SOME NEW EVIDENCE PERTAINING TO THE CHEMISTRY AND MECHANISMS OF COAL LIQUEFACTION.

Wendell H. Wiser, Department of Mining and Fuels Engineering, University of Utah, Salt Lake City, UT 84112.

Experimental observations have indicated that in solvent extraction and/or catalytic hydrogenation of bituminous coal in the range 400 - 500°C as much as 20 - 30% of the radical stabilization to produce liquid products involves hydrogen from the coal (i.e. coal pyrolysis reactions). Pyrolysis of a high volatile bituminous coal in this temperature range in a TGA apparatus with small samples (e.g. 10 mg), rapid heat-up (1 - 2 minutes) and continuously recorded weight change follows second order kinetics during 60 - 90% of the product evolution. A model compound with structure such that its pyrolysis is intended to simulate coal pyrolysis has been synthesized and pyrolyzed. The products of pyrolysis of this compound have been analyzed by MS and GC. Reaction kinetics are examined. Implications relative to coal pyrolysis kinetics and reaction paths are discussed. Reaction paths in the catalytic hydrogenation of linear (anthracene) and nonlinear (phenanthrene) condensed aromatics are considered as indicated by GC analysis of the products of these reactions.

CARBON-13 NUCLEAR MAGNETIC RESONANCE: A POWERFUL TOOL IN THE ASSESSMENT OF THE STRUCTURE OF SOLID COALS by Ronald J. Pugmire, Kurt W. Zilm, David M. Grant, Wendell H. Wiser, and Ralph E. Wood, Departments of Chemistry and Mining and Fuels Engineering, University of Utah, Salt Lake City, Utah 84112.

A number of western coals of varying rank have been studied in the solid state by means of carbon-13 NMR employing cross-polarization and magic angle spinning techniques. The solids spectra have been compared to the coal derived liquids. By means of artificially broadening the high resolution spectra of the coal derived liquids, a striking similarity in line shape and position is observed, particularly in the case of bituminous coal, when compared to the solid coal. It is noted however, that certain bands visible in the solids are no longer present in the liquid state. The significance of these results are discussed in terms of the carbon skeletal structure and changes therein associated with liquefaction reactions.

KINETICS AND MECHANISM OF SOLVENT EXTRACTION OF COAL - RELATIONS TO CHEMICAL STRUCTURE. Larry L. Anderson, Doohee Kang, Department of Mining and Fuels Engineering, University of Utah, Salt Lake City, UT 84112.

High volatile bituminous coals were extracted with tetralin in a batch-recycle reaction system. The reactions which produce benzene, hexane and pyridine soluble fractions show definite regimes which are significantly different in the way hydrogen is required from the donor solvent. Analysis of the liquid products as to chemical type and molecular weight reveal structures not present in long term reactions typical of SRC production. Oxygen structures in the primary products and the kinetics of the reaction to produce these species give information which may be related to the size of structural units in the coal and the connecting linkages.

HYDROPYROLYSIS OF COAL-DERIVED LIQUIDS AND OTHER HEAVY OILS AND SOLIDS. J. Shabtai, A. G. Oblad, Department of Mining and Fuels Engineering, University of Utah, Salt Lake City, UT 84112.

A new thermal hydrocracking process for upgrading of heavy hydrocarbon oils and solids, e.g. coal liquids, tar sand bitumens, and petroleum residues, has been developed. In a typical example, a heavy coal liquid, which contained about 45% by weight of components boiling >500°C, was hydropyrolyzed at 525°C and a hydrogen pressure of 1500 psig to yield 74% by weight of a light liquid product distilling between 60 - 380°C. The mechanism of some of the important hydropyrolytic reactions involved in the process was elucidated by parallel studies with model compounds, e.g. C_{10} - C_{16} n-paraffins, condensed arenes, and polycyclic naphthenes.