

**P7-7****Element Volatilisation During the Thermal Treatment of South African Bituminous Coals**

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The response of South African low-grade, medium rank C bituminous coals to sequential leaching with water, ammonium acetate, and hydrochloric acid has been investigated by the conventional chemical analysis of both the leached coals and the leachate solutions. The ammonium acetate treatment removed most of the Na, Ca, Mg and Mn suggestive of an organic association and occurrence as ions of carboxylate groups. Hydrochloric acid removed almost all the Ca and Fe from the coals. Close evaluation of the data suggests that some of the Al in the coals was also removed by the selective leaching process, primarily by the hydrochloric acid treatment. This may reflect a solution of organically-associated Al from the maceral components. The loss of fluxing elements (such as Ca and Mg) induced by the different leaching processes was also associated with increases in ash fusion temperatures.

Samples from the sequential leaching process were demineralised and organically-associated elements were added to the samples. The original and demineralised samples were then analysed by a series of FT-IR Raman spectroscopic experiments, which included the thermal treatment of samples at various temperatures in an external lab-scale reactor. Vapour species were detected through ZnSe windows in the reactor. This is in contrast to conventional reactor techniques where volatile species are condensed and thereafter analysed via analytical methods. The poster will present observations and results from the experiments.

**P7-8****Effect of Trace Amount of Oxygen on Removal of Stable Sulfur in Coal**

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The stable organic sulfur forms in coal such as thiophenic and dibenzothiophenic sulfurs are very stable to be removed from coal during coal conversion processes, which leads to severe environmental problems. In this work, several typical organic sulfur model compounds including thiophenic and dibenzothiophenic sulfur were pyrolyzed under 1.0% O<sub>2</sub>/He and the sulfur forms released were detected by on-line mass spectroscopy in order to investigate the effect and the mechanism of trace amount of oxygen on the removal of the stable sulfurs in coal. Furthermore, the sulfur removal during pyrolysis of one Chinese Wujiaping coal (WJP) with high organic sulfur under oxidative atmosphere was also studied. The results show that the specific peak temperature of sulfur release is decreased during pyrolysis of the model compounds with stable thiophenic sulfur under trace amount of oxygen compared to that under inert atmosphere, which indicates that the trace amount of oxygen has positive effect on removal of the stable sulfur. When WJP coal is pyrolyzed under 1.0%O<sub>2</sub>/He, the peak temperature of SO<sub>2</sub> is always lower than those of CO<sub>2</sub> and CO, indicating that the oxidation of sulfur occurred before that of organic carbon frame of coal. The coal pyrolysis tests show that the trace amount of oxygen could increase the efficiency of sulfur removal without remarkable decrease in the char yield.

**POSTER SESSION 8****GAS TURBINES AND FUEL CELLS FOR SYNTHESIS GAS AND HYDROGEN APPLICATIONS****P8-1****Solid Oxide Fuel Cell Multi-Cell Array for Parallel Testing on Direct Coal Syngas**

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Integration of solid oxide fuel cells (SOFC) and coal gasification systems is being pursued to improve energy production efficiency and enhance carbon capture capability. SOFCs are considered for integration owing to their high operating temperatures (in excess of 800°C) and reduced cleanup requirements as compared to other fuel cell technologies.

In addition to system efficiency, degradation performance must also be considered. The SOFC degradation target outlined by the U.S. Dept of Energy through the Solid State Energy Conversion Alliance (SECA) program is < 4% per 1000 hours for Phase I coal based systems. While this target has been met by SECA natural gas based systems, little system testing has been performed for SOFCs operating on direct coal syngas. Degradation due to fuelling with direct coal syngas must be considered since naturally occurring coal trace materials (Hg, Pb, Se, As, etc.) may have undesirable interaction with the SOFC anode.

The long term SECA program goals target 40,000 hours of operation while maintaining good performance. However, determination of the interaction of coal

trace species with the SOFC anode requires prolonged effort due to the low concentrations of trace materials present in direct syngas. Test durations of at least 500-1000 hours are required for accurate prediction of long term degradation after operation at 40,000 hours. Additionally, the range of trace material forms available for testing in the laboratory is a small subset of the material forms existing in direct syngas.

To enhance testing and accelerate collection of pertinent results, we have designed and deployed a mobile test skid capable of field testing SOFC button cells on direct coal syngas. The Multi-Cell Array (MCA) system simultaneously tests 12 SOFC button cells, fuelled in parallel and individually load controlled. Testing multiple specimens at once permits statistical comparison and accelerates testing compared to individual laboratory tests. The MCA system also supports an integrated GC-ICP/MS system that can provide analysis of the direct coal gas and can identify trace elements at a ppb level. The system requires a power source, and a source of coal gas, and bottled gas supplies and can operate outdoors and unattended for an indefinite period of time.

Preliminary results were obtained from initial deployment of the SOFC MCA system at the Power Systems Development Facility (PSDF) gasifier in Wilsonville, AL. The 100 hour hydrogen test indicated successful operation of 5 cells over the entire duration. The success rate was greater than 40% for this initial deployment and further improvements to the test fixture will improve this rate. Further operation of the system at the PSDF on direct coal syngas is expected later in 2008. Results from the hydrogen baseline testing and testing on direct syngas will be described in this presentation.

This technical effort was performed in support of the National Energy Technology Laboratory's on-going research in SOFC under the RDS contract DE-AC26-04NT41817.

**P8-2****Novel Sulfur and Coke Resistant Anode Catalysts for Reduced Temperature Coal Gas Fed SOFC Systems**

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Solid Oxide Fuel Cells (SOFC) are the most desirable fuel cells for stationary power generation and as auxiliary power sources in transport applications. The fuel flexibility and higher efficiency of an SOFC make it a favorable choice. They can be used for a variety of applications including small-scale, remote co-generation purposes, uninterrupted power generation in hospitals as well as eventual incorporation into large-scale distributed power generation. The higher efficiencies that can be achieved in these systems make them ideal for coal gas fed power generation systems. However, despite the degree of hydrogen purification and sulfur removal after coal gasification, there remain traces of these impurities in the feed stream. The current Ni-YSZ anode catalysts exhibit very good catalytic activity towards hydrocarbon reforming and good compatibility with the rest of the SOFC system, however they are highly susceptible to poisoning due to sulfur in the fuel. Development of sulfur and coke resistant anodes will not only bring SOFCs closer to commercialization, it will also significantly reduce costs and eliminate material issues associated with gas clean-up and pre-treatment steps. The current work examines development, performance and resistance of new formulations to sulfur and coking. Bulk and surface specific characterization techniques, including X-ray Photoelectron Spectroscopy (XPS), X-ray Diffraction (XRD) and Vibrational Spectroscopy are used to understand the catalyst chemistry and nature of interactions. Anode performance is evaluated by testing activity for various fuel side reactions.

**P8-3****Continuum Degradation Model for SOFCs Anode Material under Coal Syngas and its Implementation in FEA to Predict Long-Term Structure Integrity**

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A degradation model is developed to predict long-term structural integrity of Solid Oxide Fuel Cell (SOFC) anode exposed to coal syngas. The model incorporates thermo-mechanical degradation and coal syngas contaminants effects on the anode microstructure. The proposed model is implemented into finite element analyses through user defined subroutine. The model is validated using a NexTech Probostat™ button cell test apparatus integrated with a Sagnac optical setup and infrared thermometer. This setup is capable of simultaneously measuring surface deformation, temperature and electrochemical performance. An analytical solution is also developed for button cell under uniform pressure to establish correlation between the degradation model and experimental measurements, as well as to determine the effective anode Young's modulus due to thermal-mechanical and/or electrochemical degradation.

**P8-4****In-situ Surface Deformation and Temperature Measurement of Button Cell Under SOFC Operating Conditions**

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An experimental technique capable of simultaneously measuring in-situ surface deformation, temperature and electrochemical performance of solid oxide fuel cell