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Supplement for the Period July—September 1980

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International Coal Refining Company
Allentown, Pennsylvania

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International Coal Refining Company
Allentown, Pennsylvania

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EFFECTS ON LIQUEFACTION OF RECYCLING HEAVY SRC

by D. Kang
and E. N. Givens*

To avoid the possibility of solvent shortages in the Demonstration Plant, studies are continuing to determine if recycling SRC will generate an increased yield of recycle solvent and maintain adequate solvent quality for the plant design. During part of this 2-year investigation, we hope to determine if major operational problems may develop with SRC recycle.

The first in a series of investigations using Air Products' Coal Process Development Unit (CPDU), which simulates Demonstration Plant conditions, was detailed in the last Quarterly Report.[1] That study focused on tests using mixtures of light solvent refined coal (LSRC).

The present study ran similar tests, this time processing mixtures of Kentucky #9 coal, solvent, and heavy solvent refined coal (HSRC). To ascertain the effects of HSRC on coal liquefaction, process runs were made with HSRC/solvent, coal/solvent, and coal/HSRC/solvent. The HSRC was composed of 1% oils, 44% asphaltenes, and 55% preasphaltenes; its hydrogen content was lower than that of the LSRC produced during the same run (5.8 vs. 6.8%).

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A systematic study of HSRC recycle required the use of solvents with varying properties, so two solvents with different hydrogen contents, creosote oil (CO, hydrogen poor) and hydrotreated creosote oil (HTCO, hydrogen rich) were initially examined.

Another run has already started, in which Wilsonville recycle solvent is blended with either 15 or 25% LSRC or HSRC and processed with 38% Kentucky #9 coal at 780 and 840°F to simulate natural conditions. Results of these runs will be published in a subsequent report.

Over the 2-year period, in addition to evaluating the recycling of LSRC and HSRC in regard to SRC conversion and solvent yield, the investigation will study its impact on hydrogen consumption and solvent quality.

CONCLUSIONS

HSRC is difficult to convert, either alone or as a component in the coal slurry using HTCO as solvent. The effect on oil yield with HSRC is indiscernible at the conditions studied, within experimental error ranges. The later experimental results using CO as solvent strongly suggest that the solubility of HSRC in feed solvent played an important role, since HSRC was mainly composed of preasphaltenes, which are not easily soluble in relatively nonpolar HTCO. The high sensitivity of HSRC conversion to its concentration in HTCO indicates that addition of HSRC modifies drastically the solubility characteristics of the feed solvent.

Using both CO and HTCO as solvents clarified many of the results from the HSRC recycle runs. HSRC was found to be highly temperature-sensitive, both alone and as a solvent component in the coal slurry feed. CO has better solvency of HSRC than HTCO, although it contains less donatable hydrogen. These characteristics favor a substantial decrease in optimal process temperature yet drastically improve overall yield distribution.

We can summarize the following conclusions regarding HSRC recycle:

- Solubility considerations of HSRC in feed solvent were much more important than those of LSRC.
- Oil yield increased at favorable conditions.

- Asphaltene yield decreased.
- Preasphaltene yield decreased at favorable conditions.
- Formation of light gaseous products increased.
- Hydrogen gas consumption increased.
- Hydrogen content in the feed solvent decreased.
- Conversion slightly decreased.
- Optimum temperature was lower than demonstration conditions.

EXPERIMENTAL SECTION

Process Runs

Runs through the CPDU (designated overall as Run BCL-24) for these coal liquefaction experiments processed 30 wt % Kentucky #9 coal (-150 mesh) from the Pyro Mine with blended recycle solvents containing HSRC (15 or 25%). The HSRC had been produced in the second-stage settler of the Kerr-McGee Critical Solvent Deashing Unit at the Wilsonville Pilot Plant. Two solvents with widely differing quality were tested: creosote oil and hydrotreated creosote oil.

Process conditions for all runs were:

Run no.	BCL-24
Temperature (°F)	780/815/850
H_2 pressure (psig)	2000
H_2 rate (wt % feed slurry)	1.8
Space rate (lb/ft^3-hr)	106
Nominal residence time (min)	40
SRC:solvent	15:85
Coal:blended solvent	30:70

Condensed operating data for Run BCL-24 are summarized in Table 1. Run BCL-24 was onstream for 430 hr (in which 120 hr were on and off due to mechanical problems), during which 27 samples were taken. Workup and analytical capacity has been rate limiting for the data turnaround, which places the program plan about 3 months behind the original schedule. Our run efficiency continues to improve, but we are finding problems in equipment that was previously problem-free. Apparently, some equipment operated satisfactorily at severe conditions over short periods, but fatigued under sustained operation. Some equipment was replaced or backup equipment was installed.

Materials

Coals. Kentucky #9 coal, ground and air-dried to reduce moisture to <2%, was used in these experiments. Only particles passing 150 mesh were used. Proximate and ultimate analyses of the coal are listed in Table 2.

Solvents The process solvent was CO or HTCO blended with Kerr-McGee heavy SRC (HSRC). Since these solvents have different levels of donatable hydrogen, they were selected as one variable in this study. Hydrogen content and distribution are compared below (together with figures for a third solvent, Wilsonville recycle solvent (WRS), which will be used in subsequent studies to simulate natural conditions):

	HTCO (M-97)	CO (F-223)	WRS (F-219)
H (wt %)	7.5	6.4	8.1
H_{ar}* (%)	48.1	69.6	31.0
H_{a}* (%)	26.1	20.2	31.0
H_{o}* (%)	25.1	10.2	38.0
OH (as % O)	0.07	0.43	1.31
Aromaticity	0.74	0.87	0.62
MW	175	180	194
Boiling range (°F)	306-850	414-999	402-890
Oils (%)	98.8	98.4	98
Asphaltenes	1.2	1.6	2.0

CO contained 6.4% hydrogen (70% of which was aromatic), while HTCO and WRS contained 7.5% (48% aromatic) and 8.1% (31% aromatic) hydrogen, respectively. In terms of hydrogen content, CO seems to be the least favorable solvent. It was hoped that this negative property would sensitize the process parameters associated with HSRC conversion.

Solvent hydrogen donors are primarily naphthenic protons, which are not separable from other aliphatic protons in H_a and H_o by nuclear

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*H_{ar}, aromatic hydrogen; H_a, alpha hydrogen; H_o, other hydrogen.

magnetic resonance (NMR). (H_a and H_o are protons located at alpha and all other positions except aromatic sites (H_{ar}).)

Proton distribution data for Wilsonville solvent differ considerably from HTCO data, yet liquefaction performance of the two may not be drastically different. Wilsonville solvent contained a large number of hydrogen atoms in paraffinic side chains, phenols, and various five-membered ring naphthenes, whose protons are not as easily donated as those of simple hydroaromatic HTCO. For a meaningful comparison of solvent quality, a more detailed classification of hydrogen data needs to be developed.

HTCO contained considerably fewer phenolic species and also material with a boiling point about 100°F below that of CO. About 20% of HTCO was boiling below 450°F. Wilsonville solvent contained a much larger concentration of phenols than CO.

SRC Composition. HSRC used in Run BCL-24 was produced during Run 167 at the Wilsonville Pilot Plant, which was operating in the Kerr-McGee Critical Solvent Deashing Mode on Lafayette (Kentucky #9) coal. HSRC properties are listed in Table 3, along with an analysis of LSRC obtained during the same run.

HSRC and LSRC also differed significantly in hydrogen content: 5.7 vs. 6.7%, respectively. The proton distribution in HSRC is as follows:

	% relative	% absolute
H_{ar}	37.4	2.16
H_a	37.0	2.13
H_o	24.6	1.48
Sum	100.0	5.77
Aromaticity	0.74	

If we assume that methyls are the major alkyl chains in the SRC--a reasonable assumption for coal-derived liquids--then H_o represents one-half of the most naphthenic portion of the proton population.

There were slightly more sulfur and nitrogen heteroatoms in HSRC (S = 1.1 and N = 2.1) than in LSRC (S = 1.0 and N = 1.7), whereas oxygen atoms were similarly distributed (HSRC = 4.2 and LSRC = 4.3).

The terminal heteroatoms, measured as OH and NH, indicate the depth of heteroatom (O, N, S) conversion for SRC. From the HSRC number-average molecular weight of 640, determined by vapor pressure osmometry, we determined the molecular formula listed in Table 3. Solvent separation data showed that HSRC was predominantly asphaltenes and preasphaltenes (44 and 55%, respectively).

In the HSRC recycle runs, HSRC replaced part of the solvent relative to coal or part of the coal relative to solvent, in regard to hydrogen demand. Hydrogen distribution in the solvents and HSRC is compared in Table 4.

A comparison of Brown-Ladner structural parameters[2] for solvents and HSRC is quite informative. These parameters are defined as:

$$f_a = \frac{\frac{C}{H} - \frac{H_a^*}{X} - \frac{H_o^*}{Y}}{\frac{C}{H}} \qquad (1)$$

$$\sigma = \frac{\frac{H_a^*}{X} + \frac{H_{OH}}{H}}{\frac{H_a^*}{X} + H_{ar}^* + \frac{H_{OH}}{H}} \qquad (2)$$

$$\frac{H_{aru}}{C_{ar}} = \frac{\frac{H_a^*}{X} + H_{ar}^* + \frac{H_{OH}}{H}}{\frac{C}{H} - \frac{H_a^*}{X} - \frac{H_o^*}{Y}} \qquad (3)$$

where H_a^* = fractional alpha protons, H_o^* = fractional beta and higher protons, H_{ar}^* = fractional aromatic protons, $X = H_a/C_a$ atomic ratio, and $Y = H_o/C_o$ atomic ratio.

The aromaticity defined for the ratio of aromatic carbon atoms to total carbon atoms can be derived from proton data and elemental analyses based on equation 1 when carbon atom data are not available. H_{ar}/C_{ar} is the ratio of hydrogen atoms at the periphery of the aromatic ring to the aromatic carbon atoms. This number gives an approximate scale for the degree of the condensed aromatic ring system. For example, H_{aru}/C_{ar} ratios for benzene (a one-ring aromatic compound), naphthalene (a two-ring condensed aromatic compound), and phenanthrene (a three-ring condensed aromatic compound) are $6\ H_{aru}/6\ C_{ar} = 1$, $8\ H_{aru}/10\ C_{ar} = 0.8$, and $10\ H_{aru}/14\ C_{ar} = 0.71$, respectively. H_{aru}/C_{ar} decreases as the condensed aromatic ring system increases.

σ is defined as the ratio of substituents on the aromatic ring to the total available sites available for substitution. This will provide an estimate of the aromatic ring substitution by alkyls, naphthenics, and/or phenolics, etc. σ values for xylenes, methylnaphthalene, and phenol are $2/6 = 0.33$, $1/10 = 0.1$, and $1/6 = 0.17$, respectively.

When molecular data are combined with these parameters, the size of the aromatic ring system can be calculated, assuming the aromatic rings are katacondensed:

$$R_a = \left(\frac{C_{ar} - H_{ar}}{2}\right)_{MW} + 1$$

where R_a = the number of aromatic condensed rings, C_{ar} = aromatic carbon atoms per molecule, and H_{ar} = aromatic proton atoms per molecule.

A comparison of these structural parameters (shown in Table 5) indicates that aromaticity increased systematically between Wilsonville solvent ($f_a = 0.62$) and HSRC ($f_a = 0.74$), but the trend did not apply to the synthetic solvents HTCO and CO. This deviation appears to be the result of high σ values (0.341 to 0.350) calculated for the SRC-I process derived liquids, which reflected their highly substituted structural features as compared to those of the synthetic solvents ($\sigma = 0.127$ for CO and $\sigma = 0.222$ for HTCO). About 35% of the aromatic peripheral sites in the process-derived liquids appeared to be substituted by either aliphatic groups (linear or cyclic) or by OH and other polar groups.

The ratio of aromatic protons to aromatic carbon atoms (H_{ar}/C_{ar}) also provides a scale of the degree of fused aromaticity in a coal-derived aromatic fraction. This ratio is not affected by either alkyl or naphthenic substituents and provides a guide for solvent quality. H_{aru}/C_{ar} decreases in the order WRS > HTCO > CO > HSRC, which conforms to the increasing order of condensed aromatic structure in these materials. The solvent appears to contain an average of 3 ring-condensed aromatic clusters, whereas HSRC had an average of 11 rings. These structural parameters agree reasonably well with all the tests applied to the coal-derived aromatic liquids. The validity is statistical and based on the average properties of the materials, and appears significant only on a relative scale.

Feed Composition. The feed HSRC and HTCO component fractions as measured by solvent separation are as follows:

Solvent fractions	HSRC (wt %)	HTCO (wt %)	CO (wt %)
Oil	1.0	98.7	98.3
Asphaltenes	44.4	1.2	1.6
Preasphaltenes	54.6	0.1	0.1

However, solvent separation of a mixture of the two did not give the same proportionate amounts:

	15% HSRC/85% HTCO		25% HSRC/75% HTCO	
	Measured on whole	Measured on separate but calculated on whole	Measured on whole	Measured on separate but calculated on whole
Oils (wt %)	79.1	84.2	75.6	74.1
Asphaltenes (wt %)	9.6	7.7	14.1	12.0
Preasphaltenes (wt %)	11.3	8.2	10.1	13.6

	30% KY #9/70% HTCO		30% KY #9/ 10.5% HSRC/59.5% HTCO	
	Measured on whole	Individually measured but calculated on whole	Measured on whole	Individually measured but calculated on whole
Oils (wt %)	65.5	69.1	54.7	58.8
Asphaltenes (wt %)	1.6	0.8	5.5	5.4
Preasphaltenes (wt %)	8.1		13.6	6.0
Residue (wt %)	24.8	29.5	26.2	29.5

Clearly, experimental error could not have accounted for all of these results. It seems that solubility characteristics of the mixtures cannot be accurately predicted by partition of the individual components. These results suggest that considerable caution will be necessary when using these data in material balance and product distribution calculations.

Process Considerations

Many coal researchers feel strongly that oil formation during the solvent-refining process is the result of various intermediate product steps such as preasphaltene and asphaltene formation (although direct conversion from coal and retrograde reactions should not be totally excluded). If this is true, by recycling SRC the concentration of the intermediate species between coal and oils can be deliberately increased in order to produce more oils. In an SRC recycle mode, we are recycling primarily heavier asphaltenes and preasphaltenes.

There are arguments both for and against the recycle of LSRC or HSRC. Less work would be required to produce oil from LSRC than from HSRC, but this would be at the expense of a premium product, LSRC. Therefore, it is desirable to use the less valuable HSRC to produce oils if the penalties in doing this are acceptable. Because HSRC contains less hydrogen and more oxygen, nitrogen, and sulfur heteroatoms than LSRC, we expect that HSRC will respond differently in recycle.

Because the SRC injected into the system has a more severe time/temperature history than the newly formed SRC in the reaction system, the reactivity of the recycle SRC will be quite different from the freshly generated ones. To understand the interaction of solvent, SRC, and coal, it is worthwhile to determine the reactivity of SRC in solvent alone, to distinguish the effect of SRC without the coal slurry. This would also provide a reactivity scale for different SRC feeds that have varying reaction histories. On the other hand, the reactions of different solvents with reference SRC may provide a reactivity scale of solvents, as discussed in the previous report.[1]

RESULTS AND DISCUSSION

HTCO/HSRC

A mixture of HTCO and 15 or 25% HSRC was run through the reactor under operating conditions without coal at 780, 815, and 850°F (data are shown in Table 6).

Processing the 85% HTCO/15% HSRC mixture converted a considerable amount of HSRC to oil and lighter products, as indicated by the decrease in total HSRC concentration. First-order rate constants for HSRC disappearance show that temperature has a negative effect on conversion of the 15% HSRC.

On the other hand, when the HSRC concentration was increased to 25%, there was negligible HSRC conversion (Table 6) and no discernible temperature effect; however, the ratio of asphaltenes to preasphaltenes increased with an increase in temperature.

It thus appears that conversion is sensitive to HSRC concentration, and not simply a function of temperature. More data will be required to firmly establish the validity of the results.

With 15% HSRC, conversion of HSRC slightly increased the hydrogen content in the oil product at the expense of hydrogen in asphaltene, but it also decreased the hydrogen content of the total liquids regardless of the reaction conditions (Table 7).

With 25% HSRC in HTCO, hydrogen was depleted in all of the fractions with little apparent conversion, showing the necessity of more effective hydrogen donor availability at the higher HSRC concentration.

Brown-Ladner's structural parameters for the oils in the feeds and products are compared in Table 8 to illustrate the structural changes in the oils involved in these reactions. Refractive indices of the oils are also compared (they increase as the number of unsaturates increases). Small but definitive changes in the oils are evidenced by increases in aromaticity (f_a), refractive indices, and fused aromatic rings (R_a) in the products. Other structural parameters were not sensitive enough to provide any useful information.

Temperature sensitivity was reflected by changes in aromaticity or refractive indices in the run using the higher HSRC concentration. Increasing temperature increased the aromaticity of the oils. Molecular weight data alone provide little information (Table 9).

OH, NH, and NH_2 data for the oils and asphaltenes in the feed and products are listed in Table 10. With 15% HSRC, OH concentration in the oils decreased, whereas OH increased with 25% HSRC. In the latter case, OH formation overrides its removal from the reaction system, which clearly shows that OH groups are quite stable structures at the reaction conditions studied. OH concentrations in the product asphaltenes increased at 780°F with both 15 and 25% HSRC but decreased only at 850°F. Examination of HSRC conversion data together with these results indicates that OH concentration changes are clearly linked to the conversion of HSRC to lighter species. Evidently, the formation of OH results from the split of ether linkages.

NH and NH_2 concentrations in the product oil and asphaltenes followed a reaction severity pattern that was similar to but less definitive than that of OH. The difficulty of nitrogen heteroatom removal is shown by the NH_2 concentration increases that are concomitant with increases in both reaction temperature and HSRC concentration. At 850°F OH concentration diminished, whereas NH_2 concentration remained steady.

Coal/HTCO/HSRC

Kentucky #9 coal was reacted with HTCO mixtures containing 15% HSRC. (Detailed feed and product data are summarized in Appendix 1.) In Table 11, product distributions from the coal/HTCO/HSRC runs are compared with those from runs without HSRC.

The accuracy of the conversion data was not sufficient enough to show a clear trend of temperature sensitivity or the effects of the addition of HSRC. It appears that HSRC increased conversion at the lower temperatures (780 and 815°F) but slightly decreased conversion at the higher temperature (850°F). However, these results could fall well within experimental error range or may be caused by the artificial effects due to the varying solubility characteristics of solvent/HSRC mixtures as described previously (under Feed Composition).

As shown in Table 12, the presence of HSRC in the feed consistently increased the yields of C_1-C_4, CO + CO_2, and H_2O (similar results were observed upon LSRC addition in previous experiments[1]). The gas yields increased with temperature in every case, but the yield data for H_2S and NH_3 are less definitive compared to the others.

A comparison of data pairs with and without HSRC shows that at 780°F the presence of HSRC in the feed decreased the oil yield. However, the oil yield did increase when the temperature increased. This negative temperature effect of coal liquefaction in HTCO solvent on the oil yields contradicts previous results obtained during the BCL-22 Run[1] and raises some skepticism regarding these data. Nevertheless, the results suggest that the oil yields were marginal and were not significantly improved with the addition of HSRC at the conditions studied.

If these data accurately reflect the true nature of the reactions, the addition of HSRC produced the best yields at 815°F, with other conditions fixed. Apparently, the solvent make does not appear to be improved by the simple addition of HSRC.

In all instances asphaltene yields were substantially decreased upon HSRC addition. With HSRC, the yield was highest at a moderate temperature (815°F), while without HSRC the yield increased further with an increase in temperature (850°F).

HSRC increased preasphaltene yields in all cases. (These results confirm our previous observations that LSRC addition decreases asphaltene and increases preasphaltene yields.) Apparently, adding HSRC retards the conversion of preasphaltenes to asphaltenes. Previous LSRC recycle data had shown a slight decrease of conversion upon LSRC addition, but the impact of HSRC on conversion is not that conclusive: HSRC addition increased conversion in two cases and decreased it in a third. HTCO solubility behavior differs with and without HSRC, which might explain, at least partially, why HSRC has a tendency to increase conversion. If the mass action of the added SRC increased preasphaltene and decreased asphaltene yields, a decrease in coal conversion would be the logical consequence.

SRC sulfur content appears to be slightly reduced after HSRC addition, probably because the added HSRC was low in sulfur. To determine the impact of added HSRC on sulfur content, a continuous HSRC recycle run would be necessary, which would require an integrated KM unit.

Table 13 compares data obtained from both gaseous and solvent hydrogen consumption: one set was obtained from the elemental hydrogen balance between feed and products and the other was from the hydrogen gas balance flowing through the reactor system and solvent hydrogen. At steady state, all the hydrogen demanded by the reaction system should come from hydrogen gas; the hydrogen concentration in incoming recyle solvent should be equal to that of the existing recycle solvent. We had assumed in our one-pass-through runs that the total hydrogen consumed by the coal is equal to hydrogen gas consumption plus the amount of hydrogen depleted in the solvent during reaction. HSRC data clearly show that hydrogen consumption increased from about 1 to 2% as the process temperature rose from 780 to 850°F. The impact of the added HSRC is not certain because it is hard to distinguish between the data when values vary significantly, as was usually observed. However, the general trend, including the gas output data, suggests that added HSRC slightly increased the consumption of hydrogen, but not by a significant amount. In the previous LSRC recycle run,[1] hydrogen consumed from the solvent was not included in the estimation of total hydrogen consumption. When the solvent hydrogen consumptions were included, the results were similar to the present HSRC recycle run data.

Table 14 compares hydrogen content in the solvent mixture at start and finish. Adding HSRC improved the hydrogen acceptor property of the solvents. There was virtually no hydrogen change in the solvent with

HSRC at 780°F, whereas substantial hydrogen depletion occurred without HSRC at this temperature. This property diminishes gradually as reaction temperature increases.

Asphaltene concentration in the total slurry product decreased considerably with HSRC recycle (Table 15). The asphaltene to preasphaltene ratio in the product from HSRC recycle was about one-half that from the run without HSRC recycle. The decrease in asphaltenes relative to preasphaltenes in the product slurry may adversely impact the performance of the Kerr-McGee Critical Solvent Deashing Unit. In contrast, LSRC recycle substantially increased the ratio of asphaltenes to preasphaltenes.

The structural parameters shown in Table 16 indicate that the product oil decreased in aromaticity at 780°F from 0.74 to 0.72 in the absence of HSRC and from 0.73 to 0.72 in the presence of HSRC. As the process temperature increased, the aromaticity increased consistently in both cases. However, it is interesting to observe that with HSRC the R_a (condensed aromatic ring system) in the product oils increased slightly from 2.6 to 2.9 as the temperature increased from 780 to 850°F, while without HSRC the R_a decreased from 3.1 to 2.7 with the same temperature change. (An increase in R_a conforms to a decrease in H_{aru}/C_{ar}.) This result strongly indicates that HSRC addition creates a highly temperature-sensitive aromatization environment for the oils.

Temperature increases decreased the σ value of oil in runs with or without HSRC; this means that the aromatic ring systems in the product solvent increasingly lost substituents as temperature increased. This result is consistent with the higher gas product rate observed with increased temperatures.

The number-average molecular weights in each solvent fraction are listed in Table 17. Significant differences are displayed only by the preasphaltene molecules. Preasphaltenes in the products from the HSRC runs have lower molecular weights compared to those from runs without HSRC. This may simply be due to the large amount of unreacted HSRC reporting to the preasphaltenes, which are lower in molecular weight compared to newly generated preasphaltene molecules.

Yield data from the HSRC recycle run are summarized in Table 18.

CO/HSRC

To determine the thermal stability of CO when blended with HSRC, the feed SRC for recycle was processed with solvent under coal liquefaction conditions without coal. Shown in Table 19 are the results obtained at 780 and 850°F. At 780°F, the hydrotreatment of HSRC caused a net decrease of preasphaltenes from 8.3 to 6.6% that apparently increased oils from 83.7 to 85.4%. At 850°F, however, asphaltenes were increased about twofold in the products, from 8.0 to 16.9%, while oil content decreased from 83.7 to 74.5%. This result confirms earlier trends indicating that HSRC was unstable even with HTCO at this temperature, and it is also consistent with the LSRC/CO data reported previously.[1] HSRC altered the thermal characteristics of process solvent dramatically.

It is likely that the best process temperature for recycle of HSRC would be much lower compared to that for processing without recycle.

Coal/CO/HSRC

It is anticipated that HSRC recycle will reduce the hydrogen content of the solvent. HSRC normally contains much less hydrogen than either CO or HTCO, as illustrated in Table 4. Since CO is a less favorable recycle solvent (it contains a minimum amount of hydrogen), this study was selected to provide solutions to problems that may come up with SRC recycle regarding decreasing quality of process solvent.

Kentucky #9 coal was liquefied with CO containing 15% Kerr-McGee HSRC. The yields at three different process temperatures are summarized in Table 20, including a comparison between results with and without HSRC.

Unexpectedly, for the first time negative oil yields were observed upon conversion of Kentucky #9 coal and CO. Increasing the process temperature from 780 to 850°F gradually increased oil yield from -9 to -1% (Table 21), but decreased preasphaltene content without any significant change in conversion. However, when HSRC was added to this coal slurry (at 780°F), oil yield decreased and asphaltene and preasphaltene yields increased, which indicates that stabilization of the newly formed coal fragments was severely retarded. Without coal, the HSRC/CO system stayed stable at 780°F compared to 850°F. The results in Table 21 show that a dramatic shift in distribution was triggered by an increase in the process temperature from 780 to 815°F, but a further increase to 850°F eventually reversed the trend. The oil yields were about 20 and 16% at 815 and 850°F, respectively, accompanied by comparable decreases in asphaltene and preasphaltene yields.

These data suggest that when the feed contains HSRC the optimum process temperature lies in a narrow temperature range around 815°F. Earlier data from the reaction of Kentucky #9 coal/LSRC/CO[1] reflected a negative temperature effect on oil yield, which dropped from 29 to 7% between 780 and 850°F. Such results indicate that 850°F far exceeds the optimal temperature for oil yield. Although HSRC had no significant effect, a small but decreasing trend in conversion was noticed as the process temperature increased. The sulfur content in the SRC products appeared to decrease upon HSRC addition.

HSRC recycle consistently increased the production of light hydrocarbon gases (C_1-C_4) (Table 22), and the formation of other gases appeared to follow the same increasing trend. The measurement of non-hydrocarbon products was less accurate, as reflected in the scattered data.

Table 23 summarizes the hydrogen consumption data determined from an elemental hydrogen balance of the reaction system. As observed with HTCO, HSRC caused a minor but consistent increase in hydrogen consumption except at 780°F, which was possibly due to experimental error. The addition of 15% HSRC decreased the hydrogen content of starting solvent from 6.42 to 6.36% (Table 23). Product solvents substantially gained hydrogen, with or without HSRC. It does appear that HSRC induced more hydrogen gain in the solvent on a relative scale.

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2. J. K. Brown and W. R. Ladner, Fuels, 39, 87 (1967).

Table 1

Condensed Operating Data Summary (Run BCL-24)

Date of run M/D/Y/start/end	Product slurry ID	Temp (°F)	Pressure (psig)	Feed rate (g/hr)	H_2 feed rate (L/hr)	Product slurry (g/hr)	Total condensate (g/hr)	Product gas rate (L/hr)	H_2O (g/hr)	Organic condensate (g/hr)
1/30/80/0700/0800	147	780	2000	1705	342	1494	26.5	321	15.1	11.4
1/30/80/1400/1500	153	815	2000	1779	329	1530	34.6	310	21.2	13.4
1/30/80/2300/2400	159	850	2010	1699	348	1451	36.8	332	18.2	18.6
1/28/80/0900/1000	118	780	2000	1769	341	1484	11.3	303	6.3	5.0
1/28/80/1500/1600	122	817	1996	1687	347	1507	26.9	306	10.9	16.0
2/4/80/0100/0200	211	850	2000	1726	323	1474	31.0	301	11.9	19.1
1/29/80/1500/1600	140	780	2000	1593	335	1349	13.4	313	6.1	7.3
1/29/80/0800/0900	134	815	1998	1595	328	1418	16.5	329	7.1	9.4
1/28/80/2300/2400	129	850	2000	1487	358	1455	23.4	347	11.3	12.1
2/7/80/2000/2100	267	780	2000	1638	356	1471	9.7	347	3.2	6.5
2/7/80/1300/1400	261	815	2000	1617	338	1418	11.3	348	4.6	67.7
2/7/80/0500/0600	255	850	2000	1663	343	1436	11.5	344	5.1	6.4
2/2/80/2100/2200	194	780	1997	1819	354	1703	17.7	301	9.5	8.2
2/3/80/0400/0500	200	811	2000	1432	361	1471	22.6	290	14.0	8.6
2/3/80/1300/1400	206	850	1996	1699	339	1544	38.3	270	22.0	16.4
1/25/80/2100/2200	86	782	2000	1790	348	1598	23.4	305	17.7	5.7
1/26/80/0400/0500	92	815	1997	1752	373	1519	26.3	293	18.3	8.0
1/26/80/1100/1200	98	850	2000	1757	358	1574	32.2	288	22.4	9.8
2/2/80/0400/0500	184	780	2000	1577	346	1338	5.9	318	0.8	5.1
2/1/80/2000/2100	178	816	2008	1613	350	1463	8.3	318	2.9	5.4
2/1/80/1300/1400	172	850	2000	1606	333	1597	8.6	317	3.2	5.4
2/6/80/0600/0700	237	780	2000	1595	347	1412	5.6	337	1.6	4.0
2/6/80/1200/1300	241	815	2000	1642	344	1424	7.3	322	1.6	5.7
2/6/80/1800/1900	247	851	2000	1658	359	1477	8.6	338	3.2	5.4
2/5/80/1000/1100	229	780	2000	1674	340	1506	4.4	321	1.1	3.3
2/5/80/0200/0300	223	815	2000	1682	348	1492	5.7	324	1.2	4.5
2/4/80/1900/2000	217	848	2000	1698	368	1529	16.3	338	6.3	10.0

Table 2

Kentucky #9 Coal (Pyro Mine)

Proximate analysis	wt %
Moisture	1.54
Volatile matter	35.60
Fixed carbon	49.67
Ash	13.17

Ultimate analysis (dry basis)	wt %
Carbon	70.51
Hydrogen	4.66
Oxygen	6.23
Nitrogen	1.50
Sulfur	3.27
Sulfate S	0.04
Pyrite S	1.83
Organic S	1.08

	wt %
Sulfate ash (700°C)	13.45
Al	1.53
Fe	1.45

	ppm
Ti	570
B	590
Cl	2400
Ca	90
Mg	850
K	2700
Na	470

Table 3

Comparison of HSRC and LSRC

	HSRC	LSRC
C (wt %)	85.9	85.4
H (wt %)	5.8	6.8
O (wt %)	4.2	4.3
N (wt %)	2.1	1.7
S (wt %)	1.1	1.0
Ash (wt %)	0.1	0.1
Oils (wt %)	1.0	--
Asphaltenes (wt %)	43.5	--
Preasphaltenes (wt %)	55.5	--
MW	640	--
Molecular formula	$C_{45.8}H_{36.9}O_{1.7}N_{0.9}S_{0.2}$	--
Softening point (°F)	380	--
OH in asphaltenes (wt % OH as O)	1.49	--
NH in asphaltenes (wt % NH as N)	0.31	--

Table 4

Hydrogen Distribution

Comparison of Solvents and HSRC

	CO		HTCO	
	% relative	% absolute	% relative	% absolute
Total	100.0	6.40	100.0	7.45
H_{ar}	69.6	4.45	48.1	3.48
H_a	20.2	1.29	26.8	2.00
H_o	10.2	0.65	25.1	1.87

	HSRC	
	% relative	% absolute
Total	100.0	5.77
H_{ar}	37.4	2.16
H_a	37.0	2.13
H_o	25.6	1.48

Table 5

Structural Parameters of Various Solvents and SRC

	f_a	$\frac{H_{aru}}{C_{ar}}$	σ	R_a
CO (F-223)	0.871	0.775	0.127	2.86
HTCO (B-24-122-FL-Oil)	0.744	0.822	0.222	2.77
Wilsonville recycle oil (F-219)	0.617	0.855	0.347	2.94
HSRC (M-61)	0.744	0.631	0.350	11.11

Table 6

HSRC/HTCO Conversion Data

BCL-24 sample no.	140	134	129	267	261	255
Feed composition	85% HTCO/15% HSRC			75% HTCO/25% HSRC		
Temp (°F)	780	815	850	780	815	850
Feed						
Oils	79.1	79.1	79.1	75.6	75.6	75.6
Asphaltenes	9.6	9.6	9.6	14.1	14.1	14.1
Preasphaltenes	11.3	11.3	11.3	10.1	10.1	10.1
HSRC	20.9	20.9	20.9	24.2	24.2	24.2
Product						
Oils	86.8	81.7	81.4	76.1	76.7	74.7
Asphaltenes	7.6	10.8	10.4	13.7	13.2	16.1
Preasphaltenes	4.9	6.5	6.5	9.8	9.0	7.6
HSRC	12.5	17.3	16.9	23.5	22.2	23.7
First-order rate constant (hr^{-1})						
Oils	0.14	0.06	0.05	0.01	0.02	-0.02
Asphaltenes	-0.39	0.17	0.11	-0.05	-0.11	0.18
Preasphaltenes	-2.04	-1.24	-1.24	-0.08	-0.21	-0.54
HSRC	-0.52	-0.23	-0.27	-0.04	-0.11	-0.03

Table 7

Hydrogen Concentration Data for HSRC/HTCO Reaction

BCL-24 sample no.	140	134	129	267	261	255
Feed composition	85% HTCO/15% HSRC			75% HTCO/25% HSRC		
Temp (°F)	780	815	850	780	815	850
Hydrogen in feed (wt %)						
Total	7.6	7.6	7.6	7.2	7.2	7.2
Oils	7.4	7.4	7.4	7.5	7.5	7.5
Asphaltenes	6.7	6.7	6.7	6.2	6.2	6.2
Preasphaltenes + IOM[1]	5.3	5.3	5.3	5.6	5.6	5.6
Hydrogen in product (wt %)						
Total	7.2	7.3	7.2	7.2	7.0	6.9
Oils	7.7	7.4	7.5	6.9	7.4	7.1
Asphaltenes	6.5	6.4	6.2	6.1	5.8	6.1
Preasphaltenes + IOM	5.8	5.3	5.0	5.4	5.5	4.9

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[1] IOM, insoluble organic matter.

Table 8

Structural Parameters for HSRC/HTCO Products

BCL-24 sample no.	140	134	129	267	261	255
Feed composition	85% HTCO/15% HSRC			75% HTCO/25% HSRC		
Temp (°F)	780	815	850	780	815	850
Feed oil						
f_a	0.728	0.728	0.728	0.731	0.731	0.731
H_{aru}/C_{ar}	0.813	0.813	0.813	0.816	0.816	0.816
R_a	2.69	2.69	2.69	2.76	2.76	2.76
σ	0.222	0.222	0.222	0.220	0.220	0.220
RI	1.6053	1.6053	1.6053	1.6108	1.6108	1.6108
Product oil						
f_a	0.742	0.746	0.737	0.747	0.749	0.759
H_{aru}/C_{ar}	0.810	0.802	0.835	0.742	0.381	0.799
R_a	2.70	2.76	2.72	3.11	2.82	2.86
σ	0.227	0.210	0.224	0.242	0.223	0.201
RI	1.5925	1.6130	1.6092	1.6123	1.6153	1.6194

Table 9

Molecular Weight Data for HSRC/HTCO Reaction

BCL-24 sample no.	140	134	129	267	261	255
Feed composition	85% HTCO/15% HSRC			75% HTCO/25% HSRC		
Temp (°F)	780	815	850	780	815	850
Feed						
Total	215	215	215	260	260	260
Oils	171	171	171	172	172	172
Asphaltenes	505	505	505	510	510	510
Preasphaltenes	1735	1735	1735	1165	1165	1165
Product						
Total	204	200	194	213	210	290
Oils	179	172	177	174	183	184
Asphaltenes	509	550	453	659	595	477
Preasphaltenes	1410	1239	1725	--	--	2069

Table 10

OH, NH, and NH_2 Concentrations for HSRC/HTCO Reaction

BCL-24 sample no.	140	134	129	267	261	255
Feed composition	85% HTCO/15% HSRC			75% HTCO/25% HSRC		
Temp (°F)	780	815	850	780	815	850
Feed oil						
Oils (wt %)[1]						
OH	0.45	0.45	0.45	0.54	0.54	0.54
NH	0.10	0.10	0.10	0.17	0.17	0.17
NH_2	0.01	0.01	0.01	0.02	0.02	0.02
Asphaltenes (wt %)						
OH	1.54	1.54	1.54	1.71	1.71	1.71
NH	0.22	0.22	0.22	0.43	0.43	0.43
NH_2	0.25	0.25	0.25	0.17	0.17	0.17
Product						
Oils (wt %)						
OH	0.37	0.40	0.36	0.58	0.57	0.55
NH	0.09	0.12	0.10	0.17	0.16	0.12
NH_2	0.03	0.10	0.14	0.01	0.01	0.15
Asphaltenes (wt %)						
OH	1.77	1.47	1.53	1.73	1.71	1.67
NH	0.24	0.28	0.25	0.55	0.54	0.35
NH_2	0.40	0.59	0.65	0.28	0.10	0.51

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[1] Weight percent of OH, NH, and NH_2 as oxygen and nitrogen.

Table 11

HTCO and SRC Yields with HSRC Recycle with Coal

BCL-24 sample no.	118	112	211	147	153	159
Solvent	HTCO	HTCO	HTCO	HTCO/ HSRC	HTCO/ HSRC	HTCO/ HSRC
Temp (°F)	780	815	850	780	815	850
Conversion (wt %)	82.9	80.6	89.5	88.8	87.5	87.9
Oils	12.3	8.2	4.1	3.4	11.8	10.8
Asphaltenes	26.6	28.5	36.0	13.0	21.0	11.6
Preasphaltenes	40.1	36.3	39.8	66.8	45.4	52.3
SRC total (asph. + preasph)	66.7	64.8	75.8	79.8	66.4	63.9
% S in SRC	1.3	1.3	1.0	1.3	1.2	1.0

Table 12

Gas Yields with HSRC Recycle and HTCO

BCL-24 sample no.	118	122	211	147	153	159
Solvent	HTCO	HTCO	HTCO	HTCO/ HSRC	HTCO/ HSRC	HTCO/ HSRC
Temp (°F)	780	815	850	780	815	850
C_1-C_4	1.2	3.1	5.3	1.5	3.4	7.0
$CO + CO_2$	0.4	0.6	0.9	0.5	0.7	0.9
$H_2S + NH_3$	2.1	2.6	2.1	1.2	1.5	2.1
H_2O	0.2	1.4	1.5	2.4	3.8	3.2

Table 13

Hydrogen Consumption Data with HSRC Recycle and HTCO (Weight Percent per MAF Coal Basis)

BCL-24 sample no.	118	122	211	147	153	159
Solvent formula	HTCO	HTCO	HTCO	HTCO/HSRC	HTCO/HSRC	HTCO/HSRC
Temp (°F)	780	815	850	780	815	850
From elemental hydrogen balance						
Total	0.9	1.2	2.0	1.0	1.7	2.0
Gas	-0.5	-0.4	0.5	0.9	0.9	0.1
Solvent	1.4	1.6	1.5	0.1	0.8	1.9
From gas hydrogen and solvent hydrogen balance						
Total	2.6	3.0	2.8	0.9	1.7	3.1
Gas	1.2	1.4	1.2	0.8	0.9	1.2
Solvent	1.4	1.6	1.6	0.1	0.8	1.9

Table 14

Change of Hydrogen Content in the Solvent with HSRC Recycle

BCL-24 sample no.	118	122	211	147	153	159
Solvent formula	HTCO	HTCO	HTCO	HTCO/ HSRC	HTCO/ HSRC	HTCO/ HSRC
Temp (°F)	780	815	850	780	815	850
% solvent hydrogen						
Start	7.8	7.8	7.8	7.5	7.5	7.5
Finish	7.4	7.3	7.3	7.5	7.3	6.9

Table 15

Asphaltene/Preasphaltene Ratio in the Product Slurry with HSRC/LSRC Recycle

BCL-24 sample no.	118	122	211	147	153	159
Temp (°F)	780	815	850	780	815	850
Solvent	HTCO	HTCO	HTCO	HTCO/HSRC	HTCO/HSRC	HTCO/HSRC
A/P ratio						
Feed	16.6	16.6	16.6	0.9	0.9	0.9
Product	0.74	0.87	0.98	0.38	0.62	0.44

BCL-22 sample no.	104	96	75	83	121	50	112	42
Temp (°F)	780	850	780	850	780	850	780	850
Solvent	HTCO	HTCO	HTCO/LSRC	HTCO/LSRC	CO	CO	CO/LSRC	CO/LSRC
A/P ratio								
Feed	0.67	0.67	4.11	4.11	3.13	3.13	5.76	5.76
Product	0.56	0.59	0.60	1.00	0.54	1.15	0.86	0.70

Table 16

Structural Parameters for Coal/HTCO/HSRC Products

BCL-24 sample no.	118	122	211	147	153	159
Temp (°F)	780	815	850	780	815	850
Solvent formula	HTCO	HTCO	HTCO	HTCO/HSRC	HTCO/HSRC	HTCO/HSRC
Feed oil						
f_a	0.744	0.744	0.744	0.725	0.725	0.725
H_{aru}/C_{ar}	0.822	0.822	0.822	0.820	0.820	0.820
R_a	2.77	2.77	2.77	2.70	2.70	2.70
σ	0.222	0.22	0.222	0.222	0.222	0.222
Product oil						
f_a	0.721	0.731	0.762	0.717	0.745	0.770
H_{aru}/C_{ar}	0.759	0.782	0.809	0.830	0.838	0.795
R_a	3.05	2.88	2.69	2.62	2.63	2.90
σ	0.212	0.208	0.198	0.201	0.199	0.191

Table 17

Molecular Weight Data for HSRC/HTCO/Coal Reaction Products

BCL-24 sample no.	118	122	211	147	153	159
Solvent formula	HTCO	HTCO	HTCO	HTCO/HSRC	HTCO/HSRC	HTCO/HSRC
Temp (°F)	780	815	850	780	815	850
Feed						
Total	223	223	223	233	233	233
Oil	175	175	175	172	172	172
Asphaltenes	NA	NA	NA	472	472	472
Preasphaltenes	1402	1402	1402	653	653	653
Product						
Total	255	237	231	264	251	252
Oil	189	183	168	179	178	183
Asphaltenes	460	470	402	443	520	514
Preasphaltenes	1750	1939	902	1499	1404	1488

Table 18

Yield Data for Kentucky #9 Coal with HSRC Recycle and HTCO

BCL-24 sample no.	118	112	211	147	153	159
Solvent	HTCO	HTCO	HTCO	HTCO/ HSRC	HTCO/ HSRC	HTCO/ HSRC
Temp (°F)	780	815	850	780	815	850
Conversion (wt %)	82.9	80.6	89.5	88.8	87.5	87.9
HC gases (C_1-C_4)	1.2	3.06	5.2	1.5	3.4	7.0
H_2O	0.2	1.4	1.5	2.4	3.8	3.2
$CO + CO_2$	0.4	0.55	0.9	0.5	0.7	0.9
$H_2S + NH_3$	2.1	2.61	2.1	1.2	1.5	2.1
Oils	12.3	8.2	4.1	3.4	11.8	10.8
SRC	66.7	64.8	75.8	79.8	66.4	63.9
Asphaltenes	26.6	28.5	36.0	13.0	21.0	11.6
Preasphaltenes	40.1	36.3	39.8	66.8	45.4	52.3
Residue	18.3	20.8	11.7	12.1	13.4	13.4
Sulfur in SRC (wt %)	1.33	1.29	1.04	0.27	1.23	1.02
Solvent hydrogen (wt %)						
Start	7.8	7.8	7.8	7.5	7.5	7.5
Finish	7.4	7.3	7.3	7.5	7.3	6.9
H_2 consumption, total (wt %)	0.95	1.16	2.04	0.98	1.70	2.01
From gas	-0.45	-0.40	0.49	0.93	0.91	0.13
From solvent	1.40	1.56	1.55	0.06	0.79	1.89

Table 19

HSRC/CO Hydrotreatment Data

BCL-24 sample no.	184	172
Feed composition	85% CO/15% HSRC	
Temp (°F)	780	850
Feed (wt %)		
Oils	83.7	83.7
Asphaltenes	8.0	8.0
Preasphaltenes	8.3	8.3
HSRC	16.3	16.3
Product (wt %)		
Oils	85.4	74.5
Asphaltenes	7.9	16.9
Preasphaltenes	6.6	7.1
HSRC	14.5	24.0

Table 20

Yield Data for Kentucky #9 Coal with HSRC Recycle and CO

BCL-24 sample no.	24-86	24-92	24-98	24-194	24-200	24-206
Solvent	CO	CO	CO	CO/HSRC	CO/HSRC	CO/HSRC
Temp (°F)	780	815	850	780	815	850
Conversion (wt %)	89.8	92.5	90.2	90.6	91.2	89.1
C_1-C_4	1.22	2.57	5.32	1.48	3.09	6.24
$CO + CO_2$	0.51	0.62	0.86	0.47	0.74	0.91
$H_2S + NH_3$	1.76	2.00	2.52	1.31	2.07	2.64
H_2O	2.8	3.1	4.0	2.5	3.9	5.7
Oils	-8.5	-4.5	-1.1	-15.1	20.2	16.1
Asphaltenes	43.4	44.1	41.7	50.1	27.3	30.8
Preasphaltenes	48.7	44.5	37.0	49.8	34.0	26.7
Unconverted coal	11.4	9.8	12.1	10.6	10.8	13.3
SRC (wt %)	92.1	88.6	78.7	99.9	61.3	57.5
Sulfur in SRC (wt %)	1.51	1.52	0.98	1.20	1.16	0.96
Solvent hydrogen (wt %)						
Start	6.42	6.42	6.42	6.36	6.36	6.36
Finish	6.56	6.63	6.57	6.54	6.48	6.55
H_2 consumption (wt %)						
Total	0.88	1.01	1.36	0.61	1.17	1.76
Gas	1.28	1.60	1.78	1.10	1.51	2.27
Solvent	-0.40	-0.60	-0.43	-0.50	-0.33	-0.52

Table 21

CO and SRC Yields with HSRC Recycle with Coal

BCL sample no.	24-86	24-92	24-98	24-194	24-200	24-206
Solvent	CO	CO	CO	CO/HSRC	CO/HSRC	CO/HSRC
Temp (°F)	780	815	850	780	815	850
Conversion (wt %)	89.8	92.5	90.2	90.6	91.2	89.1
Oils	-8.5	-4.5	-1.1	-15.1	20.2	16.1
Asphaltenes	43.4	44.1	41.7	50.1	27.3	30.8
Preasphaltenes	48.7	44.5	37.0	49.8	34.0	26.7
Unconverted coal	11.4	9.8	12.1	10.6	10.8	13.3
SRC (wt %) (asphaltenes plus preasphaltenes)	92.1	88.6	78.7	99.9	61.3	57.5
Sulfur in SRC (wt %)	1.51	1.52	0.98	1.20	1.16	0.96

Table 22

Gas Yields with HSRC Recycle and CO

BCL-24 sample no.	24-86	24-92	24-98	24-194	24-200	24-206
Solvent	CO	CO	CO	CO/HSRC	CO/HSRC	CO/HSRC
Temp (°F)	780	815	850	780	815	850
wt % of MMF[1] coal						
C_1-C_4	1.22	2.57	5.32	1.48	3.09	6.24
$CO + CO_2$	0.51	0.62	0.86	0.47	0.74	0.91
$H_2S + NH_3$	1.76	2.00	2.52	1.31	2.07	2.64
H_2O	2.8	3.1	4.0	2.5	3.9	5.7

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1. Mineral matter free.

Table 23

Hydrogen Consumption with HSRC Recycle and CO

BCL-24 sample no.	24-86	24-92	24-98	24-194	24-200	24-206
Solvent	CO	CO	CO	CO/HSRC	CO/HSRC	CO/HSRC
Temp (°F)	780	815	850	780	815	850
Total (wt %)	0.88	1.01	1.36	0.61	1.17	1.76
From gas	1.28	1.60	1.78	1.10	1.51	2.27
From solvent	-0.40	-0.60	-0.43	-0.50	-0.33	-0.52
Solvent hydrogen content (wt %)						
Start	6.42	6.42	6.42	6.36	6.36	6.36
Finish	6.56	6.63	6.57	6.54	6.48	6.55

Appendix 1

Feed and Product Composition Data Summary

BCL-24 sample no.	118	122	211	147	153	159	140	134	129	267	261	255
Temp (°F)	780	817	850	780	815	850	780	815	850	780	815	850
Pressure (psig)	2000	1996	2000	2000	2000	2010	2000	1998	2000	2000	2000	2000
H_2 rate (wt % on feed slurry)	2.04	2.01	1.90	2.01	1.87	2.06	2.21	2.05	2.16	2.16	2.11	2.10
Space rate (slurry lb/hr per ft^3)	94	97	96	96	99	95	85	90	93	93	90	92
Residence time (min)	45	44	45	45	43	45	46	44	42	43	45	44
SRC/solvent ratio (wt/wt)	0/100	0/100	0/100	15/35	15/85	15/85	15/85	15/85	25/75	25/75	25/75	25/75
	HTCO	HTCO	HTCO	HSRC/HTCO	HSRC/HTCO	HSRC/HTCO	HSRC/HTCO	HSRC/HTCO	HSRC/HTCO	HSRC/HTCO	HSRC/HTCO	HSRC/HTCO
Solvent blends/coal (wt/wt)	30/70	30/70	30/70	30/70	30/70	30/70	100/0	100/0	100/0	100/0	100/0	100/0
Feed composition (wt %)	69.13	69.13	69.13	58.36	58.86	58.86	78.57	78.57	78.57	75.58	75.58	75.58
Oils	0.83	0.83	0.83	5.36	5.36	5.36	9.57	9.57	9.57	14.13	14.13	14.13
Asphaltenes	0.05	0.05	0.05	5.77	5.77	5.77	11.21	11.21	11.21			
Preasphaltenes	25.45	25.45	25.45	25.45	25.45	25.45				10.29	10.29	10.29
Insoluble organic matter	0.46	0.46	0.46	0.46	0.46							
Ash	3.95	3.95	3.95	3.35	3.95	3.95	0.46	0.46	0.46			
Product composition (wt %)												
H_2	-0.31	-0.36	-0.31	-0.22	-0.23	-0.33	-0.18	-0.05	-0.18	-0.08	-0.0	-0.13
C_1-C_4	0.29	0.67	1.28	0.37	0.84	1.72	0.14	0.36	0.85	0.21	0.53	1.15
$CO + CO_2$	0.10	0.13	0.22	0.14	0.18	0.23	0.01	0.02	0.04	0.03	0.04	0.05
H_2O	0.50	0.78	0.85	1.07	1.42	1.28	0.54	0.58	0.85	0.31	0.42	0.44
H_2S	0.48	0.59	0.48	0.30	0.36	0.49	0.06	0.11	0.16	0.05	0.08	0.11
NH_3	0.02	0.04	0.04	0.0	0.0	0.03	0.01	0.01	0.01	0.0	0.01	0.01
Oil	71.16	69.49	70.69	60.29	62.48	61.91	86.67	81.67	81.43	76.05	76.69	74.74
Asphaltenes	7.37	7.77	9.90	8.70	10.71	8.29	7.61	10.82	10.35	13.65	13.20	16.09
Preasphaltenes	9.90	8.90	10.07	22.53	17.24	18.94	4.91	6.39	6.18	9.69	8.88	7.54
Insoluble organic matter	4.51	5.07	2.93	3.04	3.38	3.35						
Ash	6.48	7.48	4.07	3.70	3.67	4.13	0.04	0.10	0.17	0.02	0.07	0.04

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