SURFACE MODIFIED COALS FOR ENHANCED CATALYST DISPERSION AND LIQUEFACTION

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I. ABSTRACT

Objective: This project investigates the surface charge properties of coals after pretreatment with various surfactants. The main objective is to ascertain and compare the dispersion and liquefaction activities of iron or molybdenum or combination of these metals on the raw coals with those loaded with coals that have been modified with surfactants.

Work done and conclusions: The coal used in this study is Illinois No.6 (DECS-24), supplied by the Penn State Coal Bank. Zeta potential results for the parent coal treated with the neutral surfactant, Triton X-100 at various pH's shows that the surfactant treated samples essentially have the same profiles as the untreated coal. This indicates that the neutral surfactant had little effect in modifying or changing the surface charge properties of the coal. This characteristic is in sharp contrast to the results obtained using cationic and anionic surfactants like sodium dodecyl sulfonate (SDS) or dodecyl dimethyl ethyl ammonium bromide (DDAB). It was observed that metal catalyst (molybdenum) adsorption on the coals was dependent upon the nature and the concentration of the surfactants. Molybdenum adsorption was most favourable at pH values of 3.5 - 4.0. Maximum catalyst adsorption was observed in the presence of DDAB compared to SDS or the untreated coal. The effect of surfactant concentration on catalyst adsorption is very pronounced in the case of DDAB with the catalyst adsorption reaching a maximum at 0.1M DDAB concentration. In the case of SDS, surfactant concentration does not seem to affect catalyst loading. Atomic force micrographs (AFM) of the raw coal and the coal that was treated with surfactants and molybdenum gave critical information about the coal surface modification and catalyst dispersion. The micrograph of the raw coal shows large areas of roughness on the surface. However micrograph of the DDAB and molybdenum treated coal shows a smoother surface with few isolated spots. The micrograph of the SDS and molydenum treated coal shows rod-like pillared structures on the coal surface. Hence the AFM results suggest that the catalyst is better dispersed on the

DDAB treated coal than the SDS sample. Liquefaction experiments were performed on Triton X-100 treated coals in the presence and absence of molybdenum catalyst. Maximum conversion of 96% to THF solubles was observed for the coal liquefied after treatment with Triton X-100 and molybdenum. This suggests that the surfactant may have enhanced the dispersion of the molybdenum catalyst.

Significance to Fossil Energy Program: An understanding of the coal surface properties will assist in developing a technique for preparing highly dispersed iron and molybdenum complexes in coal. This should make these catalysts attractive and cost-effective for coal liquefaction.

Plans for the coming year: Liquefaction and atomic force microscopy work will be carried out with other surfactants so that a complete understanding of the coal surface modification is accomplished. X-ray photelectron spectroscopy(XPS), X-ray diffraction (XRD), and Mossbauer spectroscopy will be conducted to determine metal crystallite size and catalyst dispersion.

II. HIGHLIGHT ACCOMPLISHMENTS

The effect of various surfactants and pH on the surface characteristic of the coal and its ability to adsorb molydenum catalyst has been studied. The results have been rationalized by the chemistry of coal-surfactant-catalyst interaction and interfacial phenomena. This information should assist in the preparation of well dispersed and cost-effective catalysts for large scale coal liquefaction as supplemental transportation fuel.

III. ARTICLES AND PRESENTATIONS

(1) Abotsi, G. M. K.; Bota, K. B.; Saha, G.; Mayes, S., Prep. Pap.-Am. Chem. Soc., Div. Fuel Chem. 1996, 41(3), 984 - 987.

(2) Abotsi, G. M. K.; Bota, K. B.; Saha, G., Proc. First Joint Power and Fuel Systems Contractors Conference, 38, 1996.

(3) Abotsi, G. M. K.; Bota, K. B.; Saha, G., 4th Annual HBCU/Private Sector-Energy Research & Development Technology Transfer Symposium Proc., 33-36, 1996.

(4) Mayes, S.; Abotsi, G. M. K.; Bota, K. B.; Saha, G., 5th Annual HBCU/Energy Research & Tech. Transfer Sym, Poster Presentation, Baton Rouge, LA, March 4-5, 1997.