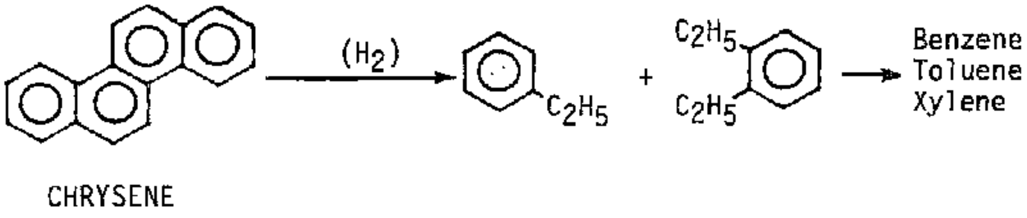
decane level (34.6 wt.%) is attractive for this use because boiling point (345°F) and energy density are favorable for this application. In general, the light liquid fraction is expected to require little upgrading beyond denitrogenation and desulfurization.

E. IMPACTING AREAS AND RECENT RESEARCH DEVELOPMENTS

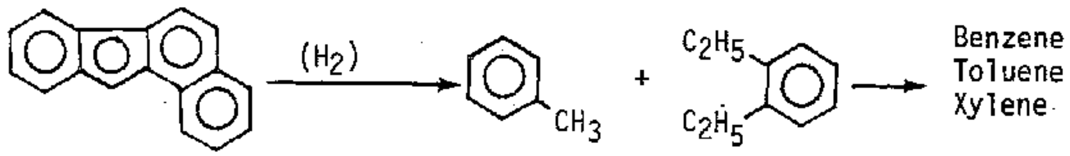
From the previous discussion, it is clear that regardless of the scheme used for upgrading heavy Coalcon coal liquids, two primary catalytic problems can be anticipated: selective cracking of four ring aromatics to single ring aromatics with minimum light gas make and minimum carbon deposition on the catalyst; and denitrogenation to acceptable levels. The potential impact of the advances in catalysis (Part 1) and related disciplines (Part 2) over the last decade in solving these problems are addressed in this section in terms of short term developments, long term developments and supporting research.

1. SHORT TERM DEVELOPMENTS

Upgrading the Coalcon heavy liquid fraction to any of the previously discussed products requires hydrotreating, the degree depending upon the wanted product. This implies selective cracking of the two primary polynuclear aromatics constituents, 1-2 benzo-fluorene and chrysene, to single ring aromatics (reactions A and B) and hydrodenitrogenation of the pyridine constituent (reaction C):

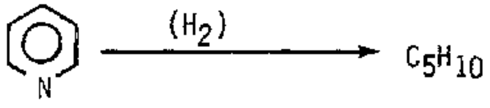


(A)



(B)

BENZOFLUORENE



(C)

PYRIDINE

For conversion to heating oils, only minimal cracking is necessary, perhaps only scission to one and two ring compounds. However, denitrogenation is still a problem. The following treatment of these problems has been divided into a discussion of activity and selectivity, and a discussion of activity maintenance.

a. Activity and Selectivity

Both selective hydrocracking and HDN require the use of bifunctional catalysts (4), i.e. the synthesis of the catalyst with the proper hydrogenation and cracking functions. If the hydrogenation activity is too high, excessive and non-selective use of costly hydrogen occurs. If it is too low, activity maintenance is a problem. Similarly, the cracking function requires careful control, depending on the process (5). One of the primary tasks of a development program designed to improve cracking and in particular HDN catalysts is catalyst characterization. This has been pointed out in Part 1 and will be discussed again in other sections in Part 3. It is a particularly important problem when bifunctional catalysts are required. It is a complex problem, and has not been studied in depth for many of the materials (e.g. supported oxides, sulfides) which would be of interest for cracking or HDN. Thus, while acidity measurements involving the amount, type, strength and distribution of acid sites can be carried out on a routine basis (6), the titration of cationic sites which are associated with hydrogenation activity (e.g. Cr^{+3}, Fe^{+2}, Co^{+2}, etc.) has only recently been studied. For example, NO chemisorption has been used to determine the number of surface cationic sites for the oxides of Co, Ni, Fe, Cu, and Cr supported on Al_2O_3 (6). This technique should have even broader applicability to other systems as well. Another adsorbent reported to be effective for measuring the number of active sites on $CoO\text{-}MoO_3\text{-}Al_2O_3$ catalysts is H_2S (7, 8). However, more work is needed to allow the routine characterization which is necessary to understand the nature of the HDN and cracking functions as well as to determine the _intrinsic_ activity for a given reaction.

In terms of catalyst improvement, the three areas which could have the most significant impact on selective cracking and HDN using _existing_ catalysts are _optimization of catalyst physical characteristics_, _variation of catalyst composition_, and _effective catalyst testing_.

Optimizing physical characteristics involves careful control of surface area, pore volume and pore size distribution for conventional HDN catalysts such as Ni-W and Ni-Mo on Al_2O_3 and mixed-oxide hydrocracking catalysts such as Ni-W, Ni-Mo, or Pd supported on zeolites, $SiO_2 \cdot Al_2O_3$, $TiO_2 \cdot SiO_2$ and $MgO \cdot SiO_2$ (9, 10).

Control of physical properties has been recognized as an important problem for HDS catalysts, and it has received considerable attention in the last few years. However, because of the more stringent conditions required for HDN (4), it is expected that the optimum HDN and HDS catalysts will differ in a number of properties, including physical characteristics. Controlled pores are important to minimize diffusion limitations and also, as mentioned below, to reduce catalyst deactivation.

With large molecules like chrysene and 1-2 benzofluorene, such diffusion problems can readily occur. They are, in general, minimized by the use of wide pore catalysts. A number of gel procedures have recently been developed which give considerable flexibility in controlling the pore size and its distribution (11). However, sometimes the requirement for large pores leads to poor mechanical properties (low crush strength). Recent work has shown that this can be remedied in some instances by proper doping with alkaline and rare earth cations (12). More work needs to be done to show the general applicability of this technique.

Variation in catalyst composition is another variable of importance in efforts to maximize the activity of existing catalysts. The need for this optimization can be seen from the fact that MoO_3/Al_2O_3 has about the same catalytic activity for HDN of pyridine as does $CoO\text{-}MoO_3/Al_2O_3$ (13). This shows that in contrast to HDS, Co is not an essential constituent for HDN, except perhaps for activity maintenance. Composition can be varied readily in a systematic manner using many of the recently developed procedures including gel precipitation, sol-gels, cogels, aerogels, and homogeneous pH change (14). Of particular interest are the latter three procedures which enable one to vary, for example, the Ni/Mo/Al ratio in $Ni\text{-}Mo/Al_2O_3$ and achieve a catalyst with homogeneous composition. The cogel procedure reportedly gives catalysts with unprecedented activity and activity maintenance for HDS and HDN of high molecular weight feedstocks (15). These catalysts are also thermally more stable (e.g. 350 m^2/g after treatment at $1200^{\circ}C$ for 2 hrs.). The stability is ascribed to the increased degree of structural homogeneity which this technique offers. It has been used to prepare $NiO \cdot WO_3$, $NiO \cdot WO_3 \cdot ZrO_2$ and $NiO \cdot WO_3 \cdot TiO_2$ catalysts, all cogelled with ultrastable zeolites (14). The cogel procedure as well as the other techniques mentioned above can be used to vary ratios of primary catalyst constituents and in conjunction with adequate catalyst characterization to improve existing catalysts.

Testing catalysts for selective hydrocracking or HDN should be done in continuous units and should use both model compounds (i.e. chrysene and 1-2 benzofluorene) as well as actual Coalcon heavy liquid product. As previously discussed, conventional trickle bed testing leads to a number of problems (16). Similarly, two-phase up-flow systems can give contacting and therefore mass transfer limitations (17). An effective reactor system for studying both general reaction variables as well as kinetics has been described by Carberry and later modified by other workers (16). This system is basically an autoclave with continuously flowing gas and liquids either over a spinning basket containing the catalyst or over a fixed catalyst bed flushed with gas and liquid by impeller motion. This type of system can optimize three phase contact and thereby give more reliable evaluation of the intrinsic catalyst activity.

b. Activity Maintenance

The importance of catalyst activity maintenance can be viewed in two ways. First, catalytic activity can decrease because of carbon deposition and/or chemical poisoning. Secondly, the catalyst can degrade mechanically or chemically because of high thermal transients either during use or during oxidative regeneration.

A number of factors control carbon deposition, particularly for processing high molecular weight feeds such as the heavy Coalcon liquid product. They include the appropriate balance of hydrogenation to cracking activity (18, 19), controlling pore size and pore size distribution of the catalyst to optimize the residence time of large molecules like chrysene within the pore structure (4), and maximizing the contacting of catalyst, hydrogen and liquid feed (20). The hydrogenation to cracking activity ratio can be controlled using the catalyst preparative procedures previously described, and thereby changing the amount of transition metal oxide hydrogenation components (e.g. NiO) or the relative amount of cracking of solid acid component (e.g. $TiO_2 \cdot SiO_2$). The control of pore size characteristics has already been discussed in conjunction with catalyst activity and selectivity. The final factor, namely optimum contacting, can be readily achieved in laboratory experiments using the Carberry type reactor (16). Commercial operation presents some difficulty, especially with the use of trickle-bed reactors which are not very effective. Ebullating bed reactors such as that used in H-oil have some advantages in this respect.

The second mode of catalyst activity loss is thermal degradation. The two primary methods of minimizing or preventing such degradation are cationic doping of the support (12) and the use of catalyst support interactions (21). Cationic doping using alkaline and rare earth ions, for example, has been used to prepare aluminas which retain a surface area of 50 m^2/g at 1250°C (12). Also, a number of ultrastable zeolites have been synthesized which can endure comparable temperatures without loss of surface area (22). Similar effects have been reported for properly prepared mixed oxide systems (14). These advances enable one to synthesize some materials which can endure repetitive oxidative regeneration even with occasionally high thermal transients, without significant degradation.

The use of catalyst-support interactions to stabilize catalysts has been growing significantly over the past five years. It is now possible to make catalysts, for example, which are used for catalytic combustion at temperatures as high as 1400°C without significant degradation (23, 24).

Many of the common HDN or hydrocracking constituents such as Ni-Mo, Ni-W, CoMo, etc. should be amenable to similar stabilization. Data of catalysts prepared by the cogel process previously described indicates that this is indeed the case (14). In another example, molybdenum oxide is known to interact very strongly with MgO to form $Mg_2Mo_3O_8$ (25) which contains Mo_3 clusters throughout an oxide matrix. Numerous other examples can be cited (26). Catalyst-support effects represent a promising approach to thermal stabilization.

2. LONG TERM DEVELOPMENTS

In considering the impact of the advances in catalysis and related disciplines on the HDN or selective hydrocracking of Coalcon heavy liquids, three broad areas can be identified. These are new synthesis procedures, new catalytic materials and reaction studies.

a. New Synthesis Procedures

As discussed in the last section, and in more detail in Section V of Part 1, numerous new procedures have been developed for catalyst preparation. The primary value of these procedures is that many of them enable the catalytic chemist to prepare new inorganic materials in high enough surface area for adequate characterization and testing. Some techniques such as the aerogel procedure developed by Tiechner (11) have been used to prepare mixed oxide solid acids such as $NiO \cdot Al_2O_3$ and $NiO \cdot MoO_3$ with surface areas as high as $600\,m^2/g$. Such high surface area allows easy doping of these materials for chemical and structural modification. A number of other procedures which will be particularly valuable in preparing new-solid acids and mixed transition metal oxides and sulfides include the cogel, aerogel, gel precipitation and homogeneous pH change techniques (11).

b. New Materials

As will be discussed in later chapters in Part 3, the high H_2S concentrations expected in liquefaction operations present a severe constraint on the choice of active catalysts. For upgrading Coalcon heavy liquids, on the other hand, the H_2S constraint is not as important since these liquids contain very low sulfur (~.03 wt.%) levels. This means that a large number of materials are available to choose from as denitrogenation and selective hydrocracking catalysts. In addition to mixed transitional metal oxides, novel materials such as borides (27), carbides (28, nitrides (28), and mixed systems (e.g. Mo_2BC) (29) are of interest. Oxides containing metal-metal bonded clusters of pertinent atoms (e.g. Mo_3 in $Mg_2Mo_3O_8$ and $Co_2Mo_3O_8$) have not been explored for HDN and cracking activity, yet offer interesting possibilities (25). Many of these materials present the possibility of varying the metal-nitrogen bond strength which effect should influence HDN activity since it is believed that C-N bond scission is the rate determining step for this reaction (30). A more extensive discussion of this possibility can be found in the section concerning upgrading of solvent refined coal, Section V.

c. Reaction Studies

A clearer understanding of the mechanisms for HDN and selective cracking of polynuclear aromatics could contribute to the development of processes for upgrading Coalcon liquids.

As discussed in Part 1, the mechanism of the HDN reaction depends on the reaction conditions. Both C-N scission (31) as well as hydrogenation of the nitrogen heterocycle (32) can be rate determining. A good example is the difference in mechanisms between HDN of quinoline (31) and indole (32). In the analysis performed to date, pyridine seems to be the primary reported nitrogen heterocycle in Coalcon liquids. This probably is a result of the oversimplified model which was used to extrapolate western coal data to that expected for eastern coals (2). However, with varying coals and process conditions, it is expected that some amount of larger heterocyclic nitrogen ring compounds will form (e.g. carbozole, indole, quinoline, etc.). Understanding the HDN mechanism would be useful in these instances, especially since little work has been reported in this area. It is particularly important to find ways to prepare HDN catalysts with significantly improved activity, as most HDN reactions go through a maximum activity with increasing temperature (33). This is because higher temperatures favor dehydrogenation of nitrogen heterocyclic compounds and the C-N bond in the dehydrogenated form cracks only with great difficulty compared to the saturated molecule.

The interaction of H_2S, NH_3, H_2O and O_2 during HDN needs to be studied in some detail. There is already some evidence, for example, that the presence of H_2S increases the rate of HDN (33, 34). This effect is not well understood, but has been attributed to improved hydrocracking activity in the presence of H_2S.

Hydrogen donor catalysis has been reported for HDS (35), and shows significant promise. In this process an active hydrogen donor such as tetralin is used in conjunction with an HDS catalyst such as $CoO \cdot MoO_3 \cdot Al_2O_3$ to hydrodesulfurize coal liquids. The hydrogen donor-catalytic system is reported to be synergistically more effective than either the catalyst or donor separately. Only a few experiments of a similar nature have been reported for nitrogen containing compounds (35). No HDN was observed. However, with the right catalyst and donor and under the proper conditions, it is conceivable that one might observe improvements in HDN activity.

The use of a hydrogen donor overcomes some of the limitation inherent in a three-phase system. Another approach, which has received little attention to date, is the use of supercritical conditions during the catalytic reaction (36). In the present case this approach is of interest primarily because of the possibility for a significant increase in the hydrogen solubility in the fluid, a parameter that is important in both HDN and hydrocracking.

Finally, something can be said about the mechanism of selective hydrocracking of polynuclear aromatics such as chrysene and 1-2 benzofluorene. Very little definitive mechanistic work has been done in this area. The steps in cracking a four ring molecule like chrysene involve hydrogenation, isomerization and cracking (37). Center ring cracking is rarely observed (38). However, some success has been reported for the cracking of phenanthrene over $Cr_2O_3 \cdot Al_2O_3$ (38). This type of work needs to be studied in more detail mechanistically, and at conditions at which the catalyst does not significantly deactivate due to carbon deposition.

3. SUPPORTING RESEARCH

Two areas of supporting research which would be helpful in furthering the development of the upgrading of Coalcon liquids is first to foster a continued effort in characterizing Coalcon liquids from various coals and obtained at different hydrogasifier conditions; and secondly to develop the emerging powerful instrumental techniques discussed in a previous review (10) for the characterization of HDN and hydrocracking catalysts for Coalcon liquids.

F. CONCLUSIONS

Only limited data have been published concerning the Coalcon Process, and particularly the characteristics of the liquid product. However, the data which have been reported indicate that the two primary areas in which catalysis could impact on upgrading Coal liquids are development of improved processes for hydrodenitrogenation, and for selective hydrocracking of polynuclear aromatic molecules to single ring aromatics. The light liquid fraction would require HDS and HDN and possibly some hydrocracking of the paraffinic constituent depending upon use. Motor gasoline and an aromatic blending stock for diesel and jet fuels are possible products. More significant HDN and hydrocracking problems are expected in upgrading the heavy liquid product. This fraction is best suited for upgrading to refined (low sulfur and nitrogen) heating and fuel oils as well as stationary turbine fuels. With substantial selective hydrocracking, it can also be used as motor gasoline and as an aromatic blending stock for jet and diesel fuels.

In short range developments, emphasis should be put on improving existing HDN and hydrocracking catalysts. This involves making use of recently developed catalyst synthesis procedures (e.g. Cogel, Aerogel, homogeneous pH change) to improve the physical properties of known catalysts. Pore volume, pore-size distribution, crush strength and thermal stability are among those properties which can be improved by these procedures. These modifications are also expected to be useful for optimizing the activity maintenance of existing catalysts. In carrying out much of this work as well as longer range programs, it is imperative that recently reported techniques for characterizing the specific surface area of oxides be further developed. Characterization of surface properties for mixed oxides (e.g. acidity characteristics, composition, specific surface areas, etc.) are necessary for determining the intrinsic activity of these catalysts.

In longer range developments, many new materials should be tested. These include new mixed oxides, oxides which contain clusters of metal atoms, borides, carbides, nitrides and numerous other compounds with promising chemical properties. Some of these may offer the possibility of modifying the interaction between heterocyclic nitrogen atoms and the surface. This could provide a means for optimizing HDN activity. Similarly, availability of many mixed oxide materials with varying surface acidity properties are going to be important in the development of new solid acid catalysts which give selective center-ring cracking of polynuclear aromatic molecules. The mechanism of both HDN and cracking needs to be investigated.

In both short and long range studies, advances in catalytic reactor design should be utilized for testing catalysts. This is particularly the case for three phase systems such as can occur for HDN or hydrocracking of Coalcon heavy liquids. The continuous flow Carberry reactor and its modifications offer one of the least expensive yet most effective means for testing catalysts for these reactions. This type of reactor operation should also be tested in conjunction with operations at supercritical conditions, and also using hydrogen donors plus catalysts. Both of these approaches provide improved contacting for multiphase systems and minimum limitations on hydrogen diffusion to the catalyst surface.

The application of many of the above mentioned advances in catalysis and related disciplines is likely to have a significant impact not only on upgrading Coalcon coal liquids, but also on HDN and selective hydrocracking in general.

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IV. REFINING COAL LIQUIDS FROM THE COED, H-COAL AND SYNTHOIL PROCESSES TO HIGH-OCTANE GASOLINE, JET FUEL AND DIESEL FUEL

A. INTRODUCTION

The central theme of this section is, in some respects, a continuation of that for Section III, namely the upgrading and refining of coal liquids to clean-burning fuels. In Section III, a detailed discussion was given for the nature of the Coalcon process, the coal liquids which are produced and the catalytic problems anticipated in upgrading these liquids to clean-burning fuels. The Coalcon process was treated separately because, although it is anticipated to progress to the commercial stage, little has appeared in the open technical literature concerning the nature of this process and the liquids produced. The present section gives an overview of the catalytic problems and research needs for refining coal liquids from three well-known liquefaction processes: COED, H-Coal and Synthoil. Refining to high octane gasoline, jet fuel and diesel fuel will be considered.

The first three parts of this section described the nature of the COED, H-Coal and Synthoil liquids, and the refining problems that have been encountered or that can be extrapolated from the chemical and physical characteristics of the coal liquids. This is followed by a discussion of those aspects from recent advances in Catalysis (Part 1) and related disciplines (Part 2) which could potentially impact on the refining of these coal liquids to high octane gasoline, jet fuel and diesel fuel.

Of the three processes, more information is available for the physico-chemical characteristics and refining of COED liquids than for liquids from

from the Synthoil and H-coal processes. COED liquids will therefore be discussed in more detail than the others. It should, however, be noted that the problems in refining the coal liquids from any of these processes are similar, differing only in degree for certain aspects. Where possible, these similarities and differences are so indicated.

B. COED LIQUIDS

The details concerning the operation of the COED process are given elsewhere (1-10). In general, coal is pulverized, dried and then heated to successively higher temperatures in a series of fluidized-bed pyrolysis reactors. In each of these reactors a fraction of the volatile matter in the coal is released. The primary reason for thermal staging is to prevent agglomeration of the coal, and therefore each reactor is heated to a progressively higher temperature which is just below the agglomeration point of the coal. Usually four stages are required with operating temperatures of 600^{o}, 850^{o}, 1000^{o} and 1500^{o}F. However, the temperatures and number of stages are dependent upon the type of coal which is processed. The heat for each of the first three reactors is provided by burning char in the fourth reactor.

The volatile oil released by the pyrolysis process is condensed and filtered to remove char fines and ash. A typical inspection for the pyrolysis oil is given in Table IV-1 for Utah and Illinois coals. The pyrolysis oil is then hydrotreated at rather severe conditions (see Table IV-2) in a fixed bed reactor to remove sulfur, nitrogen and oxygen to produce a 25-30^{o} API synthetic crude oil product. The properties of this product are discussed below.

1. NATURE OF COED LIQUIDS

Typical data for COED syncrudes derived from western and eastern coals are given in Table IV-3. Some differences in the composition of the syncrude

TABLE IV-1

TYPICAL PROPERTIES OF COED PYROLYSIS LIQUIDS (1)

	Coal Source	
	Utah A-Seam	Illinois No. 6-Seam
Properties of Derived Oil*		
Carbon, wt.%	83.8	79.6
Hydrogen, wt.%	9.5	7.1
Nitrogen, wt.%	0.9	1.1
Sulfur, wt.%	0.4	2.8
Oxygen, wt.%	5.0	8.5
Ash, wt.%	0.3	0.9
H/C Atom Ratio	1.36	1.07
API Gravity, 60°F	-3.5	-4
Moisture, wt.%	0.5	0.8
Pour Point, °F	100	100
Viscosity, SUS 210°F	390	1333
Solids, wt.%	3.8	4.0
Gross Heating Value, Btu/lb.	16,100	15,050

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(1) All percentages on dry basis.

TABLE IV-2

TYPICAL HYDROTREATING CONDITIONS FOR ILLINOIS NO. 6-SEAM COED PYROLYSIS LIQUIDS (1)

Catalyst:	NiMo on Alumina extrudates
Pressure:	1750-2500 psig
Temperature:	700-800°F
Space Velocity:	0.3-0.6 lb. oil/hr./lb. catalyst
Gas Recycle Rate:	40M to 80M SCF/bbl.
Gas Recycle Concentration:	90-95% H_2
Hydrogen Consumption:	3500 SCF/bbl.

TABLE IV-3

TYPICAL DATA FOR COED SYNCRUDES DERIVED FROM WESTERN AND EASTERN COALS (10)

Coal Source		
Mine	Illinois Peabody	Utah King
Seam	No. 6	A
Rank	HvbC	HvbB
Hydrocarbon Type Analysis, Lvol%		
Paraffins	10.4	23.7
Olefins	NIL	NIL
Naphthenes	41.4	42.2
Aromatics	48.2	34.1
API Gravity, 60°F	28.6	28.5
ASTM Distillation, °F		
Initial Boiling Point (IBP)	108	260
50% distilled	465	562
End Point (EP) (1)	746	868
Fractionation		
Yields, wt.%		
IBP-180°F	2.5	0
180-390°F	30.2	5.0
390-525°F	26.7	35.0
525-650°F	24.4	30.0
650-EP	16.2	30.0

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(1) 95% except for Illinois No. 6 which is 98%

are apparent for the two coals. The high volatility bituminous Illinois coal gives a more aromatic syncrude and much less paraffins than the western Utah coal. Both crudes are highly naphthenic (cyclic paraffins) in nature. The western coal also has a larger amount of high molecular weight fraction than the eastern coal as shown by the greater fraction boiling in the 650°F to end point range. This is in contrast to the composition predicted for Coalcon liquids which, according to the product composition model discussed in Section III, are predominantly aromatic and low in naphthenes and paraffins. As shown later, similar high aromaticity is also found for coal liquids produced by the H-coal and Synthoil processes.

A chemical analysis for the COED syncrude derived from Illinois No. 6-Seam coal is given in Table IV-4. By comparison of these data with those in Table IV-1 it is apparent that the fixed-bed hydrofining process increases the °API gravity (decreases specific gravity),(a) increases the H/C atom ratio from 1.07 to 1.58; decreases the sulfur content from 2.8 to 0.068 wt%, nitrogen from 1.1 wt.% to 324 ppm and oxygen from 8.5 to 0.64 wt.%. Table IV-4 also shows that of the 48.2 wt.% aromatic content, 14.1 wt.% is a polynuclear aromatic fraction (number of rungs $>$ 2). As discussed later the polynuclear aromatic fraction can cause severe catalyst deactivation under certain processing conditions.

Analysis of the syncrude fraction for two samples of an Illinois No. 6-Seam coal is given in greater detail for the initial boiling point (IBP) to

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(a) °API gravity and specific gravity are related at 60°F by the following relationship:

$$\text{Sp. gr. } (60^{o}\text{F}) = \frac{141.5}{131.5 + {}^{o}\text{API}}$$

TABLE IV-4

ANALYSIS OF COED SYNCRUDE DERIVED FROM ILLINOIS NO. 6-SEAM COAL (10)

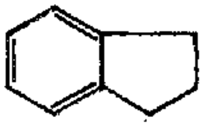
GENERAL SPECIFICATIONS

Gravity, °API at 60°F	28.6
Flash Point, °F	70
Pour Point, °F	-55
Carbon Residue (Ramsbottom), Wt. %	0.20
Hydrogen, Wt. %	11.30
Carbon, Wt. %	85.65
Sulfur, Wt. %	0.068
Nitrogen, ppm by Weight	324
Oxygen, Wt. %	0.64
H/C, Atom Ratio	1.58

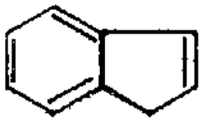
HYDROCARBON COMPOSITION

	Vol. %
Paraffins	10.4
Cyclo Paraffins	41.4
Mono Aromatics	34.1
Polynuclear Aromatics	14.1

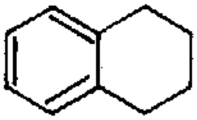
390°F fraction, the 390-650°F fraction and the 650°F^{+} fraction in Tables IV-5, IV-6 and IV-7, respectively. The IBP-390°F fraction (Table IV-5) is primarily a mixture of light and heavy naphthas and is highly naphthenic, containing 70-80 volume % mono- and dicycloparaffins. As will be indicated later, this naphtha composition is very easily converted to a high octane gasoline blending stock. The 390-650°F fraction (Table IV-6) corresponds to what might be considered a mixture of kerosene (b.p. 300-500°F) and light gas oil (b.p. 400-650°F). It is also naphthenic in character, however with an increasing fraction of polynuclear aromatics, particularly concentrated in indan, indene, tetralin and acenaphthalenes structures.



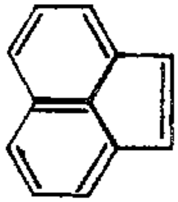
INDAN



INDENE



TETRALIN



ACENAPHTHALENE

In petroleum terminology the 650°F^{+} fraction (Table IV-7) contains medium and heavy gas oils; lube oils and waxes; and residuum. It should be noted that the total wt.% paraffins is about the same as in the other two previous fractions. The naphthene content has decreased from that in the lighter fractions and the total aromatics, particularly the polynuclear aromatics, has increased substantially. It can also be seen that significant differences can occur in the composition of the liquid fraction obtained from the same coal seam. A striking example is shown in Table IV-7 where for two different samples from No. 6-seam Illinois coal analysis gives 37.1 and 15.7 wt.% polynuclear aromatics. It is not clear at this point whether this indicates a difference in coal composition or a variation in processing conditions.

COED liquids have recently been analyzed in even greater detail with respect to specific chemical compounds for a western (Utah)(12) and eastern

TABLE IV-5

ANALYSIS OF THE IBP-390°F FRACTION OF COED SYNCRUDE FOR TWO DIFFERENT SAMPLES DERIVED FROM ILLINOIS NO. 6-SEAM COAL (10)

API Gravity, 60°F	43.8	43.3
Composition, Vol. %		
Paraffins	7.1	6.3
Monocycloparaffins	58.9	66.4
Dicycloparaffins	12.3	12.8
Tricycloparaffins	0.2	0.2
Alkylbenzenes	19.8	13.1
Indans/Tetralins	1.7	1.2
Naphthalenes	0.0	0.0

TABLE IV-6

ANALYSIS OF THE 390-650°F FRACTION OF COED SYNCRUDE FOR TWO DIFFERENT SAMPLES DERIVED FROM ILLINOIS NO. 6-SEAM COAL (10)

API Gravity, 60°F	22.5	21.7
Composition, Vol. %		
Paraffins	10.9	8.0
Monocycloparaffins	11.1	14.3
Dicycloparaffins	10.1	8.9
Tricycloparaffins	5.9	7.3
Alkylbenzenes	9.4	9.6
Indans/Tetralins	17.1	16.1
Indenes	17.3	22.0
Naphthalene	0.3	0.0
Naphthalenes	4.6	5.2
Acenaphthenes	7.3	4.5
Acenaphthalenes	5.4	3.1
Tricyclic Aromatics	0.6	1.0

TABLE IV-7

ANALYSIS OF THE 650°F$^+$ FRACTION OF COED SYNCRUDE FOR TWO DIFFERENT SAMPLES DERIVED FROM ILLINOIS NO. 6-SEAM COAL (10)

API Gravity, 60°F	11.2	13.0
Composition, Wt. %		
Total Paraffins	10.9	5.8
Monocycloparaffins	11.3	16.5
Polycycloparaffins	7.7	13.4
Total Monoaromatics	33.0	48.6
Diaromatics	13.7	9.2
Triaromatics	8.9	2.4
Tetra-aromatics	9.6	2.7
5-Ring Aromatics	4.9	1.4
Total Polynuclear Aromatics	37.1	15.7
Total Saturates	29.9	35.7
Total Aromatics	70.1	64.3

Kentucky) coal (13). The results of these studies generally agree with the more detailed data presented above in that the syncrudes analyzed contained hydrocarbon types similar to those found in petroleum crudes, however much more aromatic and naphthenic in character than petroleum crudes. The syncrudes were also found to contain substantial amounts of oxygenates and had a uniform distribution of nitrogen compounds across the boiling range unlike most petroleum crudes. These nitrogen compounds ranged from pyridine to complex carbazole structures. The sulfur content while low is contained in heterocyclic aromatic structures. Finally, the fraction of aromatics containing rings greater than two was sizeable in 390-650° and 650°F+ fractions.

The data discussed above are useful for understanding the nature of the problems involved in refining COED coal liquids. These problems are described next.

2. REFINING PROBLEMS

In considering the refining problems in converting COED syncrude to high octane gasoline, jet fuel and diesel fuel, it is useful to look at the extensive work done by Atlantic Richfield Co. (ARCO) in a subcontract from FMC Corp. (10). In this work studies were carried out on a syncrude derived from Illinois No.6-seam coal. This work included:

-Hydrogen pretreatment and reforming of naphtha fractions

-Evaluation of middle distillate oils as jet, diesel, and home heating fuels

-Fluidized-bed catalytic cracking of the atmospheric bottoms fraction.

-Hydrocracking of the atmospheric bottoms fraction.

Each of these aspects is discussed below, where appropriate, for the refining of COED syncrude to high-octane gasoline, jet fuel and diesel fuel.

a. High-Octane Gasoline

The naphthas (180-390°F) distilled from COED syncrude are highly naphthenic, containing about 70% naphthenes (cycloparaffins), 10% paraffins and 20 percent aromatics. This is an easy naphtha to process since the naphthenes readily dehydrogenate and/or isomerize over conventional reforming catalysts (e.g., Pt/Al_2O_3) to high octane aromatics. The dehydrogenation also yields a substantial amount of hydrogen (1400-2000 SCF/bbl compared to 1100-1400 SCF/Bbl for a petroleum naphtha). However, because of the presence of sulfur (~100 ppm) and nitrogen (~100 ppm), the naphtha must be hydrotreated to reduce each of these catalyst poisons to less than 2 ppm.

Because the COED naphthas are highly naphthenic in nature, they also give rise to high catalyst activity maintenance during reforming, even for conventional Pt/Al_2O_3 catalysts. The ARCO study (10) indicates that catalyst aging for COED naphthas (as measured by Δ RONC[a] per 100 hours of operation) was -0.2 to -2 units, which compares with about -4 units for petroleum naphthas. In addition the yields of reformate (gasoline blending stock) is substantially higher than from conventional petroleum naphthas. For example, operating at conditions which yield a 100 RONC product, a typical petroleum naphtha gave 75.5 volume % yield of C_5^+ fraction, compared to 91 volume % for the COED naphtha.

From the above it is clear that conventional catalytic reforming of COED naphthas to high-octane gasoline should not present a significant problem. However, it should be noted that an additional reason for the high catalytic activity maintenance in reforming a COED naphtha is the low concentration of polynuclear aromatic molecules (Table IV-5). Should these increase in

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(a) Research Octane Number Clear, measured in Δ RONC units.

concentration one would expect to see a decrease in catalyst life during reforming due to carbon deposition.

The major problems in the refining of COED liquids to high octane gasoline are encountered with the $650^{\circ}F^{+}$ fraction. Fluid cracking or fixed bed hydrocracking is required to increase the gasoline and middle distillate yield. The ARCO work (10) showed that prior to catalytic cracking of COED syncrude atmospheric residuum, it was necessary to hydrotreat this fraction to lower the polynuclear aromatics and nitrogen content. The polynuclear aromatics enhance carbon deposition on the catalyst and the nitrogen poisons the acidic cracking sites. A rather severe hydrotreatment is necessary, e.g., 0.6 WHSV, $700^{\circ}F$, 2000 psig pressure and a hydrogen rate of 6000 SCF/bbl. However, contrary to what is observed for petroleum atmospheric residuum, the corresponding fraction obtained from COED syncrude has a very low nickel and vanadium content. The latter generally results in excessive catalyst poisoning with conventional cracking catalysts. The gasoline yield from fluid catalytic cracking of the hydrotreated COED atmospheric residuum was 51% which compares favorably with a 54% yield from a Mid-Continent petroleum gas oil.

The results of the ARCO study showed the COED $650^{\circ}F^{+}$ fraction to be very difficult for hydrocracking to gasoline and middle distillates. This difficulty arises from two sources. First, the heterocyclic nitrogen (which must be reduced from 800 ppm to less than 10-20 ppm for conventional hydrocracking to prevent catalyst poisoning), is difficult to remove. High severity HDN (0.33 WHSV, $750^{\circ}F$, 2000 PSIG pressure and 6000 SCF/bbl. H_2 flow rates) did not reduce the nitrogen below about 40 ppm. Presumably this nitrogen is contained in very refractory heterocycles. The second source of processing problems results from the high content of 4 and 5 ring aromatics in the $650^{\circ}F^{+}$ fraction. These compounds adsorb very strongly on the catalyst surface, thereby promoting carbon deposition and decreasing catalyst life. The only way the 650°F$^+$ fraction could be processed by ARCO was to fractionate it into a 650-800°F cut (84%) and an 800°F$^+$ cut (16%). The latter is reportedly a reasonable blending stock for No. 6 fuel oil because of its low sulfur level and reasonable Conradson carbon and polynuclear aromatics level (10). Hydrocracking the 650-800°F fraction gives a normal product yield distribution, but involves a much higher hydrogen feed rate (12,000 SCF/bbl.) than for a corresponding petroleum feedstock (6000 SCF/bbl.). Also, the hydrocracking catalyst still underwent excessive deactivation indicating that conventional hydrocracking technology would not be feasible for COED heavy liquids.

b. Jet Fuel

The middle distillate fraction (390-650°F) from COED syncrude can be processed to both jet and diesel blending stocks. The quality of this fraction varies with the coal source. For Illinois No. 6-seam coal the middle distillate fraction is highly aromatic and therefore has poor physical and chemical properties as a jet fuel. However, hydrotreating this fraction improves the product quality somewhat so that it can be used as a jet fuel blending stock with petroleum-derived feedstocks.

As can be seen from the data in Table IV-8, the "as-distilled" 390-525°F fraction does not meet the primary jet fuel specifications for a number of parameters including density, aromatics content, smoke point, luminosity and net heating value (10). In an attempt to overcome some of these limitations the ARCO workers hydrotreated the feed. Initial hydrogenation studies were at 600-700°F, 1000-2000 psig pressure, 1.0 WHSV and 5000 SCF/Bbl H_2 flow rate. Temperatures above 650°F and pressures greater than 1500 PSIG were required to meet the minimum aromatics level specification for JP-5. However, even at these conditions the product could not meet the minimum smoke point specification. This is probably due to the very high concentration of cycloparaffins in the product. The only way in which the smoke point specification could be

TABLE IV-8

COMPARISON OF COED JET FUEL FRACTION WITH JP-5 JET FUEL SPECIFICATIONS(10)

Properties	JP-5	COED Jet Fuel (390-525°F)	
		As Distilled	2 Stage HDS (a)
ASTM 10% Distillation Point, °F	400 max.	436	412
ASTM Distillation End Point, °F	550 max.	530	526
Gravity, °API, 60°F	36-48	25.7	33.2
Sulfur, Weight %	0.4 max.	0.007	0.001
Freezing Point, °F	-51 max.	<-70 (b)	<-80 (b)
Net Heating Value, Btu/lb.	18300 min.	18070 (b)	18390 (b)
Aniline Gravity Product (c)	4500 min.	1490	4501
Aromatics, Liquid Volume %	25 max.	60.7	0 - 5
Olefins, Liquid Volume %	5 max.	0	0
Smoke Point (d)	19 min.	10	22
Luminometer Number (e)	50 min.	20.4 (b)	43.6 (b)
Flash Point	140 min.	186	156
Copper Corrosion Test (f)	1	1	---

(a) After hydroprocessing of 390-525°F syncrude fraction.

(b) Calculated.

(c) A measure of the aromaticity of an oil.

(d) A measure of the smoke and soot-producing characteristics of jet fuels.

(e) A measure of the flame temperature of jet fuels.

(f) A measure of the corrosiveness of oil to copper, a "1" designation indicates slight tarnish.

met was by using a second stage noble metal (Pt) hydrogenation to reduce the aromatic level virtually to zero. This required 700°F, 2000 psig pressure, 5000 SCF/bbl H_2 flow rate and 2 WHSV. Even this severe treatment was insufficient. It is expected that only by selective cracking of the cycloparaffins to branched and linear paraffins will all the specifications of jet fuel be achieved. It would require low temperatures and high hydrogen pressure to prevent the formation of aromatics. It is questionable whether this would be a cost-effective process because with less processing it is possible to make an aromatics feedstock for gasoline blending. Much would depend on the selectivity of a hydrocracking process which could bring about this transformation.

c. Diesel Fuel

The 525-650°F fraction distilled from COED syncrude is highly aromatic and therefore does not meet diesel specification because of high density (19° API vs. 33-37 °API) and low cetane numbers (10). Furthermore, the aromaticity of this fraction gives it high oxidation stability which makes it a poor diesel fuel.

A 390-650°F fraction can be distilled from the middle distillate cut which meets diesel fuel specifications for flash, distillation and pour point, but high aromaticity still give an unacceptably low gravity and cetane number. If the 390-525°F fraction is hydrotreated it just meets gravity specifications, but has a low final boiling point. These data are presented for comparison in Table IV-9.

The problems in converting COED syncrude to a diesel fuel are, therefore, similar to those for producing a jet fuel. It might be possible to use an active, high activity maintenance catalyst to hydrotreat the middle-distillate fraction to a paraffinic-cycloparaffinic fuel which would just

TABLE IV-9

COMPARISON OF A COED DIESEL FUEL FRACTION WITH ASTM SPECIFICATIONS (10)

Properties	Specifications	390-650°F	525-650°F	390-525°F	390-525°F Fraction 2 Stage HDS (1)
		As Distilled			
Pour Point, °F	0 Maximum	-70	-20	< -80	< -80
Flash Point, °F	130 Minimum	215	300	186	156
Sulfur, Weight %	Legal	<.001	<.001	.007	<.001
ASTM Distillation, °F					
10% distilled	460 Maximum	459	562	436	412
50% distilled	--	(5)	588	455	437
90% distilled	620 Maximum	586	626	494	483
100% distilled	660 Maximum	613	(5)	530	(5)
Gravity, °API, 60°F	33 - 37	22.5	19	25.7	33.2
Cetane Number (3)	30 Minimum	18	24	23.0	>30 (2)
Aniline Point, °C (4)	--	(5)	(5)	14.3	58.2
Aromatics, Liquid Volume %	--	(5)	(5)	58.3	5.2

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(1) After hydroprocessing of 390-525°F fraction of syncrude.

(2) Estimated.

(3) A measure of the ignition quality of diesel fuel.

(4) A measure of the aromaticity of oil.

(5) Not measured.

meet product specifications. The most desirable product (paraffins and branched paraffins) can only be made by selective hydrogenation and hydrocracking. This would require substantially greater amounts of hydrogen.

C. H-COAL LIQUIDS

The H-coal process is based on the H-oil process which was developed several years ago by Hydrocarbon Research, Inc. (HRI) for hydrotreating heavy petroleum feedstocks (14-16). The key aspect of the process is the ebullating-bed reactor into which is fed a slurry of hydrogen, coal, coal-liquids and catalyst. The catalyst is promoted cobalt molybdate with appropriately modified physical properties (e.g., attrition characteristics, pore-size distribution, etc.). The coal is hydrogenated and converted to liquid and gaseous products. Careful sizing of the coal and catalyst particles permits unconverted coal, ash, liquids and gases to leave the reactor without loss of catalyst from the reactor. Catalyst is usually added or withdrawn continuously to maintain constant activity.

An advantage of the ebullating bed is the highly effective contacting of coal, hydrogen, liquids and catalyst in this multiphase system. The product quality is a function of the operating variables, particularly temperature, pressure and catalyst to coal ratio. A brief description of the nature of the liquid product is presented next.

1. NATURE OF H-COAL LIQUIDS

Depending upon process conditions the H-coal process produces either a syncrude or low-sulfur fuel oil. A typical composition of both product types is given in Tables IV-10 to IV-12 for the liquefaction of Illinois No. 6-seam coal. As can be seen from the data in Table IV-10 the percent coal converted is about the same whether a syncrude or fuel oil is produced.

TABLE IV-10

PRODUCT DISTRIBUTION FOR H-COAL LIQUIDS DERIVED FROM ILLINOIS NO. 6-SEAM COAL (14)

	Product	
	Synthetic Crude	Low-Sulfur Fuel Oil
Normalized Product Distribution		
C_1-C_3 Hydrocarbons	10.7	5.4
C_4-400°F Distillate	17.2	12.1
400-650°F Distillate	28.2	19.3
650-975°F Distillate	18.6	17.3
975°F+ Residual Oil	10.0	29.5
Unreacted Ash-Free Coal	5.2	6.8
H_2O, NH_3, H_2S, CO, CO_2	15.0	12.8
Total (100.0 + H_2 Reacted)	104.9	103.2
Conversion, %	94.8	93.2
Hydrogen Consumption, SCF/Ton	18,600	12,200

TABLE IV-11

PRODUCT YIELD FOR H-COAL LIQUIDS DERIVED FROM ILLINOIS NO. 6-SEAM COAL (14)

	Product	
	Synthetic Crude	Low-Sulfur Fuel Oil
Wt.% of M.A.F. Coal	74.0	78.2
Barrels Per Ton of M.A.F. Coal		
C_4-400°F	1.32	0.90
400-650°F	1.64	1.14
650-975°F	0.98	0.89
975°F$^+$	0.44	1.39
	4.38	4.32

TABLE IV-12

PRODUCT INSPECTION OF C_4^+ LIQUIDS FROM H-COAL PROCESSING OF ILLINOIS NO. 6-SEAM COAL (14)

	Product	
	Synthetic Crude	Low-Sulfur Fuel Oil
°API Gravity	15.0	4.4
Hydrogen, Wt.%	9.48	8.43
Sulfur, Wt.%	0.19	0.43
Nitrogen, Wt.%	0.68	1.05

However, the latter involves a lower hydrogen consumption and therefore gives a higher molecular weight product (Table IV-11). The amount of sulfur and nitrogen present in the syncrude product (Table IV-12) is higher than that in COED syncrude. However, it should be recalled that the COED syncrude is given a rather severe hydrotreating in the fuel processing step.

A detailed compositional breakdown for various fractions distilled from the H-Coal syncrude product is given in Tables IV-13 to IV-15.

Table IV-13 shows that the C_4-400°F or naphtha fraction is somewhat similar to COED naphthas in that they are both highly naphthenic in content. However, the H-coal naphtha contains a greater fraction of polynuclear aromatic rings than a typical COED naphtha. This is shown by the approximately 8 wt.% content of indans, naphthalenes and various phenols (Table IV-13).

The middle distillate (400-650°F) fraction from H-coal is highly aromatic with 47.0 of the 59.6 wt.% aromatics being polynuclear in character (Table IV-14). The middle distillate fraction also contains about 5 wt.% heterocyclic molecules which are primarily 2 wt.% phenols, the remainder containing sulfur and nitrogen compounds.

The heavy or residuum fraction (650-919°F) consists mostly of polynuclear aromatics. Thus Table IV-15 shows that 91.6 wt.% of this fraction is aromatic and, of this, 72.8 wt.% consists of aromatic rings larger than naphthalene. The most prevelant are naphthalenes, phenanthenes, chrysenes and pyrenes. The heterocyclic content of this fraction is about 14 wt.%, containing primarily sulfur and nitrogen compounds.

Although it is probable that more detailed analyses of H-coal liquids have been done, the data is not available in the open literature.[a] Nevertheless,

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(a) A detailed analysis is about to be published by workers at the Bartlesville Energy Research Center. However, this document was not available for publication during the performance of this study.

TABLE IV-13

COMPOSITION OF C_4-400°F FRACTION FOR H-COAL LIQUIDS FROM ILLINOIS NO. 6-SEAM COAL (17)

Paraffins

Component	Wt. %
nC_4	0.10
iC_5	0.20
nC_5	0.69
C_6	2.48
C_7	2.87
C_8	2.08
C_9	1.59
C_{10}	1.19
C_{11}	0.69
C_{12}	0.10
	11.99

Alkyl Benzenes

Component	Wt. %
C_6	0.89
C_7	3.77
C_8	4.76
C_9	4.16
C_{10}	2.58
C_{11}	1.29
C_{12}	0.10
	17.55

Saturated Naphthenes

Component	Wt. %
Monocycloparaffins	42.64
Dicycloparaffins	8.50
Tricycloparaffins	0.19
	51.33

Other Compounds

Component	Wt. %
Indans	6.44
Naphthalenes	0.59
Phenols (MW)	
108	0.13
122	0.56
136	0.19
150	0.02
	7.93

Total = 100.00 Wt. %

Unsaturated Naphthenes

Component	Wt. %
Monocycloparaffins	5.32
Dicycloparaffins	4.98
Tricycloparaffins	0.90
	11.20

TABLE IV-14

COMPOSITION OF 400-650°F FRACTION FOR H-COAL LIQUIDS FROM ILLINOIS NO. 6-SEAM COAL (17)

Saturated Compounds

Component	Wt. %
n-paraffins	4.8
i-paraffins	1.7
Monocycloparaffins	14.0
Dicycloparaffins	7.9
Tricycloparaffins	2.6
	31.0

Aromatic Compounds

Component	Wt. %
Alkyl Benzenes	12.6
Indans & Tetralin	30.8
Indenes	5.7
Naphthalene	0.2
Naphthalenes	3.5
Acenaphthenes (C_nH_{2n-14})	4.0
Acenaphthenes (C_nH_{2n-16})	2.2
Tricyclics (C_nH_{2n-18})	0.4
	59.6

Unsaturated Non-Aromatic

Component	Wt. %
Monocycloparaffins	4.3
	4.3

Other Compounds

Component	Wt. %
Phenols (MW)	
108	0.04
122	0.52
136	0.98
150	0.38
164	0.07
178	0.01
Other Non-Hydrocarbons	3.10
	5.10

Total = 100.00 Wt. %

TABLE IV-15

COMPOSITION OF 650-919°F FRACTION FOR H-COAL LIQUIDS FROM ILLINOIS NO. 6-SEAM COAL (17)

Saturated Compounds

Component	Wt. %
Paraffins	1.4
Monocycloparaffins	3.1
Bicycloparaffins	0.6
Tricycloparaffins	0.7
Tetracycloparaffins	0.4
Pentacycloparaffins	0.2
Hexacycloparaffins	0.1
Phenyls	0.3
	6.8

Unsaturated Non-Aromatic

Component	Wt. %
Paraffins	0.0
Monocycloparaffins	0.5
Bicycloparaffins	0.3
Tricycloparaffins	0.2
Tetracycloparaffins	0.2
Pentacycloparaffins	0.1
Hexacycloparaffins	0.1
Phenyls	0.2
	1.6

Other Compounds

Component	Wt. %
Alkyl Benzenes	3.0
Indans &/or Tetralins	0.5
Other Aromatics*	72.8
Other Non-Hydrocarbons	13.8
	91.6
Total	100.0 Wt. %

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* An approximate breakdown of Aromatic-type compounds is given below

Component Type	Millimoles/100 grams
Naphthalenes	93.4
Phenanthrenes	91.1
Chrysenes	21.9
1-2 Benzanthracenes) 3-4 Benzphenanthrenes)	14.6
Pyrenes	15.4
5 Ringed Compounds	5.1