

New Correlations Between the Watson Characterization Factor ( $K_w$ )  
and Properties of Coal-Derived Materials

M.B. Perry and C.M. White

Division of Coal Science  
Pittsburgh Energy Technology Center  
P.O. Box 10940  
Pittsburgh, PA 15236

Introduction

Coal liquefaction products, like petroleum, are largely composed of hydrocarbons that are highly variable in properties depending on the feedstocks used and the processing conditions. In 1933, Watson and Nelson [1] emphasized that the value of physical property data on petroleum fractions is "... limited by the difficulty of correlating them into relationships of general applicability." Petroleum scientists and engineers have defined a set of mathematical and graphical expressions, or correlations, that permit the estimation of properties of these complex mixtures. Among these is a parameter termed the characterization factor ( $K_w$ ), introduced by Watson and Nelson in 1933 [1] to denote the "paraffinicity" of petroleum hydrocarbon fractions. The Watson characterization factor is defined as follows:

$$K_w = \frac{(T_b)^{1/3}}{S}$$

1)

where  $T_b$  is the mid-boiling point in degrees Rankine ( $^{\circ}R$ ) and  
 $S$  is the specific gravity at 60 degrees Fahrenheit ( $^{\circ}F$ ).

In addition to characterizing the "paraffinicity,"  $K_w$  has been used to estimate other properties. Watson and Nelson [1] demonstrated that  $K_w$  was useful for estimating the molecular weight and specific heat of petroleum fractions. Watson et al. [2] related  $K_w$  to percent hydrogen, kinematic viscosity, and critical temperature of petroleum-derived products. Smith and Watson [3] found  $K_w$  to obey mixing rules. More recently, Wilson et al. [4] demonstrated that  $K_w$  was useful for estimating the critical pressure of coal liquids.

Initially, coal scientists and engineers used the bank of correlations developed for petroleum to estimate the properties of coal liquefaction products; however, it is now accepted that estimation of properties of coal liquids from existing petroleum data can introduce large errors [5]. The deviations of properties from estimated values are believed to be caused by the higher concentration of polar compounds and by the more aromatic nature of coal liquids relative to petroleum. Since the Watson characterization factor was originally introduced to denote "paraffinicity," a high correlation with percent hydrogen and the atomic-hydrogen-to-carbon ratio is expected. That is, the contribution of aromatic constituents to the properties of the mixture should be contained in this characterization factor. Attempts to account for the contribution of polar constituents to the properties of complex mixtures are more difficult.

An assessment of the role of polar constituents in a coal liquid should ideally begin with a physical separation of the sample into functionally similar fractions. Methods used for the physical separation of coal-derived materials into chemical class fractions are numerous and varied, making the comparisons of data from the literature difficult. Because of the relatively high content of polar materials, sample components from coal-derived products may be adsorbed irreversibly onto liquid chromatographic stationary phase materials. Although specific detectors are necessary for making the fraction cuts, no suitable non-

destructive method is available for obtaining quantitative results for chemical class fractions using existing chromatographic detectors. Therefore, the fractions that are to be subjected to further characterization must be collected, the solvents removed, and the resulting fractions weighed to obtain quantitative results for the recovery of chemical class fractions. This is manpower-intensive and expensive, and can lead to imprecise results. High performance liquid chromatography (HPLC) eliminates some of the problems cited above. The speed and ease with which samples can be analyzed make HPLC appear as an attractive alternative to the more classical methods. Some major problems, however, still exist. To escape the need to pack the chromatographic column with new adsorbent after each separation, many HPLC methods require that only hexane-soluble materials are subjected to the chemical class separation; hexane insolubles are grouped into a broad, varied, and chemically undefined fraction called "asphaltenes." Asphaltenes from coal-derived materials may contain a high percentage of polar constituents that are not accounted for in polar class fractions. As mentioned previously, quantitation of the class fractions in these materials is difficult with most existing HPLC detectors. If correlations are found to be a function of the polar content of coal-derived materials, then it is necessary to characterize these constituents as carefully as possible if existing correlations are to be improved or new ones are to be developed.

This manuscript introduces a correlation between the Watson characterization factor and weight percent of polar constituents of narrow-boiling (50°F) distillate cuts of a coal-derived material from the H-Coal process. Similar correlations have been found for data previously reported by Gray et al. [5] for coal-derived distillate fractions from an SRC-II process. Finally, multiple linear least-squares treatment of the combined data from the H-Coal and SRC-II distillates correlates  $K_w$  with weight percent polars, atomic H/C, and mid-boiling point of the distillates. These new correlations relating the polar content of coal-derived liquids to the Watson characterization factor may be particularly significant because, as noted by Gray et al. [5], deviations of the observed properties of coal liquids from values predicted by correlations based on petroleum data are, in part, due to the higher concentration of polar materials in coal liquids. Therefore, any insight into the relationship between the polar content of coal liquids and other properties is valuable.

### Experimental

The H-Coal liquid was produced at the Catlettsburg H-Coal Pilot Plant on September 25, 1981, while processing Illinois No. 6 coal in the synfuel mode of operation. A blend of "light oil" and "heavy oil" products (1:1.5) was distilled by Chevron into narrow-range distillates (50°F), or pseudocomponents. Specifically, 50°F boiling-range fractions were obtained over the boiling range from 400°F to 850°F; the start to 400°F fraction and the 850°F vacuum bottoms were also obtained. The preparative liquid chromatographic separation procedure applied to the H-Coal samples was a modification of methods that have been reported previously [6,7,8,9]. Briefly, bases were first removed by a nonaqueous ion-exchange procedure [7], and the remaining acid-neutral fraction was separated by column chromatography with alumina [8]. This separation scheme produced fractions corresponding to saturates, neutral aromatics, neutral nitrogen compounds, nitrogen bases, and acids. In addition to the functional class separations, several chemical and physical measurements were made on these distillates.

### Determination of Bulk Properties

The mid-boiling point was determined by ASTM Method D-2887 [10]. Water was determined by the Karl Fischer method [11] using sodium tartrate dihydrate for standardization. Elemental analyses for carbon and hydrogen were performed as described by Houde et al. [12]. Specific gravity at 60°F was determined using a

pycnometer standardized with boiled deionized water. The atomic hydrogen/atomic carbon numbers were corrected to a dry basis using the Karl Fischer water results.

The multiple linear least-squares regressions, associated statistical parameters, and graphics were obtained on a PRO-350 (Digital Equipment Corporation) computer using a statistical software package, RS/1 (a trademark of BBN Research Systems in Cambridge, Mass.).

### Results and Discussion

A correlation does not necessarily imply a cause/effect relationship; rather, it only confirms an observed mathematical relationship for a given data set. If a correlation is found to be in agreement with measured values for a large population, it can be viewed as useful for general predictions of a given property. In the case of coal-derived materials, properties may vary as a function of the sampling point, the unit sampled, the process, and the feed coal used. The present investigation compares correlations with the Watson characterization factor from coal liquids derived from the SRC-II and H-Coal processes, both of which used bituminous feed coals. For reasons cited earlier, data from those samples significantly soluble in hexane are presented for comparison. Results from property measurements relevant to this manuscript are presented with the associated data for the correlations (Tables 1, 2, 3, and 4).

A correlation obtained using a multiple linear least-squares regression is evaluated for "goodness-of-fit" using several criteria. The software employed in this work (RS/1) prompts the operator to select the best fit that can be obtained from the input data. The best fit is characterized by having a coefficient of linear multiple determination ( $R^2$ ) close to one, a large F-Value (Regression Mean Square/Residual Mean Square), a low standard deviation, and a low significance level. Variables are selected or deleted from the multiple determination based on the partial correlation and significance level of that variable. This evaluation of property correlations with the Watson characterization factor employed comparable data from H-Coal distillates and SRC-II distillates. With noted exceptions, only the best fit, as described above, is reported.

#### Part I. Correlations of $K_w$ with H-Coal Data

A plot of  $K_w$  versus mid-boiling point (K) is given in Figure 1a, and a plot of weight percent polars (bases, acids, and neutral nitrogen compounds from Table 1) versus mid-boiling point is given in Figure 1b. The range of  $K_w$  values exhibited by these H-Coal distillates is small, 9.84 to 10.37. A comparison of these plots (Figure 1) reveals a negative correlation between total polars and  $K_w$ . A linear least-squares regression of weight percent polars versus  $K_w$  reveals a correlation coefficient (R) of -0.941, significant at the 99% confidence level for  $N = 7$ . The equation resulting from the regression is the following:

$$K_w = -0.0239 (\text{wt\% polars}) + 10.63 \quad 2)$$

A correlation based on a multiple linear regression including the H/C data with the weight percent polars versus  $K_w$  did not yield a good fit for predicting  $K_w$ ; the result of the regression is the following:

$$K_w = -0.0239 (\text{wt\% polars}) - 0.0109 (\text{H/C}) + 10.642 \quad 3)$$

The coefficient of linear multiple determination ( $R^2$ ) = 0.885 for the regression represented by Equation (3). If, however, the mid-boiling point (K) is introduced, a multiple linear least-squares fit to the same data correlates percent polars, mid-boiling point (K), and atomic H/C versus  $K_w$  with  $R^2 = 0.980$ . The multiple regression equation is the following:

$$K_w = -0.0199 (\text{wt}\% \text{ polars}) + 0.00265 (\text{mid-boiling point, K}) + 1.52 (\text{H/C}) + 7.12 \quad 4)$$

These data, including the observed, predicted, residual values, percent difference (%Δ), and associated statistical parameters, are given in Table 2.

#### Part II. Correlations with $K_w$ for Data from Distillates of SRC-II

In 1983, Gray and coworkers published a paper [5] and an extended report [13] that included the results of analyses of a series of 19 narrow-boiling distillate fractions of a product generated from SRC-II processing of Powhatan No. 5 Mine coal on Process Development Unit P-99 (located at Gulf's Research Center, Harmorville, Pa.). Chemical class fractions were obtained for each distillate fraction. Fluorescence Indicator Analysis (FIA) was applied to distillate fractions boiling below 589 K, yielding saturate, olefin, and total aromatic class fractions. "The polar fraction from FIA was calculated from three components: the phenolics content of the aromatics from a mass spectrometer analysis, nitrogen content, and sulfur content [5]." Preparative HPLC was used to separate the hexane-soluble portion of cuts boiling above 493 K into saturates and olefins, neutral aromatics, and polar aromatics. Hexane insolubles were grouped together as "asphaltenes." Results from property measurements relevant to this manuscript are presented with the associated data for the correlations (Tables 3 and 4).

A plot of  $K_w$  versus mid-boiling point (K) of the 14 distillate fractions considered is given in Figure 1a, and a plot of weight percent polars is given in Figure 1b. The range of values for  $K_w$  is larger than that for the H-Coal distillates, 9.76 to 11.74. The shape of the  $K_w$  plot appears to be slightly bimodal. As in the case of the H-Coal results (also Figure 1), comparison of the plots appears to reveal a negative correlation of total polars versus  $K_w$ . Note that the SRC-II case includes data from a much wider boiling range than was included in the H-Coal case. A linear least-squares treatment of the data derived from the SRC-II samples 1-7 in Table 3 (N=7, as in the H-Coal case) yields a correlation coefficient of -0.969, significant at the 99.9% confidence level, for weight percent polars versus  $K_w$ . However, if all 14 SRC-II distillates are included in a least-squares treatment of  $K_w$  with percent polars, the correlation coefficient is reduced to -0.5773, statistically significant at the 95% confidence level but useless for accurate property prediction. However, as shown below,  $K_w$  is not simply a function of polars present, and the dependence of  $K_w$  on other properties is more important as the boiling range covered by the pseudocomponents is increased. The resulting linear least-squares correlation for the 14 SRC-II distillates is given in Equation (5).

$$K_w = -0.0262 (\text{wt}\% \text{ polars}) + 10.87 \quad 5)$$

Equation (5), resulting from a linear least-squares treatment of the SRC-II data, is strikingly similar to Equation (2) resulting from the same treatment of the H-Coal data. A multiple linear least-squares regression of the data for the 14 SRC-II distillates correlates weight percent polars and atomic H/C versus  $K_w$  with  $R^2 = 0.9943$ . The multiple regression equation that fits the  $K_w$  data is the following:

$$K_w = -0.0118 (\text{wt}\% \text{ polars}) + 1.84 (\text{H/C}) + 8.03 \quad 6)$$

These data, including the observed, predicted, residual values, percent deviation, and associated statistical parameters, are given in Table 3. The resulting Equation (6), which represents a best fit of the SRC-II data, should be compared with Equation (3), which was a poor fit for the H-Coal data. Both data sets yield a negative correlation with total polars, but the dependence on H/C in this regression of the data is different.

Although Equation (6) represents the best fit of the SRC-II data, a good fit for the correlation of  $K_w$  with percent polars, H/C, and mid-boiling point (K) is given in Equation (7).

$$K_w = -0.0106 (\text{wt\% polars}) + 0.000651 (\text{mid-boiling-point, K}) + 2.05 (\text{H/C}) + 7.38 \quad 7)$$

The value of  $R^2$  was 0.995, and the F-Value was 605.8. A comparison of Equation (7) for SRC-II distillates and Equation (4) for the H-Coal distillates reveals the relative significance of each variable to the correlation with  $K_w$ .

### Part III. Correlations with $K_w$ for Combined H-Coal and SRC-II Data

The plots of  $K_w$  (Figure 1a) and weight percent polars (Figure 1b) versus mid-boiling point of the distillates reveal several similarities in these data sets. The  $K_w$  values are similar. In the range of mid-boiling points between 490 K and 550 K, the trends for weight percent polars are similar. The divergence of the trends for weight percent polars in the two data sets is suspect based on the similarity of  $K_w$  in the data sets. One plausible explanation can be found in the differences in the procedures used to isolate the polar fractions. Gray [13] reported 17.4% asphaltenes in the distillate cut at mid-boiling point 671.3 K. In the SRC-II case, these asphaltenes (hexane insolubles) were removed from the sample before the polars were isolated by preparative HPLC. Surely, the asphaltenes included polars as constituents that were not recovered. On the other hand, asphaltenes were not removed from the H-Coal distillates; instead, the entire sample was subjected to the complete separation scheme. The highest-boiling H-Coal distillate (mid-boiling point = 650.8 K) included in the combined data sets contained 6.9% hexane insolubles that would not have been analyzed for polars in the procedure used by Gray.

A multiple linear least-squares treatment of the combined data (combining 7 H-Coal distillates and 14 SRC-II distillates) correlates weight percent polars, mid-boiling point (K), and H/C versus  $K_w$  with  $R^2 = 0.987$ . The multiple regression equation that best fits the combined data is the following:

$$K_w = -0.00685 (\text{wt\% polars}) + 0.00278 (\text{mid-boiling point, K}) + 2.73 (\text{H/C}) + 5.28 \quad 8)$$

These data, including the observed and predicted values, are given in Table 4; the observed versus the predicted  $K_w$  are plotted in Figure 2.

### Conclusions

A negative correlation exists for the weight percent polar constituents versus  $K_w$  for distillates derived from these coal liquids. Undoubtedly,  $K_w$  is also a function of the aromatics present; but the contributions of the aromatic functionality should be contained in the H/C measurement. At least for these data sets, the weight percent of neutral aromatics does not change significantly in adjacent distillates, whereas significant concentrations of polars are confined to two distinct regions within the boiling range of the distillates (see Table 1).

The relative contributions of acids and bases to this correlation are difficult to assess. Gray and coworkers [5,13] did not separate these polar sub-fractions. However, a high correlation with polars, although not the same correlation, was found for the SRC-II data and for the H-Coal data. There is no reason to assume that the same correlation exists for acidic or basic components of the polar fraction. There is also no reason to assume that their relative contributions to  $K_w$  would not change from sample to sample. Changes in  $K_w$  attributed to the weight percent polars present may also reflect the degree of association

between the acidic and basic components. The role of both functional groups should be assessed.

It is unlikely that correlations that would be generally applicable to coal liquids can be extracted from only two data sets. However, the data sets presented were obtained on coal liquids produced from two different bituminous feed coals from different processes. Yet, an excellent correlation is found that fits the data for the characterization factor,  $K_w$ . Subbituminous feed coals may yield different fits for the Watson characterization factor.

#### Acknowledgments

We would like to acknowledge several coworkers for their contributions to this work, including Frank McCown who performed the separation of bases by non-aqueous ion exchange, Mike Ferrer who assisted in performing the alumina separations, and Joseph Hackett for performing the mid-boiling point determinations on the H-Coal distillates. We would also like to acknowledge Dennis Finseth and James Gray for illuminating discussions and advice.

A portion of the research on the H-Coal was performed while Mildred Perry was under appointment to the U.S. Department of Energy Post-Graduate Research Training Program administered by Oak Ridge Associated Universities.

#### Disclaimer

Reference in this report to any specific product, process, or service is to facilitate understanding and does not necessarily imply its endorsement or favoring by the United States Department of Energy.

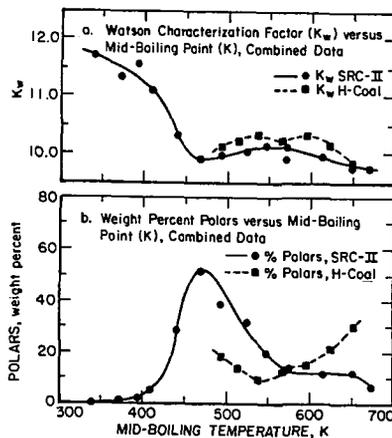


Figure 1 - Profile of  $K_w$  and Weight % Polars as a Function of Mid-Boiling Temperature (K) for Combined H-Coal and SRC-II Data.

### References

1. Watson, K.M., and Nelson, E.F. Ind. Eng. Chem., 1933, 25, 880.
2. Watson, K.M., Nelson, E.F., and Murphy, G.B. Ind. Eng. Chem., 1935, 27, 1460.
3. Smith, R.L., and Watson, K.M. Ind. Eng. Chem., 1937, 29, 1408.
4. Wilson, G.M., Johnston, R.H., Hwang, S.-C., and Tsonopoulos, C. Ind. Eng. Chem., Process Des. Dev., 1981, 20, 94.
5. Gray, J.A., Brady, C.J., Cunningham, J.R., Freeman, J.R., and Wilson, G.M. Ind. Eng. Chem., Process Des. Dev., 1983, 22, 410.
6. Perry, M.B., White, C.M., Finseth, D.H., Sprecher, R.F., and Retcofsky, H.L. Proc. NATO ASI Application of New Spectroscopic Techniques to Coal Science. B.M. Lynch, ed., Martinus Nijhoff Publishers, BV, Dordrecht, The Netherlands, to be published in 1985.
7. Green, J.B., Hoff, R.J., Woodward, P.W., and Stevens, L.L. Fuel, 1984, 63, 1290.
8. Later, D.W., Lee, M.L., Bartle, K.D., Kong, R.C., and Vassilaros, D.L. Anal. Chem., 1981, 53, 1612.
9. Schiller, J.E., and Mathiason, D.R. Anal. Chem., 1977, 49, 1225.
10. Annual Book of ASTM Standards, 1980, Part 24, 788-796.
11. Mitchell, J., Jr., and Smith, D.M. Aquametry, 2nd Ed., Part III, 1980, 5, 107-136.
12. Houde, M., Champy, J., and Furminieux, R. J. Micro Chem., 1979, 24, 300-309.
13. Gray, J.A. DOE Report DOE/ET/10104-7 (DE81025929), 1981.

Table 1.

Weight Percent of Various Compound Classes in H-Coal Distillates,  
Normalized to 100 Percent Recovery

Mid-Boiling Point, K	Saturates	Neutral Aromatics	Bases	Acids	Neutral Nitrogen
493.6	30.0	51.0	8.76	10.0	0.24
513.6	31.0	55.0	5.50	6.5	2.00
538.0	29.5	60.5	3.15	6.5	0.35
566.9	25.5	61.0	7.90	4.5	1.10
595.8	22.5	61.5	7.29	8.5	0.21
623.0	13.9	63.9	11.50	6.3	4.40
650.8	13.0	56.0	22.06	8.0	0.94

Table 2.

Results of Multiple Linear Least-Squares Regression of  $K_w$  Using Weight Percent Polars, Mid-Boiling Point, and Atomic H/C for H-Coal Distillates

$$K_w = -0.019876(\text{wt\% polars}) + 0.00265(\text{mid-boiling point, K}) + 1.521086(\text{H/C}) + 7.118681^a$$

Mid-Boiling Point, K	Weight Percent Polars	H/C (dry)	$K_w$ (observed)	$K_w$ (predicted)	Residual <sup>b</sup>	% $\Delta$ <sup>b</sup>
493.6	19.0	1.375	10.15	10.140	0.009	0.092
513.6	14.0	1.351	10.26	10.256	0.003	0.033
538.0	10.0	1.360	10.37	10.414	-0.044	0.429
566.9	13.5	1.235	10.25	10.231	0.018	0.182
595.8	16.0	1.277	10.34	10.322	0.017	0.173
623.0	22.2	1.198	10.17	10.150	0.019	0.189
650.8	31.0	1.076	9.84	9.864	-0.024	0.244

Variable Name	Coefficient Value	Standard Deviation	Sig. Level
Weight Percent Polars	-0.019876	0.003605	0.011745
Mid-Boiling Point, K	0.002650	0.000696	0.031869
H/C (dry)	1.521086	0.459905	0.045481

## Analysis of Variance Table

	Sum of Squares	DF	Mean Square	F Value	Sig. Level	Multi R <sup>2</sup>	Std Deviation of Regression
Regression	0.183857	3	0.061286	49.88	0.0016	0.9803	0.0351
Residual	0.003686	3	0.001229				

$$\% \Delta = (|\text{Residual}| / K_w \text{ observed}) \times 100$$

<sup>a</sup>Coefficients and constant term generated by RS/1 before adjusting to appropriate significant figures.

<sup>b</sup>Calculated before rounding off  $K_w$  (predicted).

Table 3.

Results of Multiple Linear Least-Squares Regression of  $K_w$  Using Percent Polars and Atomic H/C for SRC-II Distillates

$$K_w = -0.011807(\text{wt\% polars}) + 1.840546(\text{H/C}) + 8.028509^a$$

Mid-Boiling Point, K	Weight Percent Polars	H/C (dry)	$K_w$ (observed)	$K_w$ (predicted)	Residual <sup>b</sup>	$\% \Delta^b$
339.7	0.00	2.040	11.74	11.783	-0.045	0.387
372.4	1.60	1.846	11.36	11.408	-0.046	0.406
393.6	2.50	1.898	11.59	11.493	0.095	0.824
410.2	5.70	1.699	11.12	11.088	0.035	0.319
439.7	29.50	1.487	10.33	10.417	-0.085	0.824
468.6	52.00	1.353	9.92	9.905	0.012	0.129
493.0	39.55	1.316	9.99	9.985	0.002	0.028
524.7	32.40	1.279	10.05	10.001	0.053	0.527
547.4	20.95	1.315	10.16	10.201	-0.044	0.442
571.9	13.80	1.131	9.92	9.948	-0.032	0.328
573.0	14.45	1.208	10.13	10.082	0.050	0.497
615.2	12.10	1.090	9.96	9.892	0.062	0.630
650.2	12.85	1.027	9.76	9.767	-0.003	0.038
671.3	7.30	1.015	9.76	9.810	-0.055	0.564

Variable Name	Coefficient Value	Standard Deviation	Sig. Level
Weight Percent Polars	-0.011807	0.001115	0.0001
H/C (dry)	1.840546	0.051536	0.0001

Analysis of Variance Table

	Sum of Squares	DF	Mean Square	F Value	Sig. Level	Multi R <sup>2</sup>	Std Deviation of Regression
Regression	6.521707	2	3.260854	959.38	0.0001	0.9943	0.0583
Residual	0.037388	11	0.003399				

$$\% \Delta = (|\text{Residual}| / K_w \text{ observed}) \times 100$$

<sup>a</sup>Coefficients and constant term generated by RS/1 before adjusting to appropriate significant figures.

<sup>b</sup>Calculated before rounding off  $K_w$  (predicted).

Table 4.

Results of Multiple Linear Least-Squares Regression of  $K_w$  for Combined Data:  
SRC-II (Rows 1 to 14) and H-Coal (Rows 15 to 21)

$$K_w = -0.006847(\text{wt\% polars}) + 0.002776(\text{mid-boiling point, K}) \\ + 2.734032(\text{H/C}) + 5.279782^a$$

Sample No.	Weight Percent polars	H/C (dry)	Mid-Boiling Point, K	$K_w$ (observed)	$K_w$ (predicted)	Residual <sup>b</sup>	% $\Delta$ <sup>b</sup>
1	0.00	2.040	339.7	11.74	11.800	-0.062	0.533
2	1.60	1.846	372.4	11.36	11.351	0.010	0.096
3	2.50	1.898	393.6	11.59	11.546	0.042	0.369
4	5.70	1.699	410.2	11.12	11.024	0.099	0.891
5	29.50	1.480	439.7	10.33	10.363	-0.031	0.310
6	52.00	1.353	468.6	9.92	9.924	-0.006	0.066
7	39.55	1.318	493.0	9.99	9.977	0.010	0.102
8	32.40	1.279	524.7	10.05	10.013	0.040	0.407
9	20.95	1.315	547.4	10.16	10.251	-0.094	0.932
10	13.80	1.131	571.9	9.92	9.867	0.048	0.492
11	14.45	1.208	573.0	10.13	10.076	0.056	0.559
12	12.10	1.090	615.2	9.96	9.886	-0.069	0.701
13	12.85	1.027	650.2	9.76	9.805	-0.041	0.427
14	7.30	1.015	671.3	9.76	9.869	-0.113	1.161
15	19.00	1.375	493.6	10.15	10.279	-0.129	1.274
16	14.00	1.351	513.6	10.26	10.303	-0.043	0.423
17	10.00	1.360	538.0	10.37	10.423	-0.053	0.513
18	13.50	1.235	566.9	10.25	10.137	0.112	1.096
19	16.00	1.277	595.8	10.34	10.315	0.024	0.236
20	22.20	1.198	623.0	10.17	10.132	0.037	0.367
21	31.00	1.076	650.8	9.84	9.816	0.023	0.243

Variable Name	Coefficient Value	Standard Deviation	Sig. Level
Weight Percent Polars	-0.006847	0.001725	0.0010
H/C (dry)	2.734032	0.237914	0.0001
Mid-Boiling Point, K	0.002776	0.000667	0.0010

$$\% \Delta = (|\text{Residual}| / K_w \text{ observed}) \times 100$$

<sup>a</sup>Coefficients and constant term generated by RS/1 before adjusting to appropriate significant figures.

<sup>b</sup>Calculated before rounding off  $K_w$  (predicted).

Table 4. (Continued)

Analysis of Variance Table							
	Sum of Squares	DF	Mean Square	F Value	Sig. Level	Multi R <sup>2</sup>	Std Deviation of Regression
Regression	6.875659	3	2.291886	437.59	0.0001	0.9872	0.0724
Residual	0.089038	17	0.005238				

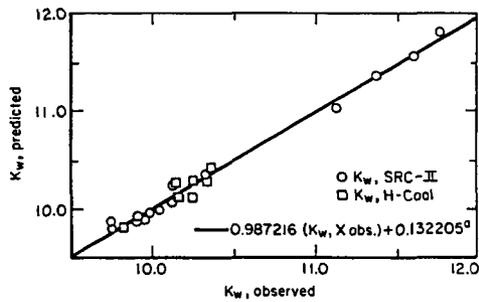


Figure 2 - Plot of  $K_w$  (observed) for Combined SRC-II and H-Coal Data versus  $K_w$  (predicted) by Multiple Regression).

<sup>a</sup>Equation for linear least-squares line of best fit.