

Predictors of Isothermal Fluid Properties of Coals

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Fluidity, which typically develops in the range 380-420°C, is a unique property of mid-ranked coals. Coals of similar rank and composition, however, often exhibit Gieseler fluidities differing by several orders of magnitude. The objective of this study is to seek to identify predictively useful correlations between other well-defined parameters and the fluid properties of hvb coals.

In the standard Gieseler plastometer analysis (1) the coal is heated at a constant 3 deg C/min throughout the run. There are, however, several advantages to be gained by operating the plastometer in an isothermal mode, among them the more accurate determination of melting and coking slopes and the determination of the activation energies associated with these slopes and with maximum fluidities (2). In this study we use the isothermal fluid characteristics of a group of hvb coals as the dependent variables. We will examine a number of standard and nonstandard characterizations of coals for their predictive power with regard to these fluid properties.

Twenty-nine coal samples were collected from eastern mid-continent seams (mostly from western Kentucky), from active mines and from coal cleaning plants using freshly mined coal of known local origin. To minimize adventitious weathering of the samples, all coals were reduced, split and stored in sealed heavy plastic under inert gas at freezer temperatures prior to testing. The proximate, ultimate and short petrographic characterizations are given in Table 1. More detailed source information is available elsewhere (3).

For each of these coals a number of isothermal Gieseler determinations (at least 18) has been made. Both melting and coking slopes follow Arrhenius dependencies (2,4), as do $\ln(\text{maximum observed fluidity})$ and $\ln(\text{intersection maximum fluidity})$ (2). For direct coal-to-coal comparison it is convenient to make an interpolation or short extrapolation of temperature to a benchmark value such as 400°C. Table 2 summarizes the fluidity characteristics of these coals, with slope and fluidity data estimated for 380, 400 and 420°C. The maximum Gieseler fluidities (by slope intersection) of these coals cover a wide range, ranging at 400°C from 62,300 ddpm (coal 25) to 1.8 ddpm (coal 28).

In addition to the characterization data summarized in Table 1, several nonstandard measurements have been made. These are described below.

When small portions (3-5 mg) of coal are pyrolyzed at a high ramp (500 deg C/sec) and low ceiling temperature (450°C) onto a nonpolar chromatographic column, the resulting chromatogram provides information in two distinct regions, a gaseous product mixture which quickly elutes from a 50 cm silicone (OV 101) column at 60°C, and a larger vapor product mixture eluting at 200-250°C. A standard pyrolysis/GC procedure has been developed (5), wherein the integrator signals in several one-minute windows are found to correlate significantly with observed fluid properties. This is a reasonably reproducible procedure, with standard deviations

(quadruplicate analyses) averaging 6.5% of the total integrator signal per microgram coal.

Total organic material extractable by refluxing tetrahydrofuran (THF) and refluxing N,N-dimethylformamide (DMF) has been determined for all coals by Soxhlet extraction in triplicate. The average amount extracted by THF (dry ash-included basis) is 14.3%, average standard deviation 0.29%. The average amount extracted by DMF (same basis) is 25.1%, average standard deviation 0.85%. It is necessary to heat residues to 150°C under 1 torr in order to obtain complete desorption of the nitrogen base (6).

Two other kinds of data were obtained and found to have no predictive value with regard to plasticity. If fluid properties were related to low covalent crosslink densities, then the swelling (7,8) of DMF extraction residues by cold DMF might be expected to correlate with fluidities. Residues from four coals were swelled to equilibrium by direct contact with liquid solvent in a simple apparatus adapted from Larsen (7). The four coals had ASTM maximum fluidities ranging from 35 to over 30,000 ddpn. The swelling ratios were all between 2.1 and 2.5, with the most fluid coal having one of the lower swelling ratios. This observation seems to rule out the possibility that fluidity differences among hvb coals arise from differences in covalent crosslink densities.

The second experiment productive of negative results was that of FTIR examination of selected coals and their THF extracts, using the procedure described by Painter (9,10) and the H(aromatic)/H(aliphatic) ratio technique of Solomon (11). Two low-fluidity coals, 03 and 24, and two highly fluid coals, 22 and 34, were compared. The aromatic/aliphatic ratios are slightly different for the raw coals (0.43 and 0.45 for the low-fluidity coals and 0.47 and 0.49 for the high-fluidity coals), and are identical for the THF extracts (0.33 for all four coal extracts). This appears to rule out the view that variations in fluid behavior reflect substantial variations in the chemical characteristics of the sol fractions.

The following 'independent' variables were collected for first-round prediction testing:

16 classical characterizations, including seven petrographic measurements;

6 semistandard characterizations (ash sulfate, organic and pyritic sulfur, aliphatic/aromatic ratio, and DMF and THF extractables);

25 measures (with considerable redundancy) of the pyrolysis/GC chromatograms; and

9 sets of values derived from the above (five estimates of reactive macerals, 2 estimates of H/C ratio, an empirical formula for estimating liquefaction reactivity from % hydrogen and organic sulfur, and an estimate of extractable 'preasphaltenes' as [DMF-THF]).

These parameters were examined separately by simple linear regression, using the SAS (12) R-square test, to reduce the candidate independent variables to a manageable number. The number of variables was reduced to 13, using two criteria. A candidate variable is rejected if the fraction of the total sums of squares accounted for by a simple linear regression using the candidate variable is less than 0.1, and/or the variable is redundant with another variable which has stronger predictive power. (For example, pyritic sulfur is less predictive than total sulfur, and with total sulfur present in the analysis pyritic sulfur does not

provide sufficient additional predictivity.) The variables surviving this screening are shown in Table 3.

The best single predictor of fluidity at 400-420°C is the 4-5 min pyrolysis/GC signal (the gas signal from fast pyrolysis to 450°C), which affords correlation coefficients of .850 at 420 and .867 at 400°C. In the absence of pyrolysis/GC data the next best predictor is total DMF-extractables, affording correlation coefficients of .851 at 420 and .812 at 400°C.

The expansion of the regression equation to include additional independent variables always increases the goodness of fit. After the third variable is added, however, improvement in the correlation coefficient R becomes quite small. In predicting ln(maximum intersection fluidity) at 400°C, for instance, the values of R with the successive addition of the 4-5 min pyrolysis/GC signal, vitrinite reflectance, THF-extractables and total sulfur are .867, .895, .920 and .935. When pyrolysis data are excluded, the successive inclusion of DMF-extractables, vitrinite reflectance, THF-extractables and % resinite yields R values of .812, .856, .890 and .901. In these and other cases the improvement obtained by adding the fourth predictive variable is of marginal statistical significance. The following observations are based upon the most consistent three-variable regressions provided by this database.

When only classical and petrographic data are available the best three-term linear regressions provide fits with R in the vicinity of 0.7-0.8 (Table 4). This is illustrated by the regression plot for ln(maximum intersection fluidity) at 400°C (Figure 1). The variables used here are heating value, total sulfur, and maximum vitrinite reflectance.

With the addition of quantitative Soxhlet extraction data, a regression on the same fluidity data using vitrinite reflectance, THF-extractables and DMF-extractables provides a reasonably good fit (Figure 2), with R = .890.

With the further addition of the pyrolysis/GC data, inclusion of the 4-5 min pyrolysis signal, along with vitrinite reflectance and THF-extractables, provides a still better fit (Figure 3), with R = .920. The predictions at 420°C are comparably good (Table 4).

An important test for the adequacy of any predictive model is the examination of residuals for possible patterning. A plot of the residuals from the regression of Figure 3 is shown in Figure 4. The substantially random distribution of these residuals suggests that most of the data scatter of Figure 3 represents random error (sample inhomogeneity and errors of sampling, analysis, and possibly adventitious sample ageing during the various analyses).

Discussion.

It has not proven to be possible to predict fluid properties of coals on the basis of a single chemical or petrographic characterization. Even solvent extraction with pyridine or quinoline (13) appears to be little more than roughly indicative. In the present study DMF-extractables constitute an approximate predictor ($R > 0.8$), and a part of the 450°C pyrolysis gas signal is a slightly better predictor.

The above data (Table 4) show reasonably good prediction (R 's > 0.9) of maximum fluidity and melting and coking slopes by multiple linear regression equations using three predictive variables. The data fits are not quite as good when pyrolysis or extraction data are excluded. The correlation coefficient falls to 0.85 when both pyrolysis and extraction data are excluded (Figure 1).

The measurements with the greatest significance for our data are the 4-min. pyrolysis/GC signal (or other nearly equivalent pyrolysis data), THF-extractables, DMF-extractables, heating value and vitrinite reflectance. Increases in the values of any of the first four correlate with increasing the melting slope; increasing reflectance makes little change in melting slope but diminishes the coking slope. Increases in any of these variables correlate with increased maximum fluidity.

The relative importance of predictive variables varies with the situation. DMF-extractables is a considerably better single predictor than THF-extractables; yet in most multivariate cases THF-extractables make a larger Type IV contribution to regression sums of squares than do the DMF data. It is tentatively suggested that the DMF data are partially redundant with the pyrolysis data. We are not yet able to offer a specific mechanistic interpretation of these observations.

After examination of a number of expressions containing predictors raised to other than the first power, and a number of expressions with cross-terms containing products of two predictors, the simple first-order linear equations of Table 4 seem to be as good as any. We are continuing to apply factor analysis to these data, with the objective of characterizing more clearly the underlying physicochemical features controlling fluid behavior in coals.

This work is part of a larger study of coal plasticity, for which we acknowledge with thanks the support of the U.S. Department of Energy (3).

References

1. ASTM Method D 2639, Amer. Soc. for Testing and Materials, Phila., PA, 1982.
2. W. G. Lloyd, J. W. Reasoner, J. C. Hower and L. P. Yates, Amer. Chem. Soc., Divn. Fuel Chem., preceding paper.
3. W. G. Lloyd, J. W. Reasoner, J. C. Hower, L. P. Yates, C. P. Clark, E. Davis, A. Fitzpatrick, S. Irefin, A. Jimenez, T. McC. Jones, C. L. Reagles, L. P. Sturgeon, J. M. Whitt and G. Wild, 'Predictors of Plasticity in Bituminous Coals', Final Techn. Rept., U. S. Dept. of Energy Contract DE-FG22-81PC40793, January 1984.
4. W. G. Lloyd, H. E. Francis, M. R. Yewell, Jr., R. O. Kushida and V. D. Sankur, Amer. Chem. Soc., Divn. Fuel Chem. Preprints, 25, no. 2, 128 (1980).
5. J. W. Reasoner, J. C. Hower, L. P. Yates and W. G. Lloyd, submitted to Fuel.
6. A. W. Fort (Univ. of Kentucky), private communication.
7. J. W. Larsen, 'Coal Structure and Reactivity', USDOE Contractors' Conf., Pittsburgh, PA, Oct. 1982.
8. N. A. Peppas, L. M. Lucht, M. E. Hill-Lievense and D. T. Hooker, II, 'Macromolecular Structural Changes in Bituminous Coals during Extraction and Solubilization', Final Techn. Rept., U. S. Dept. of Energy Contract DE-FG22-80PC30222, August 1983.
9. P. C. Painter, R. W. Snyder, M. Starsinic, M. M. Coleman, D. W. Kuehn and A. A. Davis, Appl. Spectroscopy, 35, 475 (1981).
10. P. C. Painter, R. W. Snyder, M. Starsinic, M. M. Coleman, D. W. Kuehn and A. A. Davis, 'Coal and Coal Products: Analytical Characterization Techniques', in E. L. Fuller, ed., ACS Symp. Ser. 205, Amer. Chem. Soc., Washington, DC, 1982.
11. P. R. Solomon, Amer. Chem. Soc., Divn. Fuel Chem. Preprints, 24, no. 3, 184 (1979).
12. Statistical Analysis System, SAS Institute, Inc., Cary, NC.
13. K. Ouchi, K. Tanimoto, M. Makube and H. Itoh, Fuel, 62, 1227 (1983).

Table 1¹

coal	rank	moist.	ash	VM	%C	%H	%N	%S	pyrS	orgS	Btu	FSI	vit ²	lip ³	min ⁴	refl ⁵
02	hvBb	7.86	10.77	42.6	71.67	5.05	1.62	3.41	1.43	1.96	12620	4.5	66.4	7.2	13.5	0.42
03	hvBb	6.75	5.40	41.6	77.60	5.38	1.60	2.02	0.98	1.02	13720	4	85.2	5.0	7.0	0.70
04	hvBb	5.33	6.44	46.8	76.48	5.37	1.60	3.29	2.22	0.92	13650	3.5	74.4	7.6	8.8	0.59
06	hvBb	5.02	7.86	44.5	72.19	5.09	1.11	3.68	1.38	2.27	13300	6	78.4	4.2	10.5	0.57
07	hvBb	5.21	6.48	44.8	76.46	4.78	1.04	3.20	1.08	2.08	13590	3.5	81.9	2.7	8.8	0.60
09	hvBb	7.76	8.79	41.4	73.16	5.43	1.52	3.13	1.25	1.99	13050	4.5	75.4	4.2	11.6	0.58
10	hvBb	6.32	8.49	41.7	75.08	4.30	1.13	3.14	1.18	1.85	13330	4	75.5	2.8	10.9	0.57
11	hvBb	5.94	17.71	38.4	63.32	4.61	1.25	3.40	1.61	1.63	11770	2.5	69.7	3.2	21.0	0.56
14	hvBb	6.70	7.60	41.1	74.12	5.21	1.35	2.75	0.93	1.76	13410	4	79.1	3.1	9.7	0.54
15	hvBb	6.31	10.38	41.3	73.18	5.47	1.54	3.77	1.62	2.10	12850	4.5	71.7	3.7	13.3	0.61
18	hvBb	7.09	8.36	40.6	74.08	5.11	1.50	3.59	1.47	1.86	13020	4.5	77.3	3.9	11.0	0.54
20	hvBb	7.77	9.70	43.5	74.06	5.28	1.22	2.92	0.92	1.71	12910	5	79.9	2.9	11.8	0.53
21	hvAb	2.57	8.68	40.3	75.41	5.27	1.07	3.35	1.33	1.93	13540	8.5	75.5	4.3	11.2	0.71
22	hvAb	2.45	9.60	39.4	75.98	5.42	1.44	2.91	1.45	1.35	13490	8	76.0	3.7	12.0	0.73
24	hvBb	7.87	7.15	42.8	75.68	5.55	1.51	3.56	1.22	2.27	13300	4	80.2	3.2	9.7	0.60
25	hvAb	1.68	6.79	40.2	77.79	5.33	2.04	1.38	0.19	1.17	14250	7	75.7	5.7	8.1	0.87
26	hvAb	2.12	14.20	32.2	69.87	4.43	1.50	2.76	0.48	2.20	12610	7	72.2	2.7	17.3	0.87
27	hvAb	2.86	8.12	40.0	76.18	5.17	1.54	3.53	0.48	2.97	13650	7	71.1	3.6	10.7	0.76
28	hvCb	10.96	8.26	42.2	76.65	5.78	1.58	1.42	0.80	0.59	13240	2.5	69.0	7.8	9.7	0.64
30	hvBb	6.44	8.95	48.7	74.67	5.41	1.54	4.01	1.46	2.23	13010	4.5	68.4	9.6	11.9	0.58
32	hvAb	2.94	7.23	42.8	76.05	5.37	1.65	3.00	0.92	2.05	13730	5	78.5	3.1	9.5	0.65
34	hvAb	2.28	8.03	41.0	74.36	5.25	1.45	2.77	1.08	1.67	13670	6.5	80.5	3.9	10.2	0.69
35	hvBb	6.59	10.61	39.3	73.77	5.10	1.25	4.06	2.05	1.91	12775	6	77.5	2.7	13.7	0.58
36	hvBb	7.00	12.58	38.2	70.38	4.91	1.29	4.06	2.22	1.72	12470	4.5	76.2	2.5	15.8	0.58
37	hvAb	3.30	12.48	37.2	72.88	4.91	1.53	2.90	1.70	1.16	12740	4.5	75.3	2.4	15.1	0.66
38	hvBb	9.89	3.41	40.5	81.75	5.64	1.65	0.83	---	---	14170	3	76.7	8.4	3.9	0.67
39	hvBb	7.63	13.41	38.5	70.57	5.12	1.56	1.91	---	---	12530	3	72.2	7.6	15.6	0.65
40	hvBb	9.29	3.75	39.6	81.33	5.68	1.73	0.80	---	---	14150	2.5	80.1	7.9	4.6	0.70
41	hvBb	7.78	2.77	42.1	80.73	5.74	1.61	1.06	---	---	14280	3	85.7	7.2	3.3	0.67

¹ Moisture is as determined; other analyses are on a dry ash-included basis. ² Vitrinite and pseudovitrinite.

³ Exinite and resinite. ⁴ Mineral matter content by Parr procedure. ⁵ Vitrinite maximum reflectance in oil at 546 nm.

Table 2

coal	exptl T range, °C	melting slope, min ⁻¹		coking slope, min ⁻¹		ln(max observed fluidity)		ln(max intersection flu)							
		@380°	@420°	@380°	@400°	@380°	@400°	@380°	@400°						
25	404-420°	0.246	0.631	1.535	0.379	1.05	0.276	9.52	9.93	10.34	2.	11.10	11.04	10.99	0.
34	390-409	0.371	1.232	3.823	0.653	1.74	4.36	8.24	9.74	11.40	7.	7.60	10.10	13.19	12.
32	389-411	0.392	1.187	3.373	0.797	2.06	5.06	5.56	8.40	12.39	18.	6.92	9.23	12.11	13.
27	379-404	0.197	0.875	3.564	0.565	1.53	3.91	4.37	8.43	15.65	29.	5.64	8.81	13.40	20.
21	387-410	0.340	1.023	2.885	0.567	1.79	5.26	4.84	8.11	13.19	23.	5.91	8.68	12.46	17.
22	389-413	0.193	0.702	2.375	0.429	1.31	3.74	4.05	6.71	10.78	22.	4.96	7.84	12.07	20.
35	400-419	0.263	0.656	1.551	0.912	2.45	6.24	3.63	5.87	9.21	21.	4.36	6.49	9.46	17.
06	393-418	0.156	0.518	1.606	0.620	2.05	6.34	2.96	5.67	10.47	28.	3.59	6.11	10.09	23.
07	404-426	0.219	0.505	1.109	0.614	2.06	6.45	2.58	4.43	7.36	24.	3.36	5.15	7.69	19.
37	406-432	0.179	0.431	0.986	0.648	1.95	5.49	1.98	3.40	5.62	24.	2.72	4.23	6.42	19.
36	404-425	0.140	0.382	0.982	0.829	2.40	6.56	2.00	3.46	5.79	24.	2.53	4.11	6.49	21.
14	398-422	0.215	0.466	0.966	0.942	2.73	7.45	1.61	3.03	5.48	28.	2.42	3.88	6.04	21.
15	400-427	0.137	0.350	0.844	1.02	2.76	7.06	2.10	3.47	5.56	22.	2.26	3.78	6.13	22.
41	412-438	0.088	0.240	0.616	0.435	1.41	4.29	1.95	3.20	5.10	22.	2.35	3.68	5.63	20.
04	406-431	0.070	0.252	0.842	0.475	1.68	5.54	1.33	2.84	5.80	33.	2.04	3.66	6.33	26.
39	410-435	0.101	0.267	0.667	0.565	1.67	4.60	1.74	3.03	5.11	24.	2.04	3.43	5.58	23.
26	412-436	0.113	0.280	0.661	0.363	1.09	3.04	1.18	2.23	4.07	28.	1.92	3.11	4.89	21.
38	411-436	0.044	0.155	0.505	0.341	1.19	3.85	1.49	2.70	4.75	26.	1.73	3.07	5.26	25.
40	417-443	0.278	0.424	0.631	0.587	1.61	4.18	0.476	1.09	2.37	36.	1.99	2.89	4.11	16.
20	401-428	0.221	0.420	0.769	0.993	2.72	7.04	0.616	1.61	3.97	42.	1.42	2.67	4.85	28.
10	405-429	0.222	0.442	0.846	0.588	2.14	7.23	0.651	1.57	3.61	39.	1.18	2.38	4.62	31.
30	399-426	0.191	0.400	0.803	0.965	2.67	6.94	0.287	0.967	3.03	53.	1.01	2.12	4.26	32.
18	398-424	0.195	0.396	0.773	0.889	2.70	7.67	0.428	1.26	3.47	47.	0.907	2.06	4.47	36.
24	405-431	0.282	0.435	0.653	1.09	2.84	7.01	0.394	0.916	2.03	37.	1.02	1.76	2.94	24.
11	412-432	0.286	0.493	0.824	0.486	1.79	6.11	0.631	1.28	2.48	31.	0.856	1.75	3.42	31.
09	403-427	0.174	0.352	0.683	0.592	2.07	6.71	0.252	0.813	2.45	51.	0.484	1.34	3.48	44.
03	408-433	0.092	0.235	0.569	0.368	1.36	4.67	0.273	0.704	1.72	41.	0.445	1.14	2.76	41.
02	406-423	0.176	0.316	0.546	0.611	2.21	7.39	0.380	0.852	1.82	35.	0.408	1.04	2.50	41.
28	413-437	0.201	0.394	0.743	0.123	0.670	3.29	0.160	0.339	0.687	33.	0.314	0.585	1.05	27.

1 Activation energy in kcal. The average standard deviation of E(a) of 1.9 kcal.

Table 3
Variables Retained for Multiple Linear Regression Analysis

Class:		R^2 in simple regression*
Classical	FSI	.260
	BTU	.122
	% Sulfur	.031 ¹
Petrographic	Exinite	.128
	Resinite	.105
	Pseudovitrinite	.290
	Max Vitrinite Reflectance	.246
Extraction	DMF-extractables	.554
	THF-extractables	.199
Pyrolysis/GC	4-5 min signal % ²	.595
	2-5 min signal counts ²	.572
	14-16 min signal counts ³	.572
	13-17 min window counts ³	.565

* Averages for six estimates: max observed fluidity at 400° and 420°, and E(act), and max intersection fluidity at 400° and 420°, and E(act).

¹ Retained owing to good predictive power for coking slopes.

² The 4-5 min signal % and 2-5 min signal counts are substantially redundant.

³ The 14-16 min and 13-17 min signal counts are substantially redundant.

Table 4
Best-fit Three-value Multiple Linear Regression Equations

Equation ¹	Corr. coeff.
<u>CLASSICAL AND PETROGRAPHIC DATA ONLY:</u>	
MELT400 = -1.128 +1.309E-4 * BTU -8.857E-2 * EXIN +2.531E-1 * RESI	.785
MELT420 = -5.986 +5.793E-4 * BTU -2.758E-1 * EXIN +6.919E-1 * RESI	.692
COKE400 = +0.078 +1.582E-5 * BTU +3.356E-2 * SULF -3.018E-1 * REFL	.806 ²
COKE420 = +0.757 +2.401E-5 * BTU +6.273E-2 * SULF -1.103E0 * REFL	.913 ²
FCAL400 = -44.32 +2.419E-3 * BTU +1.815E0 * SULF +1.789E+1 * REFL	.721
FCAL420 = -54.54 +3.101E-3 * BTU +2.643E0 * SULF +1.962E+1 * REFL	.723
<u>WITH EXTRACTION AND PYROLYSIS/GC DATA AVAILABLE:</u>	
MELT400 = -0.311 +1.224E-1 * RESI +3.168E-2 * THF +3.287E-1 * PYR4	.906
MELT420 = -1.369 +2.388E-1 * RESI +1.025E-1 * THF +1.285E0 * PYR4	.904
FCAL400 = -9.998 +1.102E+1 * REFL +3.374E-1 * THF +3.369E0 * PYR4	.920
FCAL420 = -11.59 +1.134E+1 * REFL +5.767E-1 * THF +3.731E0 * PYR4	.912

¹ Abbreviations: MELT400 and MELT420 - melting slopes at 400° and 420°C; COKE400 and COKE420 - coking slopes at 400° and 420°C; FCAL400 and FCAL420 - ln(intersection maximum fluidity) at 400° and 420°C; BTU - heating value; EXI - % exinite; REFL - % maximum vitrinite reflectance; RESI - % resinite; SULF - % sulfur; THF - % extractable by THF. ² Best three-variable fit.

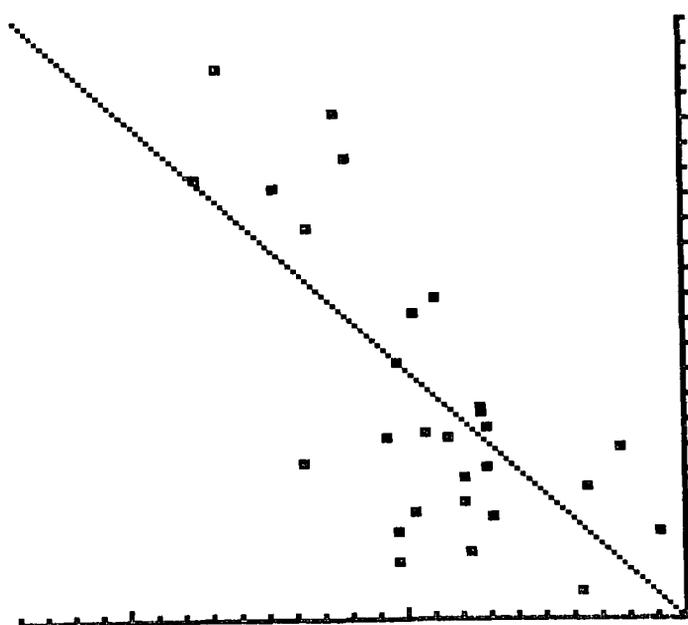


FIGURE 1. PREDICTION OF LN(MAXIMUM FLUIDITY) AT 400°C, EXCLUDING EXTRACTION AND PYROLYSIS DATA. Horizontal: ln(observed dpm). Vertical: ln(predicted dpm). Both scales 0 to 12. Independent variables: heating value, total sulfur, maximum vitrinite reflectance. $R^2 = .520$ (29 coals).

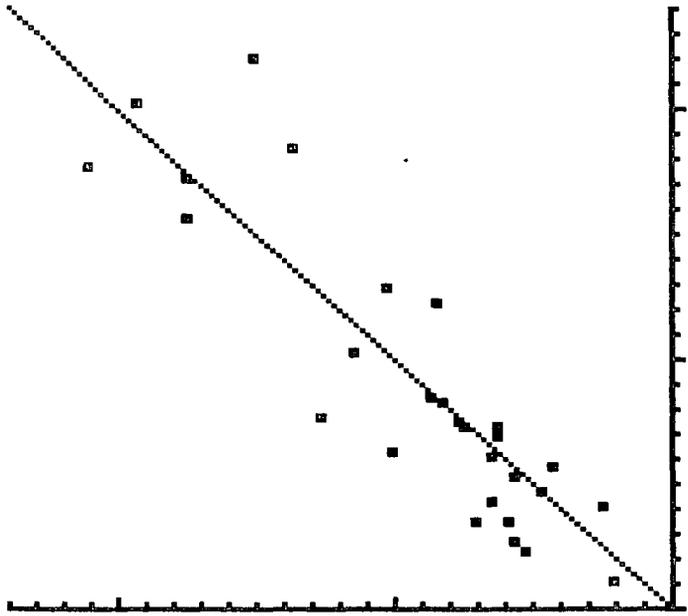


FIGURE 2. PREDICTION OF LN(MAXIMUM FLUIDITY) AT 400°C, INCLUDING EXTRACTION DATA. Horizontal: ln(observed dpm). Vertical: ln(predicted dpm). Both scales 0 to 12. Independent variables: maximum vitrinite reflectance, DMF-extractables, THF-extractables. $R^2 = .792$ (29 coals).

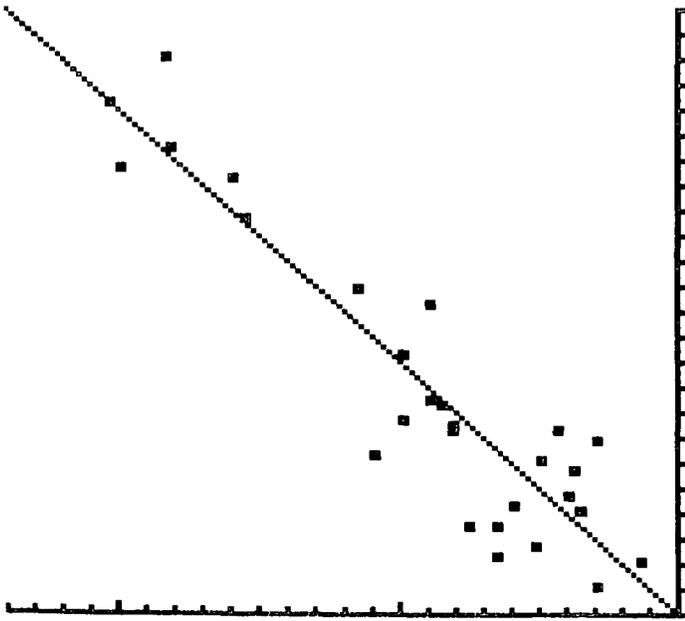


FIGURE 3. PREDICTION OF LN(MAXIMUM FLUIDITY) AT 400°C, INCLUDING PYROLYSIS DATA. Horizontal: $\ln(\text{predicted ddpm})$. Vertical: $\ln(\text{observed ddpm})$. Both scales 0 to 12. Independent variables: maximum vitrinite reflectance, THF-extractables, 4-5 min pyrolysis/GC signal. $R^2 = .847$ (29 coats).

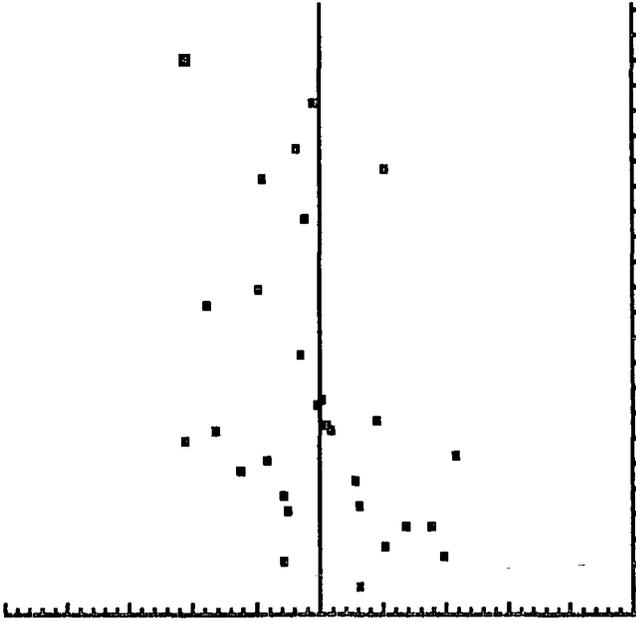


FIGURE 4. ANALYSIS OF RESIDUALS IN THE REGRESSION OF FIGURE 3. Horizontal: $\ln(\text{observed fluidity, ddpm})$, scale 0 to 12. Vertical: residuals from regression [observed - predicted], scale -5 to +5.