero-gel production is crucial. In this study, by using fly ash from coal fired power plants as the feedstock, a new silica aerogel composites reinforced by glass-fiber were synthesized at ambient pressure. The synthesis process included alkali dissolution and ion exchange, surface hydrophobic treatment of the wet-gel followed by drying of the wet-gel at ambient pressure. Synthesis parameters were optimized based on systematic experiments. BET, SEM and FTIR were used to investigate the structure and characteristics of the silica aero-gel samples. The results indicated that silica aero-gel produced in this study had uniform mesoporous structure, high porosity (89%), high surface area (736 m<sup>2</sup>/g), and low density (0.09 g/cm<sup>3</sup>). It is therefore technically and economically feasible to produce silica aero-gel from coal fly ash.

## Comparative Study on Changes of Oxidation Products Accompanying Self-heating of Chinese and Indonesian low-rank coals

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Coal, especially low-rank coal, is easily oxidized in air at low-temperature to release heat, which increase the susceptibility to spontaneous combustion. During oxidation of the coal, the formations of some gaseous and solid oxidation products (i.e. CO<sub>2</sub>, CO, oxygenated compounds) are accompanied by the self-heating of coal in response to oxidation reactions. This study systematically investigated the low-temperature oxidation characteristics of Indonesian (YN) and Chinese low-rank coals (SH) by using a dual fixed-bed quartz reactor to measure the separation point temperature (SPT) and the crossing point temperature (CPT). The changes in the chemical structures of coal were analyzed using Fourier transform infrared spectroscopy (FTIR). The yields of CO<sub>2</sub> and CO at the outlet were measured using gas chromatograph (GC). The link between gas products, solid oxygenated compounds and residual water in coal with the heat release during low temperature oxidation was investigated. The changes of coal temperature from SPT to CPT reflected the heat release caused by oxidation reactions. The results showed that a high yield of CO<sub>2</sub> before CPT was obtained when coal contained higher moisture. Correspondingly, more heat was generated in the coal bed at higher moisture contents. However, the yield of CO during coal self-heating did not follow the same trend. Water desorption released more methylene sites, leading to the decrease in the ratios of CH<sub>3</sub>/CH<sub>2</sub>, C=O/C<sub>ar</sub> and COOH/C<sub>ar</sub> with increasing oxidation temperature up to SPT. The heat loss due to water desorption limited self-heating of coal until coal temperature reach to the SPT. Compared with YN coal, the SH coal exhibited higher oxidation reactivity and stronger oxygen absorption capacity as indicated by the higher CO<sub>2</sub> yield and the increases of C=O/C<sub>ar</sub> and COOH/C<sub>ar</sub> ratios at higher oxidation temperatures.

**Keywords:** Oxidation; Low-rank coal; Moisture content; Functional groups.

## Mechanistic study on formation of phenolics-rich oil via catalytic co-pyrolysis of lignite and stalk biomass

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Lignite accounts for nearly half of global coal resources and accounts for 15% of China's coal resources. Lignite is an important energy resource in China and its molecular structure is rich in benzene rings. Stalk biomass as a major by-product in the farming is abundant in some agricultural countries and its main components are lignin, cellulose and hemicellulose. Therefore, the production of high-yield and high-quality tar rich in phenolic compounds through co-pyrolysis of lignite and stalk biomass is one of the efficient utilization methods of lignite and stalk biomass. In this study, the production of tar rich in phenolic compounds via catalytic co-pyrolysis of Hailar lignite and stalk biomass was investigated. The tar yield of Hailar lignite pyrolysis was about 10 wt.% at 600°C, that of soybean stalk and corn stalk were about 40 wt.% and 46 wt.% respectively. The yield of phenolic compounds in these tar increased with increasing temperature from 400°C to 700°C. The co-pyrolysis of lignite and stalk biomass did not increase the tar yield, but increased the yield of phenolic compounds in tar, thereby improving the tar quality. The addition of activated carbon as catalyst reduced the tar yield but significantly increased the yield of phenolic compounds in the tar. Due to the porous structure of the activated carbon, the chemical reaction is selective for both the reactants and the products. The porous structure of activated carbon has a strong selectivity for different adsorbents, which promotes the formation of phenolic compounds during the pyrolysis and co-pyrolysis.

# Modeling Characteristics of Coal Decomposition in Microwave Pyrolysis Systems

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Predicting chemical changes within a complex heterogeneous mixture of organic materials is a complex process of pyrolysis. Chemical changes in coal under conditions including but not limited by temperature, heating rate, rank, grade variation and geological factors can dramatically alter reaction mechanisms and pathways which is not yet understood extensively. Deterministic modeling of microwave pyrolysis has also not been understood and investigated.

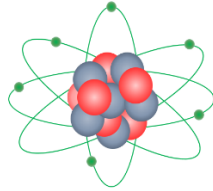
The focus of this research is to advance the limited understanding in modeling bond cleavage and radical reaction theory undergone during coal pyrolysis in to a comprehensive knowledge. A fortran compiler will be applied with open source codes CPD and DAE already developed. The source codes modified in this research will need to explain radical behavior during bond cleavage analytically during various operating conditions.

A specific set of batch experiments in a 2kW industrial microwave will be undertaken. Coke samples from each experiment will be analysed using GC-MS, TG-FTIR, SEM and XRD for identifying the chemical species present and species distribution. The eventual aim is to validate these experiments with model predictions under identical parameters.

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