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LAWRENCE BERKELEY LABORATORY
Room: 128 Bldg.: 70 Ext.: 6241

December 8, 1980

TO: Charles Grua

FROM: Amos Newton and Phyllis Fox

RE: Monthly Progress Report for November
Environmental Effect and Control for
Coal-Water Systems
LBID-321

PHENOLS AND SLURRY WATER

The difficulty in methylating phenols in slurry water from Illinois No. 6 coal has been solved. After spiking the water with an internal standard of perdeutero phenol and adding NaOH, the solution is pre-extracted with methylene chloride and hexane. These solvents remove the unidentified material in this slurry water which catalyzes the hydrolysis of dimethyl sulfate. When dimethyl sulfate is added to the cooled, pre-extracted solutions and the mixture is stirred overnight, the yield of anisole from the perdeuterated phenol is adequate.

No such problem was found with Peabody Black Mesa coal. The methylation of the slurry water from this coal was similar in behavior to that from Wyodak Coal.

Table 1 shows a compilation of results of phenol yield and the absorption of various phenolics by the three coals under investigation. This table shows that the three coals behave differently. Wyodak coal yields close to the same phenol concentration in the slurry water whether or not phenol is added before slurry preparation. Phenol is freely absorbed by and extracted from Wyodak coal. Illinois No. 6 and Black Mesa coals yield much less free phenol in coal slurry water and when phenol is added to the water before slurry preparation, they do not absorb to the same concentration as was found without added phenol. The behavior of Black Mesa coal shows less absorption of the phenolics in general, though 1-naphthol and 5-phenyl phenol are almost completely absorbed. This behavior must be checked.

POLYNUCLEAR AROMATIC HYDROCARBONS IN COAL SLURRY WATER

It was previously found that perdeutero phenanthrene is absorbed from water and the concentration of phenanthrene in coal slurry water is less than 5 ppt (parts per trillion). All coals were checked for the absorption of a variety of polynuclear aromatics with the results shown in Table 2. Black Mesa coal shows incomplete absorption. Whether this is caused by lack of absorptive capacity or simply a slow rate of absorption must be checked. Even this coal removes more than 99.7% of the added material.

NITROGENOUS COMPOUNDS IN COAL SLURRY WATER

Several nitrogenous compounds which might be derived from coal were added to water at a concentration of 100 ppm each before slurry preparation. As shown in Table 3, these were each absorbed by the coal. Only quinoline was positively identified in the slurry water from Wyodak coal. More than 99.9% of each component was removed from the water by coal of any type tested.

Table 1. Phenol and phenolics in coal slurry waters from various coals made with and without added phenolics before slurry preparation.

Compound[a]	ppb compound in coal slurry water from:		
	Wyodak Coal	Illinois No. 6 Coal	Black Mesa Coal
phenol (no addition)	9.0	<2.0	1.2
phenol (added)	11.0	4.5	12.9
o-cresol (added)	<0.5	0.02	7.4
2,6 dimethyl phenol (added)	<0.5	<0.01	14.5
Resorcinol (added)	<0.5	<0.005	23.8
1-naphthol (added)	<0.5	<0.005	<0.1
4-phenyl phenol (added)	<0.5	<0.005	<0.1

[a]The initial concentration of each added component was 100 ppb.

Table 2. Absorption of polynuclear aromatic hydrocarbons from water during coal slurry formation.

Compound[a]	ppb concentration of compound in slurry water from:		
	Wyodak Coal	Illinois No. 6 Coal	Black Mesa Coal
acenaphthene-D_{10}	0.009	0.04	0.27
phenanthrene-D_{10}	<0.005	0.01	0.21
pyrene-D_{10}	<0.003	<0.01	0.13
1,2 Benzanthracene-D_{12}	<0.003	<0.01	0.15
chrysene-D_{12}	<0.003	<0.01	0.14
p-Terphenyl-D_{14}	0.003	<0.01	0.12
perylene-D_{12}	<0.008	<0.01	0.10

[a]The initial concentration of each component was 100 ppb.

Table 3. The absorption of nirtogenous compounds from water during coal slurry preparation.

Compound[a]	ppb concentration of compound in slurry water from:		
	Wyodak Coal	Illinois No. 6 Coal	Black Mesa Coal
pyrrole	<0.01	<0.1	<0.1
pyridine	<0.01	<0.1	<0.1
aniline	<0.01	<0.1	<0.1
quinoline	0.08	<0.1	<0.1
diphenyl amine	<0.05	<0.1	<0.1

[a]The initial concentration of each component was 100 ppb.

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