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International Coal Refining Company
Allentown, Pennsylvania

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MASTER

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PARTICLE SIZE AND BULK DENSITY OF K-MAC

J. R. O'Leary*

Samples of Kerr-McGee ash concentrate (K-MAC) from Wilsonville were recently analyzed at Air Products' Linwood Laboratory and at GKT to determine the magnitude and cause of particle size and bulk density variations resulting from the following process operations:

- Normal 3-day run at steady operating conditions.
- Different runs, including low-SRC-recovery operation.
- Runs made with and without deashing solvent (DAS) injection.
- Runs using different ash concentrators.

The following conclusions can be drawn from the studies:

- The particle size variation over a 3-day period at constant conditions is small and within the accuracy of the sampling and analytical methods. GKT feels that the six samples they analyzed from the 3-day period were less variable than that expected from coal mine samples.
- Different runs exhibit substantial variations in particle size and bulk density. The median particle size of the samples analyzed varied from 16 to 67 microns.
- The particle size increases as the percent cresol insolubles in the K-MAC increase; this correlation is probably related to the viscosity of the first-stage heavy phase.

*International Coal Refining Co. (ICRC).

- ° Injecting DAS upstream of the letdown valve reduces the particle size of the K-MAC. More controlled experiments must be made to quantify the effect.
- ° The effect of the letdown vessel on K-MAC particle size is inconsistent.
- ° The compacted bulk density of the K-MAC (0.36 to 0.72 g/cm³) is roughly proportional to the particle size. Drying the K-MAC before analyses does not affect the bulk density of the material.
- ° The extremes of particle sizes are consistent with the range previously given to GKT for design purposes.
- ° The particle size measured by the GKT wet sieve technique is much finer than the particle size measured by the APCI Wet Microtrac technique for the same K-MAC samples. That this difference exists must be considered in future discussions with GKT concerning design particle size and particle size variation.

DEFINITION OF SAMPLES

In support of the GKT design efforts, approximately 50 samples of K-MAC were collected from Wilsonville runs 219 to 230 (an operating period from October 1980 to June 1981) and analyzed at the APCI Linwood Lab to determine the magnitude and cause of particle size and bulk density variations. The samples were selected to examine particle size variation associated with the following process operations:

- ° Normal 3-day period at steady operating conditions.
- ° Different runs, including low-SRC-recovery operation.

- ° Runs made with and without deashing solvent (DAS) injection.
- ° Runs using different ash concentrators.

To study the first process operation, 12 samples were collected over a 3-day material balance period during run 229 to determine both particle size and bulk density. Each sample was obtained from a separate drum on a predetermined time schedule. Six of the samples were also sent to GKT to be analyzed by their methods. To study the second process operation, composite samples were obtained for all material balances (MB) over the 9-month period from October 1980 to June 1981. Only a particle size analysis was done on these samples. To study the third process operation, triplicate samples from two different operating periods were selected with and without DAS injection at otherwise identical operating conditions. Both bulk density and particle size analyses were carried out. To study the fourth process operation, samples were taken from the continuous and batch ash concentrators during the same operating periods. The triplicate samples at the two operating conditions mentioned above were also used for this study. Table 1 summarizes the samples obtained.

SAMPLING AND ANALYTICAL METHODS

Most K-MAC samples were scooped from the top of the specified drums and shipped to APCI's Linwood Lab in quart cans; GKT samples were shipped in gallon cans. MB samples used in study 2 were composites from the top of each drum collected during material balance runs. To determine if the samples were representative of the entire drum, nine samples were systematically taken from a well-handled drum and analyzed. The median particle size of all nine samples agreed within ± 3 microns (Table 2), which is the normal precision of the analytical technique. Therefore, the scooping technique was assumed adequate.

Particle size was determined by the Wet Microtrac particle analyzer, which uses a laser light source to optically measure the particle size of the K-MAC, slurried in water. Each injected sample was analyzed twice. One sample of K-MAC was analyzed for particle size

distribution five times to determine the reproducibility of the method. That is, five samples were removed from the quart-can sample and separately injected into the Wet Microtrac analyzer, which then analyzed each of the five samples in duplicate. The median particle size of the samples was within ± 3 microns (Table 3).

Packed bulk density was obtained by using a simple machine tapping device. The K-MAC was poured into a cylinder mounted on the rotary device that tapped the sample several thousand times. The weight and final volume were then used to determine the bulk density. Bulk density of a single sample was also analyzed five times. The reproducibility was $\pm 0.007 \text{ g/cm}^3$, as shown in Table 3.

GKT analyzed their samples by using a wet sieve for particle size and a comparable packed density device.

RESULTS AND CONCLUSIONS

Study 1

Table 4 and Figure 1 summarize the analyses of the 12 samples obtained during the 229AB material balance. Numbers in parentheses are the result of selective reruns. Figure 2 shows the range of particle-size distributions for the 12 samples, as well as the extremes of particle sizes measured in study 2.

Several conclusions can be drawn from these data:

- The range of particle sizes for the 12 samples is within the normal precision of the sampling and analytical methods.
- The APCI Microtrac analyzer measures a significantly coarser particle size than does the GKT wet sieve for the same sample.
- The APCI packed-bulk density shows substantial variability.

As reported earlier (Wilkins and Reighard, 1981), GKT personnel were astonished at the homogeneous nature of material they analyzed, and commented that the data were less variable than that expected from coal mine samples. All material as received suggested that particle size classification was not required.

The data therefore indicate that particle size fluctuations are not a major concern as long as the plant is running at steady conditions. It is recommended that extreme care be used in baseline, contact, and design discussions with GKT concerning particle size, since their results and those of ICRC are different.

It was suggested that the bulk density fluctuations measured at Linwood may have been caused by varying moisture/DAS content in the samples. To better understand the effect of moisture/DAS content, the two extreme samples (points 4 and 6 on Figure 1) were reanalyzed as received, after drying and after humidifying to 2% moisture. Table 5 clearly indicates that drying of the sample did not affect the bulk density. More work must therefore be done to explain the variability.

Study 2

Although particle size distribution during steady-state operation varied little, distribution during different runs varied substantially. Table 6 summarizes available data from the different material balance samples. The median particle size ranged from 16 microns during run 230 to 67 microns during run 227CD. These extremes are also shown in Figure 2.

Based on previous literature review, viscosity of the heavy phase before pressure letdown was considered one of the possible key variables affecting particle size.¹ Since no direct measurement of heavy-phase viscosity was available, evaluation focused on the cresol-insoluble portion of the K-MAC, since that is indirectly related to the solids content and thus the viscosity of the heavy phase. Figure 3 plots the median particle size against the cresol-insoluble material of the K-MAC. Although there is scatter in the data, it is evident that the higher the solids loading (higher viscosity) the larger the particle size. Figure 4 shows the same effect with weight % particles less than 88 microns.

To better understand the effect of viscosity on particle size, the installation of a viscosity indicator in the first-stage underflow at Wilsonville has been discussed. The indicator will not give a true

¹Memo to G. C. Rappe (ICRC), July 30, 1981.

viscosity, but may give a correlatable number for predicting particle size. An on-line particle size analyzer is also being reviewed for possible installation at Wilsonville to aid in this effort.

The major conclusion from study 2 is that the processing conditions in the SRC liquefaction and CSD units do affect the particle size of the K-MAC, which necessitates the development of an on-line means of predicting the magnitude of changes in particle size. One favorable result of this study is that the extremes generated are consistent with the extremes that have been used for the past year in the GKT design work.

Study 3

DAS injection into the first-stage underflow to cool the K-MAC and produce a dry, free-flowing powder has been proposed for the demonstration plant. Study 3 was designed to determine the effect of this injection on the particle size. It should be remembered when reviewing these results and the results of study 4 that the samples were not generated during controlled tests to specifically study the effects of DAS injection. Rather, the samples were collected from material remaining from earlier tests during which operating conditions other than DAS injection may have varied. Consequently, all the results are not consistent. Table 7 summarizes the data obtained for studies 3 and 4. The asterisked data seem to be out-of-line. DAS injection data from Table 7 are averaged and summarized in Table 8. The data suggest that DAS injection does lower the particle size of the K-MAC. This is expected since the DAS probably lowers the viscosity of the underflow stream and causes more turbulence at and downstream of the letdown valve. Additional controlled experiments have recently been run at Wilsonville when DAS injection was varied over a wide range at otherwise constant conditions. These results are not yet available. In addition to its cooling effect, DAS injection may diminish viscosity variations and yield a more constant particle size. Future testing is required to support this theory.

Study 4

At Wilsonville, the first-stage heavy phase can flow from the letdown valve to one of two vessels. The continuous ash concentrator

consists of a relatively large-diameter vessel into which the letdown stream flashes. The batch ash concentrator has a much smaller diameter. The inlet to both vessels is tangential. If agglomeration of the K-MAC affects the final particle size, then the smaller vessel should yield a larger diameter particle. Therefore, study 4 was proposed as a possible means of determining agglomeration effects. The same data used in study 3 were used in this study (Table 7). These data are averaged and summarized in Table 9 to show the ash concentrator effect; it is evident that the results are inconsistent, and that more controlled studies are required to establish whether there is an effect.

All samples from studies 3 and 4 and the samples from runs 220 and 230 were also analyzed for bulk density. Figure 5, which is a plot of all bulk density data as a function of particle size, shows a rough correlation between larger particle size and higher bulk density.

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Table 1
Summary of Samples

Date	Wilsonville run no.	Samples	Vessel	Process study
July 6	230	3	batch	2
June 16-18	229AB	12	continuous	1
May 30-31	228AB	1	continuous	2
May 7	227G	3	continuous	3,4
		3	batch	3,4
May 3-4	227E	1	continuous	2
April 15-17	227CD	3	continuous	3,4
		3	batch	3,4
April 14-15	227A	1	continuous	2
Feb 15	225I	1	continuous	2
Feb 12-13	225G	1	continuous	2
Feb 11-12	225F	1	continuous	2
Jan 30-31	225BC	1	continuous	2
Jan 1-4	222ABC	1	continuous	2
Dec 27	221G	1	continuous	2
Dec 19-21	221ABC	1	continuous	2
Nov 7-9	220DE	3	continuous	2
Oct 28-29	220AB	3	continuous	2
Oct 20-21	219AB	1	continuous	2

Table 2
Particle Size Throughout Single Drum

Sample location	Particle size at stated % (μ)		
	90%	50%	10%
top - right	68	28	7
middle - right	63	26	6
bottom - right	59	25	5
top - center	64	26	7
middle - center	74	31	8
bottom - center	66	26	6
top - left	69	28	6
middle - left	61	26	6
bottom - left	66	27	7

Table 3

Precision of Linwood Methods

a. Wet Microtrac analyzer (Sample 227G)

Sample no.	Median particle size (μ)		
	1st analysis	2nd analysis	Avg
1	27.4	27.7	27.6
2	30.7	30.4	30.6
3	26.3	22.7	24.5
4	31.2	29.7	30.5
5	27.3	27.9	<u>27.6</u>
			28.2 Avg

b. Packed bulk density (Sample 229B)

Sample no.	Packed bulk density (g/cm^3)
1	0.351
2	0.345
3	0.348
4	0.354
5	<u>0.358</u>
	0.351 Avg

Table 4

Summary of Steady-State Results from
K-MAC Study 1^a

Date	Time	APCI	GKT	Particle size		Bulk density (g/cm ³)
		sample no.	sample no.	50% (μ)	<88 μ (%)	
6/16/81	0455	71526	71529A	30	89	0.444
6/16/81	0555	71526F	71529B	34(30) ^b	83(91)	0.415
6/16/81	0655	71526B	71529	29	88	0.409
6/16/81	0755	71526E	-	26	92	0.445
8/17/81	1400	71526D	-	27	90	0.388
6/17/81	1500	71527D	-	28	91	0.360
6/17/81	1600	71527B	-	30	92	0.382
6/17/81	1700	71527C	-	21(25)	100(91)	0.436
6/18/81	1900	71527A	71528B	28	87	0.394
6/18/81	1950	71526C	71528	24(30)	100(92)	0.391
6/18/81	2045	71527	-	26	92	0.379
6/18/81	2140	71526A	71528A	<u>28</u> 27.6	<u>91</u> 91	0.395

^aLinwood results from analysis of Wilsonville run no. 229AB.

^bParenthetical value is the result of sample reanalysis.

Table 5
Effect of Drying/Humidification
on K-MAC Bulk Density

Sample condition	Packed bulk density (g/cm ³)	
	Sample no. 71526E	Sample no. 71527D
As received initially	0.445	0.360
As received retested	0.429	0.362
After drying	0.425	0.361
After humidifying to 2%	0.449	0.398

Table 6

Summary of Material Balance Results from
K-MAC Study 2

APCI sample no.	Wilsonville run no.	Particle size		% cresol insoluble ^b
		50% (μ)	<88 μ (%)	
61638	219AB	56	72	69.1
71525-B	220AB	59 ^a	68	69.2
62534-B	220DE	49 ^a	75	70.4
63315	221ABC	32	87	67.5
63550	221G	37	89	64.3
64106	222ABC	27	93	63.2
64985	225BC	34	84	68.3
65601	225F	45	84	67.0
65931	225G	28	88	64.0
65783	225I	36	81	66.2
67245	227A	49	69	69.8
61519-B	227CD	52 ^a	74	66.1
68346	227E	48	74	65.2
69661	228AB	35	81	67.4
71526-F	229AB	28 ^a	91	65.0
71521-B	230	18 ^a	98	63.3

^a Average of 3 or more samples.

^b DAS-free K-MAC.

Table 7

Summary of DAS Injection and Letdown Vessel Results from
K-MAC Studies 3 and 4

APCI sample no.	Wilsonville run no.	Ash concentrator	DAS inj	Particle size 50% (μ)	<88 μ (%)	Bulk density (g/cm ³)
71519	227CD	continuous	no	55	74	0.549
71519A	227CD	continuous	no	52	70	0.549
71519B	227CD	continuous	no	<u>50</u>	<u>77</u>	<u>0.505</u>
				53	74	0.534
71524	227CD	batch	no	67	65	0.625
71524A	227CD	batch	no	59	64	0.640
71524B	227CD	batch	no	<u>39</u> ^a (40) ^b	<u>83</u> ^a (78)	<u>0.542</u> ^a
				55	71	0.602
71523	227G	continuous	yes	31*	85*	0.539
71523A	227G	continuous	yes	49	73	0.531
71523B	227G	continuous	yes	<u>47</u>	<u>75</u>	<u>0.437</u> *
				42	78	0.502
71522	227G	batch	yes	28	84	0.591
71522A	227G	batch	yes	24	91	0.566
71522B	227G	batch	yes	<u>41</u> *(35)	<u>80</u> (82)	<u>0.537</u>
				31 (29)	85(86)	0.565
70536		continuous	no	28	89	
71128		batch	no	42	64	

^aAsterisk indicates values that are out-of-line.

^bParentetical value is the result of sample reanalysis.

Table 8

Effect of DAS Injection
on K-MAC Particle Size

DAS injection	Median particle size	
	Case 1	Case 2
Yes	42	29
No	53	55

Table 9

Effect of Ash Concentrator
on K-MAC Particle Size

DAS injection	Median particle size		
	Case 1	Case 2	Case 3
Continunus	42	53	28
Batch	30	55	42

Figure 1
K-MAC Properties Fluctuation at Steady Process Operation
(Run 229 MB)

Figure 2
Extremes of Particle Size in K-MAC Samples
Analyzed by Wet Microtrac Technique
(Wilsonville Run Nos. 219-230)

Figure 3
Particle Size vs. % Cresol Insolubles

Figure 4
K-MAC Particle Size vs. % Cresol Insolubles

Figure 5
Bulk Density vs. Median Particle Size

IMPACT OF SRC RECYCLE ON PLANT DESIGN

D. Kang* and D. H. S. Ying*

ICRC is conducting an experimental program to examine the effect of recycling solvent-refined coal (SRC) on dissolver performance under various process conditions. In addition, the program is attempting to develop accurate recycle-run data required to determine solvent balance during integrated recycle runs. The program was initiated in October 1981 to expand the existing data base on the effect on liquefaction of recycling light SRC (LSRC) and to determine the impact on the design and operation of the SRC-I Demonstration Plant. The program continues work from an earlier study in which a closed-loop experiment, designed to accurately measure solvent balance, was not completely successful because of the poor performance of the recycle still.

During this quarter, a numerical simulation of SRC recycle using the sequential kinetic model has been conducted. The results of this study indicate that the rate constants developed from the base-line data set for no SRC recycle are inadequate to describe the SRC recycle data. The model underestimates the preasphaltene yield but overestimates the asphaltenes yield. Although the model also predicts that oil yield strongly depends on process temperature, this prediction conflicts with the experimental results. Therefore, an experimental plan for future LSRC recycle runs has been restructured to cover broader experimental conditions.

SIMULATED SRC RECYCLE RUNS

During this reporting period, a numerical simulation of SRC recycle runs has been conducted by using the sequential reaction kinetic model.

*International Coal Refining Company (ICRC).

The purpose of this study was to evaluate the prediction of yield distribution to provide guidelines for a future experimental program.

The simulation study covered three concentrations (0, 15, and 25%) of both light SRC (LSRC) and heavy SRC (HSRC) in the recycle solvent through a temperature range of 750-880°F. The yield-distribution prediction was compared with the experimental data for the BCL-29 SRC recycle run (Kang and Givens, 1981a) made from Kentucky #9 coal, as shown in Figures 1 to 10. The operating conditions of this SRC recycle run and the coal composition are summarized as follows: 2,000-psig pressure; 780-840°F temperature; 40-min residence time; 0, 15, and 25% SRC concentration in solvent; 38 wt % slurry concentration; 10% coal mineral matter; 96% organic matter in reactive coal; and 15 wt % pre-asphaltenes in feed coal.

The composition of SRC is summarized below:

	<u>LSRC</u>	<u>HSRC</u>
Solvent	22.3	-
Oil	7.1	1.2
Asphaltenes	65.2	58.6
Preasphaltenes	5.0	40.2

For a detailed discussion of SRC composition, refer to Kang and Givens (1981a). Solvent was determined from the simulated distillation data of pentane-soluble oils (Kang and Givens, 1980).

Three different sets of kinetic parameters derived from different data bases were used to examine the effect of varying the type and concentration of SRC on the yield structure. The first set of rate constants (K-Ky #9) shown in Table 1 was based on the liquefaction of Kentucky #9 coal in Wilsonville recycle solvent (WRS).¹ The second set of constants (K-default), shown in Table 2, was derived from liquefying Kentucky #9/14 coal in a synthetic solvent consisting of a mixture of hydrotreated creosote oil and creosote oil (Martin, 1979). The third set of rate constants (K-SRC), shown in Table 3, was determined from data from the SRC recycle run of Kentucky #9 coal, WRS, Kerr-McGee ash

¹R. Sivasubramanian, ICRC, personal communication.

concentrate (K-MAC), and SRC. Both LSRC and HSRC were used in developing the third set of constants.

The sequential kinetic model predicts that increased recycling of LSRC or HSRC increases the oil yield but reduces asphaltene and pre-asphaltene yields for all three sets of rate constants tested. For example, by injecting 15% LSRC in the recycle solvent at 840°F and 40-min residence time, the kinetic model predicts a 9% increase in net oil yields from Kentucky #9 coal. A 25% increase in LSRC concentration results in an additional 7% net increase in oil. The predicted effects of adding LSRC during liquefaction of Kentucky #9/14 coals are similar to those when Kentucky #9 is liquefied, but the increase in oil yield is smaller. In general, the experimental data follow these trends: increasing oil yield but decreasing asphaltene and preasphaltene yields as SRC-recycle concentrations increase. However, Figures 1 to 10 show that the kinetic model fails to fit the absolute values of most experimental data.

The predicted effect of process temperature heavily depends on which rate-constant data base is used. According to the first set of rate constants (K-Ky #9), asphaltene yield from Kentucky #9 coal increases slightly between 750 and 810°F and then decreases rapidly at higher temperatures, as shown in Figure 2. In contrast, the second set of rate constants (K-default) predicts that asphaltene yield from Kentucky #9/14 coals increases as temperature increases (750-870°F), although the increase becomes less profound for higher SRC concentrations. Preasphaltene yield, however, always decreases with increasing process temperature. Furthermore, the sequential kinetic model predicts that recycling HSRC will yield more oils and fewer asphaltenes and preasphaltenes than recycling LSRC under all process conditions, except when temperature is below 810°F and Kentucky #9 coal is used.

Comparing experimental data with values predicted by the model shows that the model significantly underestimated preasphaltene yields, whereas it overestimated asphaltene yields. Whereas the model using the base-line kinetic constants (K-Ky #9) predicts that oil yield strongly depends on temperature, experimental oil yields from SRC recycle runs (BCL-29) with Kentucky #9 coal were only weakly influenced

by this variable. Contrary to the model's prediction, oil yields occasionally decreased as temperature increased, especially at high SRC-recycle rates (Figure 3). In all cases, the predicted values depart greatly from the experimental data at high temperature.

Better agreement was obtained between experimental data from the SRC recycle run and model prediction by using the third set of rate parameters, as shown in Figures 7 to 9. Although the agreement has improved considerably, the model slightly underestimates preasphaltene yields at higher temperatures, asphaltene yields at lower temperatures, and oil yields at higher SRC-recycle concentrations. Without SRC recycle, oil yield is a strong positive function of temperature. At low SRC recycle rates, the yields are a weak function of temperature, whereas, at high SRC recycle rates, temperature has a negative influence on yields. More data are needed to arrive at a firm conclusion about the adequacy of the sequential kinetic model to predict the yield from SRC recycle.

In addition, simulating steady-state SRC recycle² with the sequential kinetic model shows that negligible changes in yield distribution occur between the first and second passes of SRC recycle runs and that steady state arrives within two passes of SRC recycle (Table 4). Again, these results conflict with those from the experimental data of multiple-pass recycle runs (BCL-34 and BCL-35) in which significant changes of yield data were observed (Kang and Givens, 1981b).

This study clearly shows that we need more extensive data on SRC-recycle runs to expand our fundamental understanding of the kinetic behavior of coal/SRC mixtures. In the future, the kinetic model should describe not only base-line runs, but also recycle runs.

²J. S. Zabrenski. Internal memorandum to K. S. Upadhye. SRC dissolver simulation. June 18, 1980.

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Table 1

Rate Constant Data Based on
Kentucky #9 Coal Base-Line Data Set, K-Ky #9 Values^a

Conversion	Constant
Coal to preasphaltenes	$K = 7.143 \times 10^{-5} \exp[-1.765 \times 10^4 / (T + 459.69)]$
Preasphaltenes to asphaltenes	$K = 3.134 \times 10^3 \exp[-1.452 \times 10^4 / (T + 459.69)]$
Preasphaltenes to C ₁ -C ₄ gases	$K = 1.508 \times 10^8 \exp[-3.477 \times 10^4 / (T + 459.69)]$
Asphaltenes to heavy distillate	$K = 6.543 \times 10^8 \exp[-3.154 \times 10^4 / (T + 459.69)]$
Asphaltenes to C ₁ -C ₄ gases	$K = 1.508 \times 10^8 \exp[-3.477 \times 10^4 / (T + 459.69)]$
Heavy distillate to kerosene	$K = 0.0 \exp[-1.093 \times 10^4 / (T + 459.69)]$
Heavy distillate to C ₁ -C ₄ gases	$K = 1.508 \times 10^7 \exp[-3.477 \times 10^4 / (T + 459.69)]$
Kerosene to light oil	$K = 0.0 \exp[-1.893 \times 10^4 / (T + 459.69)]$
Kerosene to C ₁ -C ₄ gases	$K = 2.215 \times 10^7 \exp[-3.236 \times 10^4 / (T + 459.69)]$
Light oil to C ₁ -C ₄ gases	$K = 2.215 \times 10^7 \exp[-3.236 \times 10^4 / (T + 459.69)]$
Organic sulfur to sulfur in SRC	$K = 1.742 \times 10 \exp[-1.1640 \times 10^4 / (T + 459.69)]$
Initial oxygen to oxygen in preasphaltenes	$K = 1.742 \times 10 \exp[-1.164 \times 10^4 / (T + 459.69)]$

^aReaction rate constants are defined as $K = A \exp[-E/R(T + 459.69)]$ with the following units: E is Btu/lb-mol; R is Btu/(lb-mol. °F); T is °F; A is min⁻¹; and K is min⁻¹.

Table 2

Rate Constant Data Based on
Kentucky #9/14 Coal, K-Default Values^a

Conversion	Constant
Coal to preasphaltenes	$K = 7.143 \times 10^{-5} \exp[-1.765 \times 10^4 / (T + 459.69)]$
Preasphaltenes to asphaltenes	$K = 3.115 \times 10^3 \exp[-1.515 \times 10^4 / (T + 459.69)]$
Preasphaltenes to C ₁ -C ₄ gases	$K = 2.215 \times 10^7 \exp[-3.236 \times 10^4 / (T + 459.69)]$
Asphaltenes to heavy distillate	$K = 1.939 \times 10^2 \exp[-1.275 \times 10^4 / (T + 459.69)]$
Asphaltenes to C ₁ -C ₄ gases	$K = 2.215 \times 10^7 \exp[-3.236 \times 10^4 / (T + 459.69)]$
Heavy distillate to kerosene	$K = 2.365 \times 10 \exp[-1.093 \times 10^4 / (T + 459.69)]$
Heavy distillate to C ₁ -C ₄ gases	$K = 2.215 \times 10^7 \exp[-3.236 \times 10^4 / (T + 459.69)]$
Kerosene to light oil	$K = 2.956 \times 10^3 \exp[-1.893 \times 10^4 / (T + 459.69)]$
Kerosene to C ₁ -C ₄ gases	$K = 2.215 \times 10^7 \exp[-3.236 \times 10^4 / (T + 459.69)]$
Light oil to C ₁ -C ₄ gases	$K = 2.215 \times 10^7 \exp[-3.236 \times 10^4 / (T + 459.69)]$
Organic sulfur to sulfur in SRC	$K = 1.674 \times 10^4 \exp[-1.650 \times 10^4 / (T + 459.69)]$
Initial oxygen to oxygen in preasphaltenes	$K = 1.021 \times 10^4 \exp[-1.611 \times 10^4 / (T + 459.69)]$

^aReaction rate constants are defined as $K = A \exp[-E/R(T + 459.69)]$ with the following units: E is Btu/lb-mol; R is Btu/(lb-mol. °F); T is °F; A is min⁻¹; and K is min⁻¹.

Table 3

Rate Constant Data Based on
SRC Recycle Run of Kentucky #9 Coal, K-SRC^a Values^a

Conversion	Constant
Coal to preasphaltenes	$K = 6.723 \times 10^{-3} \exp[+4.749 \times 10^4 / (T + 459.69)]$
Preasphaltenes to asphaltenes	$K = 5.053 \times 10^6 \exp[-2.516 \times 10^4 / (T + 459.69)]$
Preasphaltenes to C ₁ -C ₄ gases	$K = 1.114 \times 10^8 \exp[-3.389 \times 10^4 / (T + 459.69)]$
Asphaltenes to heavy distillate	$K = 3.793 \times 10^{-2} \exp[-3.368 \times 10^3 / (T + 459.69)]$
Asphaltenes to C ₁ -C ₄ gases	$K = 1.114 \times 10^{-8} \exp[-3.389 \times 10^4 / (T + 459.69)]$
Heavy distillate to kerosene	$K = 0.0 \exp[-1.093 \times 10^4 / (T + 459.69)]$
Heavy distillate to C ₁ -C ₄ gases	$K = 1.114 \times 10^8 \exp[-3.389 \times 10^4 / (T + 459.69)]$
Kerosene to light oil	$K = 0.0 \exp[-1.893 \times 10^4 / (T + 459.69)]$
Kerosene to C ₁ -C ₄ gases	$K = 2.215 \times 10^7 \exp[-3.236 \times 10^4 / (T + 459.69)]$
Light oil to C ₁ -C ₄ gases	$K = 2.215 \times 10^7 \exp[-3.236 \times 10^4 / (T + 459.69)]$
Organic sulfur to sulfur in SRC	$K = 2.459 \times 10^2 \exp[-1.030 \times 10^4 / (T + 459.69)]$
Initial oxygen to oxygen in preasphaltenes	$K = 7.201 \times 10^7 \exp[-2.738 \times 10^4 / (T + 459.69)]$

^aReaction rate constants are defined as $K = A \exp[-E/R(T + 459.69)]$ with the following units: E is Btu/lb-mol; R is Btu/(lb-mol. °F); T is °F; A is min⁻¹; and K is min⁻¹.

Table 4

Yield Data from the Steady-State SRC Simulation Model^a

	Base line (wt %)	SRC recycle, percentage of solvent			
		15% LSRC		30% LSRC	
		1st pass	2nd pass	1st pass	2nd pass
Conversion	93.83	93.83	93.83	93.83	93.83
Unconverted coal	6.17	6.17	6.17	6.17	6.17
Preasphaltenes	32.81	32.61	32.79	32.41	33.06
Asphaltenes	33.53	27.21	26.97	20.90	20.09
Oils	22.77	29.28	29.31	35.78	35.92
Hydrocarbon gases	3.95	3.75	3.75	3.75	3.75
Other gases	0.99	0.99	0.99	0.99	0.99

^a Conditions were: reactor = CSTR, temperature = 840°F, residence time = 40 min, and rate constants = Kentucky #9 coal base-line data set from Table 1. The simulation model was described in an earlier report (J. S. Zabrenski; see footnote 2 to text).

Figure 1
Predicted vs. Observed Yields of Preasphaltenes by Using
Rate Constants Based on Kentucky #9 Coal Base-Line Data

Figure 2
Predicted vs. Observed Yields of Asphaltenes by Using
Rate Constants Based on Kentucky #9 Coal Base-Line Data

Figure 3
Predicted vs. Observed Yields of Oils by Using
Rate Constants Based on Kentucky #9 Base-Line Data

Figure 4
Predicted vs. Observed Yields of Asphaltenes by Using
Rate Constants Based on Kentucky #9/14 Coal Base-Line Data

Figure 5
Predicted vs. Observed Yields of Preasphaltenes by Using
Rate Constants Based on Kentucky #9/14 Coal Base-Line Data

Figure 6
Predicted vs. Observed Yields of Oils by Using Defaulted
Rate Constants Based on Kentucky #9/14 Coal Base-Line Data

Figure 7
Predicted vs. Observed Yields of Asphaltenes by Using
Rate Constants Based on Recycled Kentucky #9 Coal Data

Figure 8
Predicted vs. Observed Yields of Preasphaltenes by Using
Rate Constants Based on Recycled Kentucky #9 Coal Data

Figure 9
Predicted vs. Observed Yields of Oils by Using
Rate Constants Based on Recycled Kentucky #9 Coal Data

Figure 10
Simulated Distillation Curve for LSRC Oil