HOKKAIDO UNIVERSITY

Title	Center for Advanced Research of Energy Technology. Summary International Report, July 1995-June 1996
Citation	Memoirs of the Faculty of Engineering, Hokkaido University, 19(3), 568-571
Issue Date	1996
Doc URL	https://hdl.handle.net/2115/38069
Type	other
File Information	19(3)_568-571.pdf



Hokkaido University Collection of Scholarly and Academic Papers : HUSCAP

8th International Conference
on Coal Science, September
10-15, 1995, Oviedo, Spain

Change in the conformation of lignite molecule during moisture release process

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Effects of drying conditions on the conformation of lignite molecule has been investigated. Volumetric shrinkage and recovery of the lignite were measured with a swelling apparatus at 30°C. ^{1}H-NMR and L-band EPR measurements were also done for the moisture controlled samples and readsorped ones. Volumetric change of lignite is sensitive to the moisture release process. For dewatering process, volumetric change of lignite is reversible up to 12% of moisture loss (so-called free water removing) and is irreversible for the bonded water removing. For drying process, the change is irreversible over the whole range of moisture loss so far tested. T_2 values for three components (two Gaussian and one Lorentzian) were obtained by deconvolutions of NMR FID. Change in spin-spin relaxation times (T_2) of protons in lignite molecule and associated water molecule showsa good agreement with volumetric change in lignite during moisture release and readsorption process. Spectral intensities with L-band EPR measurement increase rapidly beyond 20% of moisture loss. These results suggest the structure change of lignite during moisture release is affected with drying conditions.

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A Model Structure of Zao Zhuang Bituminous Coal

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A model structure of Zao Zhung (Chinese bituminous) coal based on the structural analyses and the computer simulation was suggested. The coal was extracted with carbon

disulfide-N-methyl-2-pyrolidinone mixed solvent and the extract obtained was further fractionated. The extract fractions were hydrogenated using Adkins catalysis under mild condition at 430°C. The oils obtained from each fraction were analyzed by column separation followed by FID/GC and FD/MS. Molecular models of each fraction were constructed based on the structural data. Associated structures for heavy fractions including the extraction residue have been suggested. All model molecules included in each fraction were placed in a basic cell randomly, and CAMD (computer aided molecular design) was applied for the construction of the raw coal model using periodic boundary condition. A model structure suggested is a strained and anisotropic structure. Physical density of the raw coal model was estimated by previous improved method and the calculated density was 1.22(g/cm^3), in good agreement with that observed experimentally.

8th International Conference on Coal Science September 10-15, 1995, Oviedo, Spain

Interaction Between Coal and Mixed Solvent System by Means of L-band EPR

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To elucidate the synergy between pyridine and CS_2, a new technique with L-band EPR is introduced. The intensity and line width of an EPR spectrum have been determined for a coal sample immersed in the solvent as a function of the mixing ratio of pyridine and CS_2. Upper Freeport and Beulah Zap lignite, Argonne premium coal samples, were used in this study. The results of the EPR experiments showed the following. In the pyridine/CS_2 mixed solvent system, the interaction between the model compound with radical and solvent changed with the ratio of pyridine/CS_2. That is, EPR spectral intensity intensity and line width varied with the ratio of pyridine and CS_2(50/50) for Upper Freeport coal. The line width is also altered as a function of the solvent ratio. The advantage of L-band EPR technique is that signal acquisition is available from coal immersed in the solvent with high electric permittivity. The technique described here will give an insight into coal molecules surrounding solvent or water.

45th Canadian Chemical Engineering Conference, Quebec city, October 15-18, 1995

Chlorination Characteristics of Minerals in Coal Ashes

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Three bituminous coals, a lignite and a brown coal ashes having different mineral compositions were chlorinated by exposure to Cl_2 gas. The ash samples were prepared by burning coal in a muffle furnace at 1088 K (high-temperature ash; HTA) and in O_2 plasma asher (low-temperature ash; LTA). Change in the ash weight with time due to chlorination and volatilization of minerals was directly measured in a thermobalance reactor with a heating of 10 K/min up to a holding temperature of 1273 K in atmospheric Cl_2 gas flow.

Changes in the ash weight with increasing temperature widely varied for the type of the initial ash. The variation was explained on the basis of the initial contents of metal oxides and carbonates. The chlorination treatment resulted in a significant reduction of differences in the mineral compositions, melting-point temperatures and acid-base indices of residual solids from HTAs derived from the bituminous coals.

8th International Conference on Coal Science, Oviedo, SPAIN, 10-15, September. 1995

Vapor Pressure Estimation of Hydrocarbons in a Coal Derived Liquid

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The vapor pressure as well as the boiling point is one of the most fundamental properties for process design and control. In spite of many studies on vapor pressure estimation for pure compounds, their applicability to coal derived liquids has never been confirmed yet.

It was clarified that the difference (dlogP) of logarithmic values of the vapor pressure of hydrocarbon homologue with those of straight alkanes having the same total carbons was

almost constant at a given temperature regardless of change in the total carbon number. The value of dlogP was found to be directly proportional to the reciprocal of temperature with the slope being negative and gradually becoming gentle with increasing numbers of aromatic or naphthenic rings. The value of slope reflects influence of aromatic or naphthenic rings to the vapor pressure. A correlation is proposed based on these considerations. Application of the method to a recycle solvent gave a good agreement between the calculated and observed vapor pressures. Hence, it is now possible to estimate the vapor pressure of various hydrocarbons such as alkanes, aromatics, hydroaromatics and their alkyl derivatives, in both forms of pure substance and mixture, over a range of total carbon number from 6 to 20.