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PRODUCTION OF JET FUELS FROM COAL-DERIVED LIQUIDS

Vol VIII - Heteroatom Removal by Catalytic Processing

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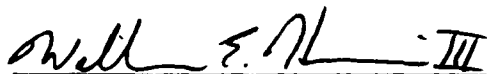
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In September 1986, the Fuels Branch of the Aero Propulsion Laboratory at Wright-Patterson Air Force Base, Ohio, commenced an investigation of the potential of the production of jet fuel from the liquid by-products streams produced by the gasification of lignite at the Great Plains Gasification Plant in Beulah, North Dakota. Funding was provided to the Department of Energy (DOE), Pittsburgh Energy Technology Center (PETC), to administer the experimental portion of this effort. This report details the program with the University of North Dakota Energy and Mineral Research Center (UNDEMRC) to study the removal of heteroatoms and the saturation of aromatics found in the Great Plains tar oil stream. UNDEMRC tested a processing approach consisting of multiple-stage hydrogenations. Testing was conducted in a one-gallon, hot-charge, semi-batch autoclave. Statistical experiments were conducted to select optimum process conditions.			
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FOREWARD

In September 1986, the Fuels Branch of the Aero Propulsion Laboratory at Wright-Patterson Air Force Base, Ohio, commenced an investigation of the potential for production of jet fuel from the liquid by-product streams produced by the gasification of lignite at the Great Plains Gasification Plant located in Beulah, North Dakota. Funding was provided to the Department of Energy (DOE) Pittsburgh Energy Technology Center (PETC) to administer the experimental portion of this effort. This report details the effort of the University of North Dakota Energy and Mineral Research Center (UNDEMRC), who, as a contractor to DOE (DOE Contract Number DE-AC22-87PC90016), modeled the heteroatom removal of the liquids via hydrogenation technologies. DOE/PETC was funded through Military Interdepartmental Purchase Request (MIPR) FY1455-86-N0657. Mr. William E. Harrison, III, was the Air Force Program Manager, Mr. Gary Steigel was the DOE/PETC Program Manager, and Mr. John Rindt was the UNDEMRC Program Manager.

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EXECUTIVE SUMMARY

In an effort to assure adequate supplies of aviation turbine fuels in the event of a petroleum shortage, the U.S. Air Force has investigated the use of coal-derived liquids to produce synthetic aviation fuel. This report details the results of research performed at the University of North Dakota Energy and Mineral Research Center on liquid by-product streams from the Great Plains Gasification Plant (GPGP) in Beulah, North Dakota. The primary research objective was to assess the technical and economic feasibility of producing aviation turbine fuels from coal liquids streams. A secondary objective was to assess the possibility of converting the by-product streams into a new, higher-density aviation fuel. To accomplish these objectives, the by-product streams were characterized to determine which streams, if any, were suitable for upgrading; the tar oil stream was found to be suitable. A two-stage upgrading method was chosen; heteroatoms were removed in the first, more severe, stage and hydrogenation took place in the second stage. Processing was performed in a one-gallon, hot-charge autoclave system. A statistical experimental design was used to efficiently determine the "optimum" conditions necessary for heteroatom removal during the first-stage processing. Verification runs performed at the indicated optimum conditions resulted in virtually complete removal of heteroatoms. The total mass balance on liquid product corroborated the analytical workups. Second-stage processing of the first-stage product did not result in the necessary increase in aliphatic content. The fact that the aliphatic content did not increase is probably a result of choice of catalyst and/or the conditions under which the second-stage processing was performed. The results of this research indicate that catalyst choice may greatly influence the product obtained. The first-stage products which were obtained appear to be excellent candidates for high-density fuels due to their high aromaticity; however, the second-stage catalysts which were used were not effective in converting aromatics to cyclic aliphatics to produce a product with the required low aromatic content.

INTRODUCTION

Domestic production currently supplies only approximately 60 percent of the United States' petroleum requirements, and future oil supplies, both domestic and foreign, will continue to be unreliable. Synthetic liquid fuels are therefore an essential part of an energy scenario which provides the United States with a means to reduce its reliance on imported oil. The Department of Defense is the largest single consumer of liquid fuels in the United States, with the U.S. Air Force using approximately 240,000 barrels of Grade JP-4 turbine fuel daily for aircraft operations. A naphtha-based fuel, JP-4 is used primarily in the U.S., while a kerosene-type fuel, JP-8, is used abroad. Because of the need to assure adequate supplies of both JP-4 and JP-8 fuels at acceptable costs, the Air Force has investigated the characteristics, cost, and yield of these fuels when produced from tar sands, shale oil, and heavy oils, and is seeking similar data for coal-derived liquids.

One producer of coal-derived liquids is the Great Plains Gasification Plant (GPGP) in Beulah, North Dakota. The plant currently produces over 150 million cubic feet per day of high-Btu synthetic natural gas (SNG) from North Dakota lignite. In addition, GPGP generates three liquid streams (rectisol naphtha, crude phenol, and tar oil) which are candidates for upgrading to jet fuel.

PROJECT OBJECTIVES

The primary objective of this project was to assess the technical and economic feasibility of producing aviation turbine fuels from the GPGP by-product streams. A secondary project objective was to assess the possibility of converting the by-product streams into a new, higher-density aviation fuel.

SPECIFICATIONS OF AVIATION FUELS

Aviation turbine fuels have a specific gravity of approximately 0.7-0.8, a minimum hydrogen content of approximately 13.0 weight percent, a maximum boiling temperature of approximately 320°-330°C, and a maximum aromatic content of 25 volume percent. The properties of the JP-4 and JP-8 aviation turbine fuels used by the U.S. Air Force are listed in Table 1. The table also compares the properties of these fuels to the preliminary specifications for the higher-density near-term JP-8X.

FEEDSTOCK CHARACTERISTICS

As mentioned previously, three liquid streams (rectisol naphtha, crude phenol, and tar oil) are produced at the GPGP as a result of coal gasification. Complete characterizations of the three streams were performed and reported by Knudson (1) and Rossi (2). An overview of the characteristics of these streams is presented here.

The rectisol naphtha stream contains primarily benzene and toluene, the crude phenol stream contains primarily phenols and cresols, and the tar oil stream is comprised mainly of methylated one- and two-ring aromatics. Table 2 presents the results of elemental analyses and, Table 3 presents the results of NMR analyses of the three streams.

The tar oil stream is the only stream with enough material in the correct boiling range to warrant consideration for upgrading to jet fuel. The rectisol naphtha stream is very volatile, and only a small portion of it is in the volatility range of a jet fuel. The distillation distribution of the crude phenol stream overlaps that of aviation fuel; however, due to its composition (primarily phenol and the cresols), it would produce cyclohexane and methylcyclohexane during hydrogenation and would therefore consume a large quantity of hydrogen. The results of ASTM D86 distillations performed on the three coal liquid streams and an aviation fuel, AV Jet A, are presented in Table 4. As the table shows, the tar oil stream contains sizable fractions in the aviation fuel distillation region. The ASTM D86 distillation profile of the tar oil stream is compared to the profiles of JP-4 and JP-8 in Figure 1.

As recovered, the tar oil stream is somewhat variable, depending on coal properties, gasifier operation, gas quenching, and product storage (3,4). It is fairly typical of the products of low-rank coal pyrolysis or carbonization in that it is largely hydrogen-deficient and oxygen-rich in comparison to either direct liquefaction or petroleum products (5,6,7). This tar oil stream contains significant hydroxyl functionality, aiding its retention of 1-4 weight percent water. It can also contain several weight percent coal and char fines, which are dependent upon gasifier operation and, to a lesser extent, upon coal quality (4).

TABLE 1
PROPERTIES OF JP-4, JP-8, AND JP-8X AVIATION TURBINE FUELS

Property	JP-4 ^a	JP-8 ^a	Near Term JP-8X
Specific Gravity @ 15°C/15°C	0.710 - 0.802	0.788 - 0.845	0.850 min
Hydrogen, min wt %	13.6	13.5	13.0
Boiling Range, °C (ASTM D-2887)	Report - 320	Report - 330	Report - 330
H _C , Net Btu/gal x 10 ⁻³	-- ^b	120.9 min	130 min
Freezing Point, °C max	-56	-50	-47
Aromatics, max vol %	25.0	25.0	25.0
Paraffins, vol %	---	---	---

^a Specification properties from "Handbook of Aviation Fuel Properties," CRC Report No. 350, Coordinating Research Council, Inc., Atlanta, GA, 1983.

^b Not specified.

The results of the D86 distillation illustrate another problem associated with upgrading the tar oil: the bottoms are unstable at moderate temperatures. Distillation bottoms content can range from under 4 weight percent to over 20 weight percent, depending on the heating rates. This drawback can be easily corrected using any one of a number of mild hydrotreating processes that are commercially proven (8).

The high heteroatom (oxygen, sulfur, and nitrogen) content of the tar oil stream will require well over a thousand scf of hydrogen to remove. The data also show that distillation by itself will not produce clear-cut fractions between high and low oxygen functionality. However, effective fractionation using solvent extraction processes such as the Pitt-Consol or Phenoraffin has been demonstrated commercially with similar streams (8). Thus it appears that removal of the phenols from the tar oil stream by solvent extraction would be the preferred processing option. The phenols could be included with the crude phenol stream for sale as

TABLE 2
RESULTS OF THE ELEMENTAL ANALYSIS
OF THE GPGP LIQUID BY-PRODUCTS STREAMS^a

Element	Tar Oil	Crude Phenol	Rectisol Naphtha
Carbon	83.76	72.18	87.65
Hydrogen	8.83	7.49	10.12
Nitrogen	0.52	0.28	0.00
Sulfur	0.39	0.04	0.00
KF-water ^b	1.20	4.48	
THFI ^c	0.11	0.00	

^a Given in weight percent as-received sample.

^b Water determined by Karl Fisher titration.

^c Tetrahydrofuran insolubles (0.5 micron filter).

phenols or cresylic acids. The remaining two-thirds of the tar oil stream could be hydrotreated to produce jet fuel.

UPGRADING COAL LIQUIDS TO JET FUEL

To produce specification-grade jet fuel from coal-derived liquids, the concentration of oxygen, sulfur, and nitrogen in the feedstock must be reduced to virtually nil, and most of the aromatic rings must be saturated. If saturation can be accomplished without destroying the ring structures, the most economical use of hydrogen is assured.

Upgrading of the coal-derived liquids may be accomplished in a high-severity single stage or in multiple stages (9,10). Product composition can be controlled to a large degree by reaction severity; i.e., temperature, pressure, space velocity, or catalyst composition. The single- or first-stage hydrotreating is designed to remove the heteroatoms from the feedstock. Typical operating conditions include a temperature of approximately 370°C, a pressure of about 2000 psig, and liquid hourly space velocities below 1.0 hr⁻¹ over a commercial Ni-Mo catalyst (10,11). Hydrogenation generally takes place during the second stage. This processing requires less severity than either the first-stage or single-stage processing and it may use noble metal catalysts. The high oxygen concentration in the GPGP feedstocks will require a high hydrogen feed ratio during this step (11).

EXPERIMENTAL DESIGN

Determination of "optimum" processing conditions via a one-at-a-time testing method is costly, both in terms of time and project dollars. To gain the maximum amount of information in the most efficient manner, testing was

TABLE 3
PROTON AND CARBON-13 NMR DATA FOR GPGP LIQUID STREAMS

Carbon Type	NMR Region, ppm	Tar Oil Area %	Crude Phenol Area %	Rectisol Naphtha Area %
<u>PROTON NMR</u>				
Aromatic	9.0 - 5.9	28.3	50.2	38.9
Phenol	4.4 - 3.5	2.4	16.9	0.4
Acenaphthene	3.5 - 3.3	0.5	2.1	1.9
-CH ₂ -alpha	3.3 - 1.9	28.4	23.5	22.2
-CH ₂ -beta	1.9 - 1.5	5.3	1.3	10.5
-CH ₂ -	1.5 - 1.0	23.4	4.8	13.9
-CH ₃	1.0 - 0.1	11.7	1.2	12.2
Total Area %		<u>100.0</u>	<u>100.0</u>	<u>100.0</u>
-CH ₂ -/-CH ₃		2.0	4.0	1.1
<u>CARBON-13 NMR</u>				
Aliphatic, C=	240 - 187		1.0	2.0
Aromatic, C=O	187 - 160		0.1	1.1
Phenolic	160 - 149		10.2	0.0
Aromatic, =C=	149 - 138		8.3	2.7
Aromatic, =C-	138 - 95		65.8	66.7
Methoxyl	95 - 60		0.2	1.1
Aliph., -CH ₂ -	50 - 36		1.4	4.3
C	36 - 27		2.3	9.7
alpha C	27 - 17		5.2	8.0
-CH ₃	17 - 0		5.5	4.4
Total Area %			<u>100.0</u>	<u>100.0</u>

performed using a statistical experimental design to enable prediction of the conditions at which heteroatom removal during first-stage processing would be virtually complete. The choice of a particular statistical experimental design is made based upon whether or not the results of the testing are expected to be linear in nature. It was not expected that the heteroatom content of the product of the first stage would be a linear function of the temperature and pressure of the process. For this reason, a central composite design for two factors was used to collect the experimental data. This design allowed the fitting of a general quadratic equation for smoothing and prediction of the data. This class of design allows the experimenter to build upon a two-level factorial design and adds a set of axial points. These axial points, along with a center point, allow the estimation of all pure quadratic terms.

TABLE 4
RESULTS OF ASTM D86 DISTILLATIONS PERFORMED ON GPGP
LIQUID STREAMS AND AV JET A

	Tar Oil	Crude Phenol	Rectisol Naphtha	AV Jet A
Bar. Press (mm Hg)	756	742	731	742
Rm. Temp. ($^{\circ}$ C)	23	23	24	23
Vol % Distilled				
IBP	93	97	43	82
5%	135	98	63	173
10%	170	185	69	183
20%	195	190	76	197
30%	210	193	79	205
40%	225	193	83	213
50%	250	196	86	220
60%	263	201	89	228
70%	285	210	94	235
80%	297	229	102	245
90%	303	263	119	260
95%			132	268
Max. Temp. ($^{\circ}$ C)	303	265	132	274
Max. Vol %	92	95	96	98
Residue (wt %)	9.66	5.75	2.80	2.20
Recovery (wt %)	87.68	92.45	96.35	96.21
Lost (wt %)	2.66	1.80	0.85	1.59
Specific Gravity	1.02	1.06	0.82	0.82

Table 5 shows the matrix which was designed for use in the first-stage data collection. For these experiments, Shell 424 was used as the catalyst, and the ranges of temperature and pressure that were evaluated were 328 $^{\circ}$ -387 $^{\circ}$ C and 1500-2500 psig, respectively. The matrix was randomized to ensure that all results were independent. Actual run conditions of the tests as they were performed are listed in Table 6.

After the engineering and analytical data were collected, the responses were analyzed via computer regression analysis. The full model was fit, and a check was made for outlying data points. Following this, a check was made for lack of fit of the quadratic equation and unnecessary terms were eliminated, resulting in a mathematical model.

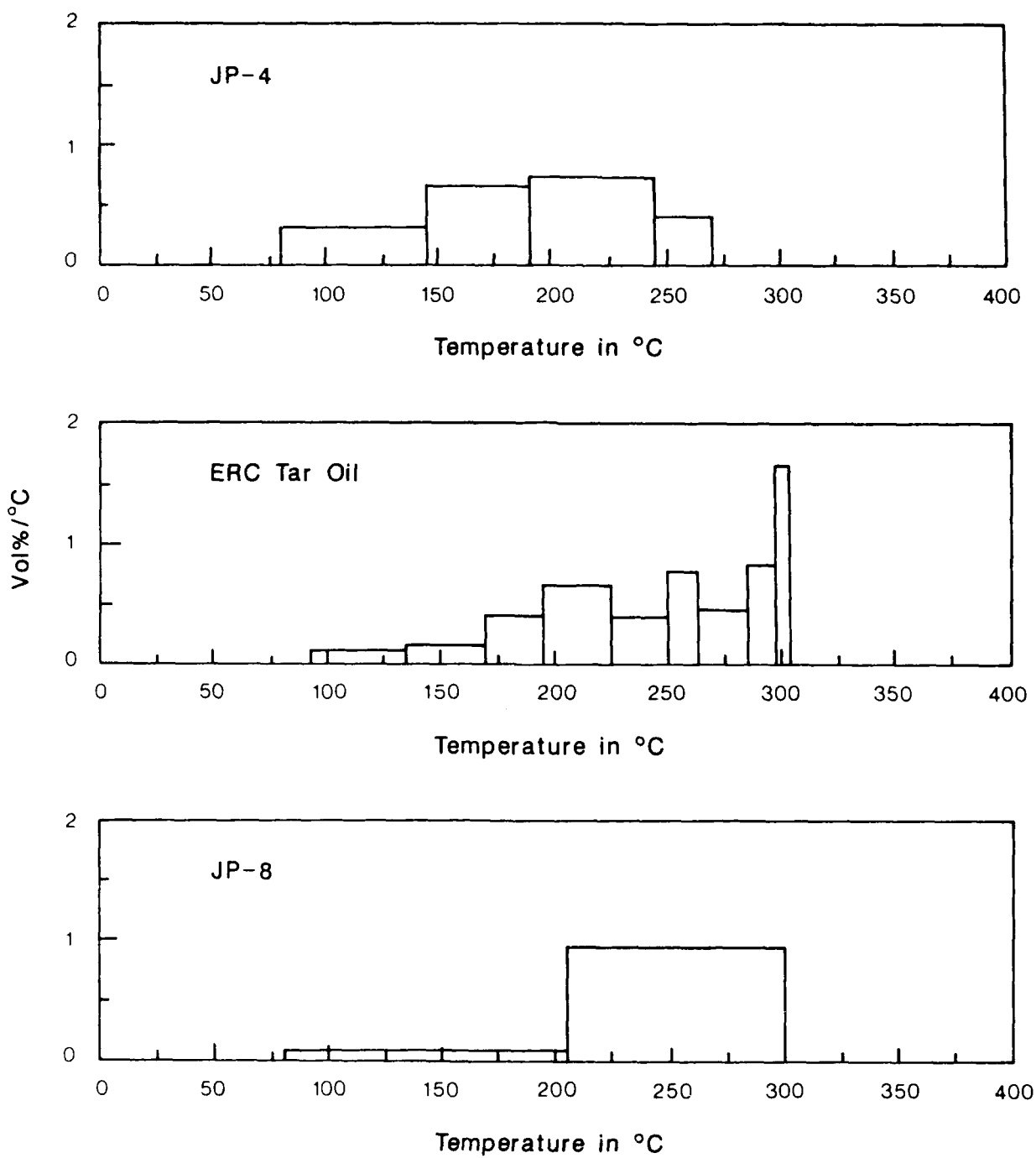


Figure 1. Comparison of ASTM D86 distillation profiles of JP-4, JP-8, and GPGP tar oil stream.

TABLE 5

MATRIX FOR STUDYING EFFECTS OF TEMPERATURE AND PRESSURE
IN FIRST-STAGE PROCESSING TO REMOVE HETEROATOMS

Run	Temperature (°C)	Pressure (psig)
1	387	2500
2	387	1500
3	328	2500
4	328	1500
5	357	2710
6	357	1300
7	400	2000
8	316	2000
9	357	2000
10	357	2000

TABLE 6

RUN CONDITIONS FOR FIRST-STAGE TESTING

Run	Date	Catalyst	Temperature (°C)	Pressure (psig)
First-Stage Tests				
N-408	8/05/87	Shell 424	374	2675
N-409	8/11/87	Shell 424	385	1435
N-410	8/13/87	Shell 424	394	2235
N-413	8/28/87	Shell 424	357	1300
N-414	9/01/87	Shell 424	387	2500
N-415	9/02/87	Shell 424	357	2000
N-416	9/03/87	Shell 424	329	1491
N-417	9/04/87	Shell 424	358	2012
N-418	9/09/87	Shell 424	367	1500
N-421	9/22/87	Shell 424	345	1975
N-432	6/02/88	Shell 424	395	2384
N-433	6/09/88	Shell 424	380	2250
Single-Stage Tests				
N-418	9/09/87	NT550	354	2000
N-419	9/11/87	NT550	390	1997
N-420	9/15/87	Katalco 660	394	2023

MATERIALS, EQUIPMENT, AND EXPERIMENTAL PROCEDURES

First-stage testing took place in the Energy and Mineral Research Center (EMRC) one-gallon, hot-charge, semi-batch autoclave system shown in Figure 2. Gas flowed through the system at the equivalent rate of 6500 scf/bbl. Three catalysts were used during these tests: Shell 424, NT550 (nickel-tungsten on an alumina support), and Katalco 660 (nickel-tungsten on an experimental silicon dioxide support). One hundred grams of catalyst and 1 kg of tar oil were used for each test. The catalyst was pre-sulfided at reaction temperature and was batch-charged fresh each run. In the autoclave, the catalyst exhibited high-contact, free-floating behavior. The tar oil-to-catalyst ratio of 5.3 g/g was maintained for each run in an effort to have enough feedstock relative to catalyst such that the catalyst would be seen as if it were in an ebulating bed reactor.

The tests were one hour in duration at reaction temperature, followed by a cooldown to 200°C. To prevent undesirable condensation reactions, the system was held stable at this temperature for 20 minutes, and then was allowed to cool to room temperature. Periodic liquid samples were taken during the run from the bottom of the autoclave, while gas samples were collected in a diaphragm accumulator. Hydrogen flowed through the system continuously during the test.

For each test, a suite of time samples was created by taking a sample every three minutes. Time samples were also taken at the beginning and the end of the 200°C stabilization period. Bulk liquid samples were taken of the feedstock and the endpoint, the liquid and solid materials remaining in the reactor at the end of the run after cooldown to room temperature. In addition, two bulk gas samples were obtained for GC analysis. This type of sampling procedure was used because it provided samples often enough to follow changes in both chemical composition and heteroatom concentration, and, when appropriate, to develop kinetic information on the rates of the reactions taking place.

Analyses which were performed on the liquid time samples included percent aromatics and C, H, N, and S elemental analyses. These analyses were performed on samples taken at 3, 6, 9, 18, 27, and 36 minutes during the run and at both the beginning and the end of the stabilization period following cooldown to 200°C. The endpoint samples received more scrutiny, undergoing C, H, N, and S elemental analyses, distillation analysis, GC/MS, and other detailed analyses when appropriate. Samples which are listed in Table 7 were sent to Western Research Institute for detailed nitrogen analysis because the analytical equipment available at the EMRC was not sensitive enough to detect the very low nitrogen contents which were expected.

The purpose of the first stage in this type of processing is to remove the heteroatoms from the feedstock prior to hydrogenation. The conditions at which heteroatom removal should most effectively occur were determined using the results of the tests performed as a part of the statistical matrix.

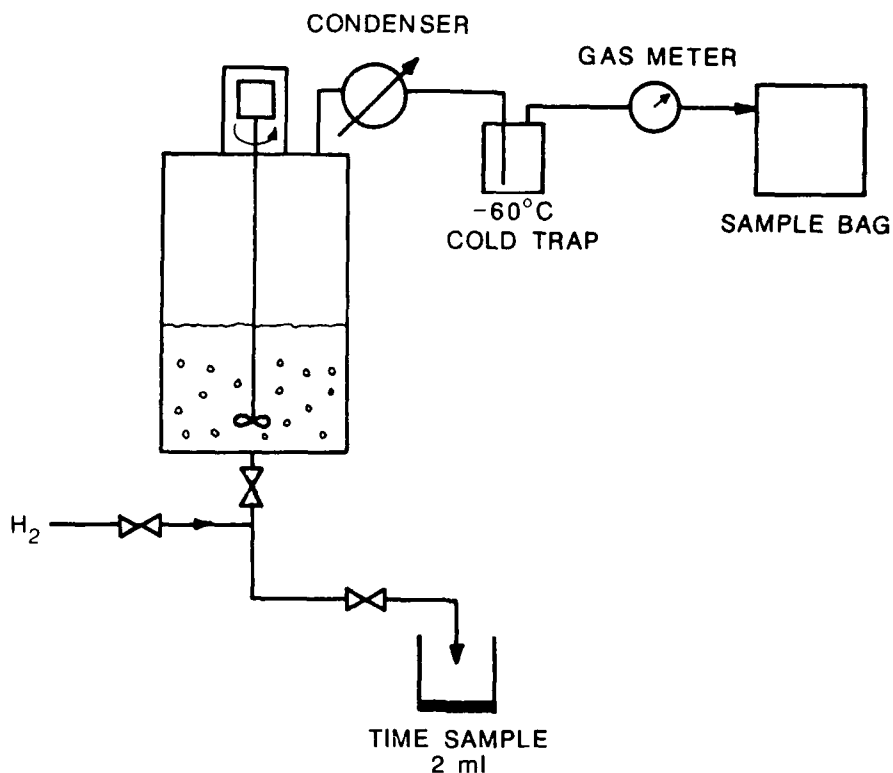


Figure 2. Autoclave system used during tar oil upgrading.

TABLE 7

SAMPLES SENT TO WESTERN RESEARCH INSTITUTE FOR NITROGEN ANALYSIS

Run	Time Sample Number
N-408	1,4,7,10,13,16,19,22,endpot
N-409	1,4,7,10,13,16,19,22,endpot
N-410	endpot
N-413	endpot
N-414	1,4,7,10,13,16,19,22,endpot
N-415	1,4,7,10,13,16,19,22,endpot
N-416	1,4,7,10,13,16,19,22,endpot
N-417	endpot
N-418	endpot
N-419	endpot
N-420	endpot
N-421	endpot
Feed	

RESULTS OF STATISTICAL MATRIX TESTING

To arrive at the mathematical models listed in the following subsections, the computer first estimated the parameters. The computer then performed a regression analysis using all of the possible terms: intercept, x , y , x^2 , y^2 , and xy . The computer determined which terms had Prob > F values which were not significant; i.e., had large values. In a backward elimination procedure, the computer dropped the variable which produced the least significant term. The procedure was repeated over and over with the computer dropping terms until all of the remaining terms had significant Prob > F values. The parameters which were estimated when the computer determined that all terms were significant are the coefficients used the final model equation.

Total Heteroatom Content

The results indicate that the heteroatom content of the product is a linear function of the temperature and pressure of the first-stage reaction. This function is defined by Equation (1).

$$HC = 3.43 - 2.04 * X_1 - 0.67 * X_2 \quad (1)$$

where $X_1 = (T - 360)/30$, $X_2 = (P - 2000)/500$, and temperature and pressure are expressed in $^{\circ}\text{C}$ and psig, respectively. Equation (1) shows that a 10°C change in temperature produces a change in heteroatom content that is equivalent to the change produced by a 500 psig change in pressure. The equation was plotted as a function of temperature over the entire range of pressures included in the statistical matrix. This plot is shown in Figure 3. As the plot clearly shows, a total heteroatom content of zero occurs only at a temperature of 400°C at pressures of 2650 psig or greater.

Nitrogen Content

Nitrogen content was determined by the statistical analysis to be a nonlinear function of temperature and pressure defined by Equation (2).

$$N = 0.000104 + (0.000041 X_1) - (0.000661 X_2) - (0.000722 X_1 X_2) + (0.000655 X_1^2) + (0.000602 X_2^2) \quad (2)$$

where X_1 and X_2 are the same variables as were defined for Equation (1). This equation was plotted as a function of temperature over the entire range of pressures included in the statistical matrix, and the plot is presented in Figure 4. It is difficult to determine optimal conditions for nitrogen removal from this plot; therefore, the portion of the plot which indicates that nitrogen contents approaching zero are possible was enlarged, and is shown as Figure 5. This plot clearly shows that any of the temperatures which were tested could result in a nitrogen content approaching zero if the proper pressure is selected. Generally, though, the optimal conditions appear to be between 360° and 380°C and 2275 and 2425 psi.

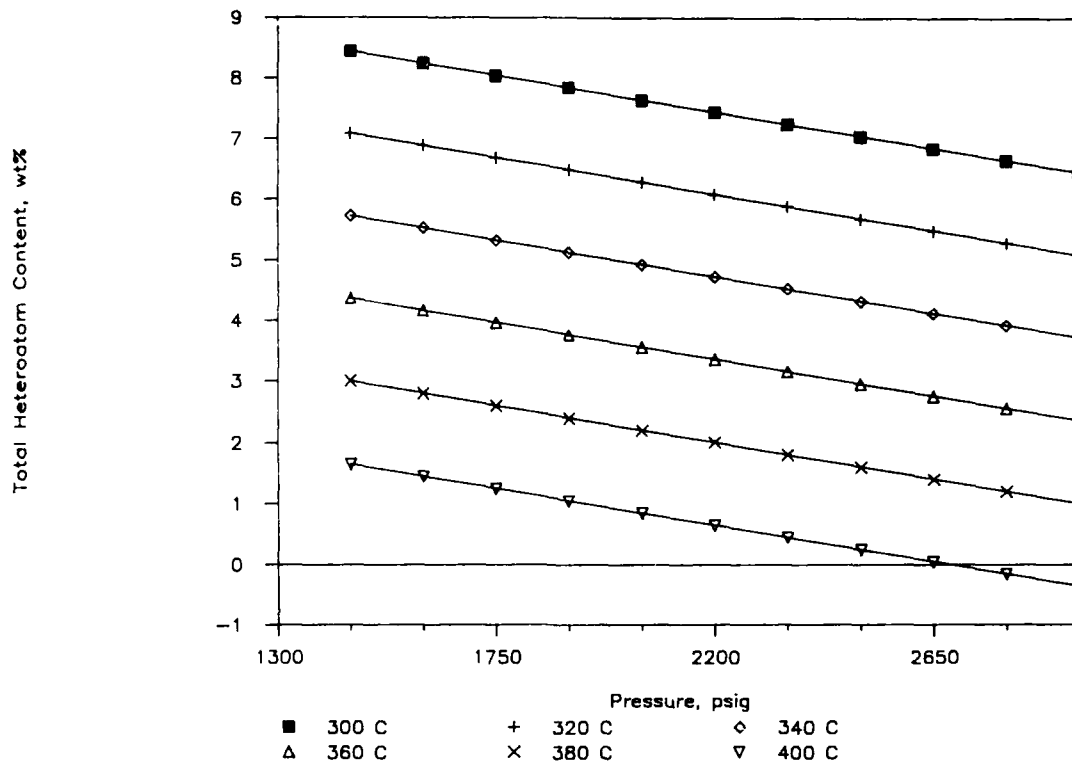


Figure 3. Effect of temperature on total heteroatom content over the entire pressure range tested.

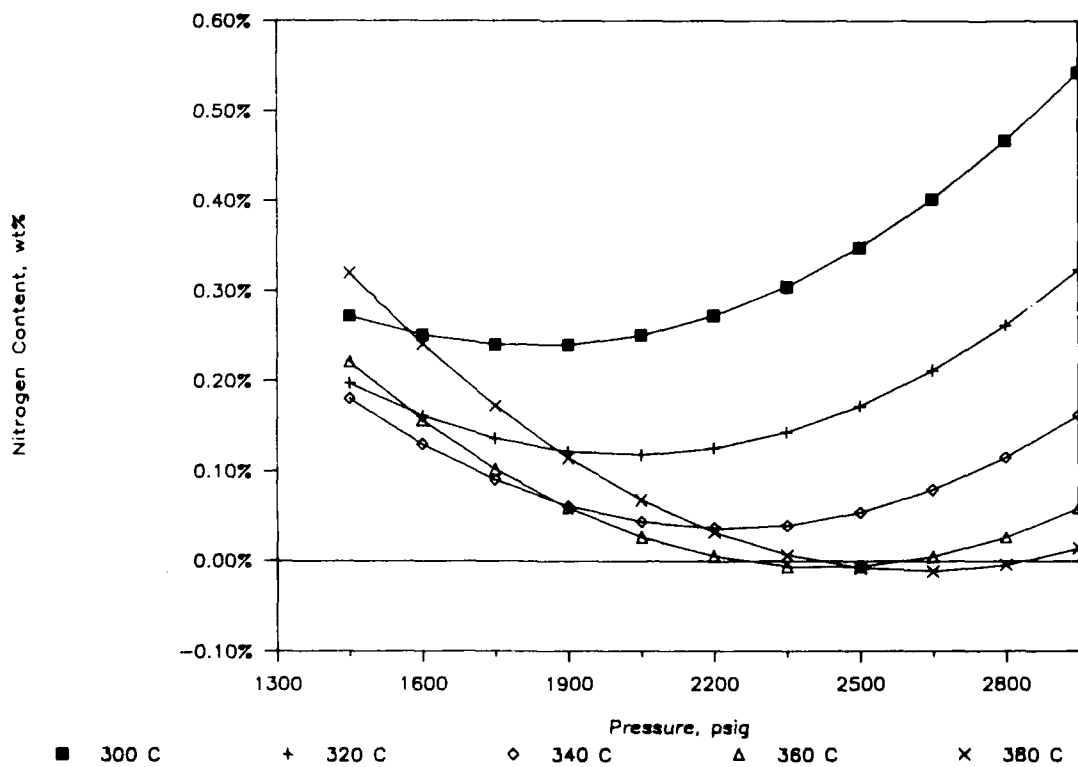


Figure 4. Effect of temperature on nitrogen content over the entire pressure range tested.

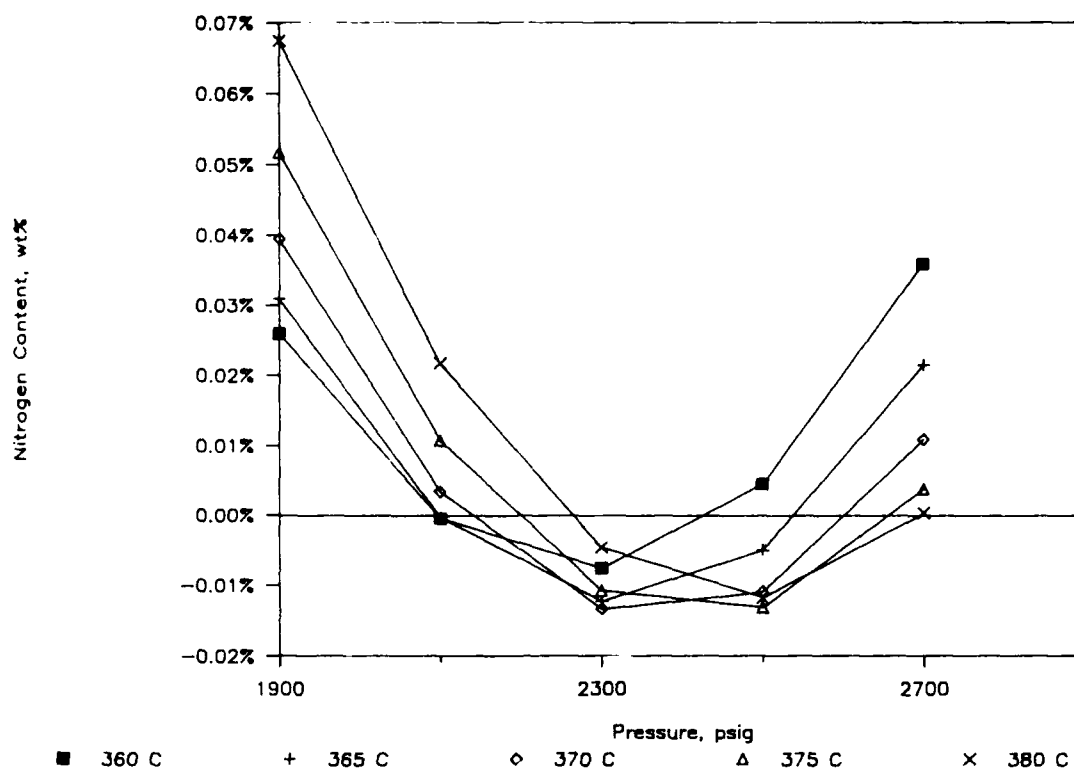


Figure 5. Detail of the best nitrogen removal conditions.

Sulfur Content

The results of the statistical analysis indicated that sulfur content is temperature independent, following the nonlinear function given in Equation (3).

$$S = 0.000159 - 0.000150 X_2 + 0.000427 X_2^2 \quad (3)$$

where X_2 is defined as for Equation (1). Equation (3) was plotted over the entire pressure range; the result is shown in Figure 6. As the plot shows, the lowest sulfur content, 0.015 percent, can be expected to occur at a processing pressure of 2050 psi. Even at the best conditions for nitrogen removal (i.e., approximately 2300 psi), the sulfur content would be expected to be approximately 0.025 percent.

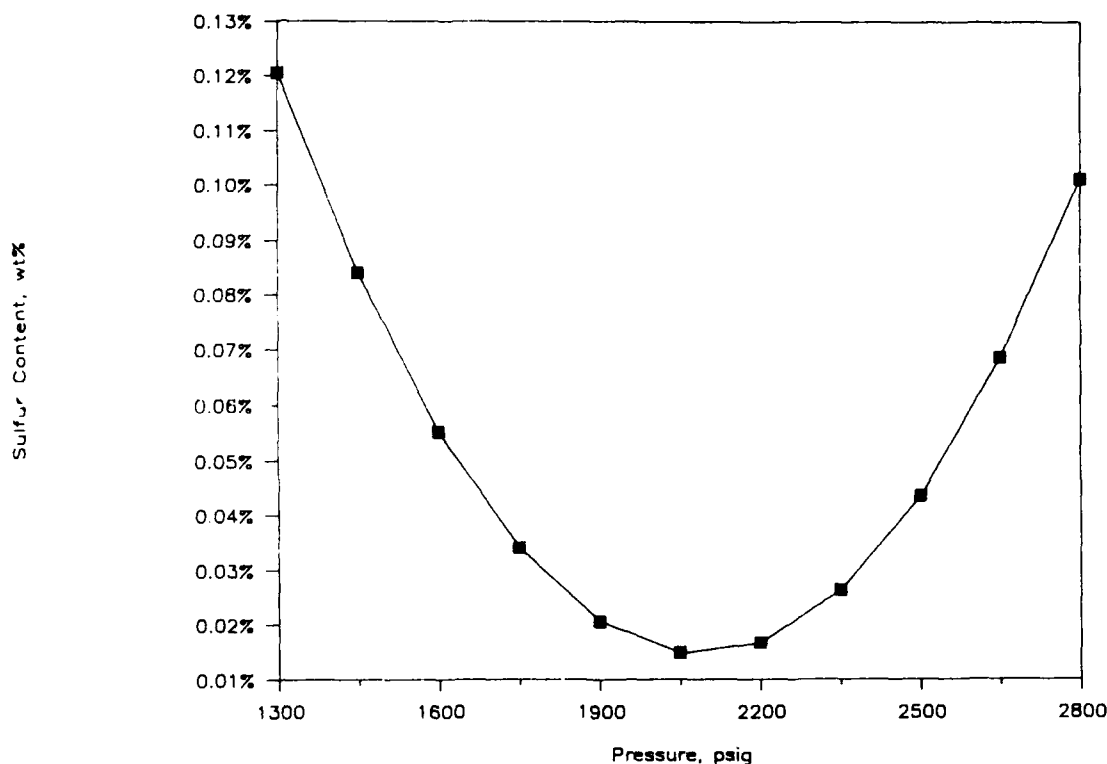


Figure 6. Effect of a change in pressure on sulfur content.

Aliphatic Content and Aromatic-to-Aliphatic Ratio

Equations describing the relationship of temperature and pressure with aliphatic content and aromatic-to-aliphatic ratio were also determined using the analysis of variance. The aliphatic content (ALI CON) of the first-stage product was found to be a linear function of temperature and pressure defined by Equation (4).

$$\text{ALI CON} = 48.492 + 3.871 X_1 + 2.409 X_2 \quad (4)$$

where X_1 and X_2 are defined as for Equation (1). The aromatic-to-aliphatic ratio (ARO:ALI) was defined as a linear function of temperature and pressure by Equation (5).

$$\text{ARO:ALI} = 1.082 - 0.176 X_1 - 0.099 X_2 \quad (5)$$

where X_1 and X_2 are again defined as for Equation 1. Equations (4) and (5) were plotted over the ranges of temperature and pressure which were used in the testing, resulting in Figures 7 and 8, respectively. From Figure 8, it can be seen that the highest aliphatic content of the first-stage product is approximately 57 percent, occurring at 400°C and 2800 psi. These are, of course, the conditions at which the aromatic-to-aliphatic ratio is the lowest, as shown in Figure 8.

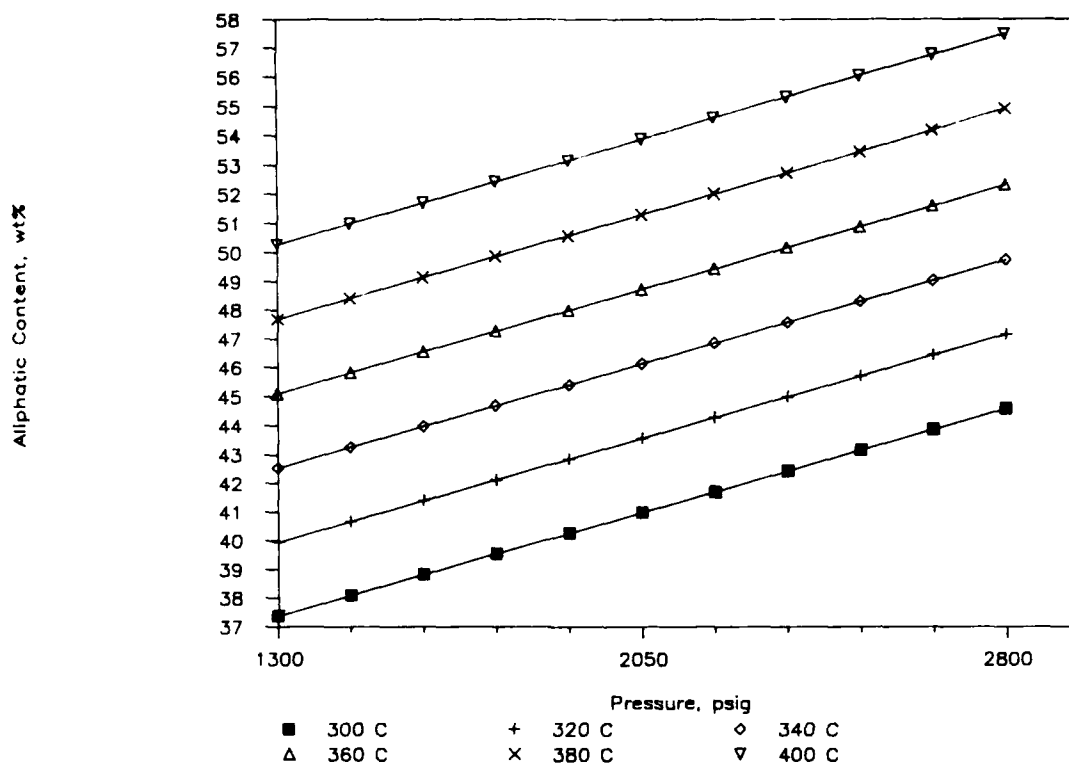


Figure 7. Effect of temperature on aliphatic content over the entire range of pressures tested.

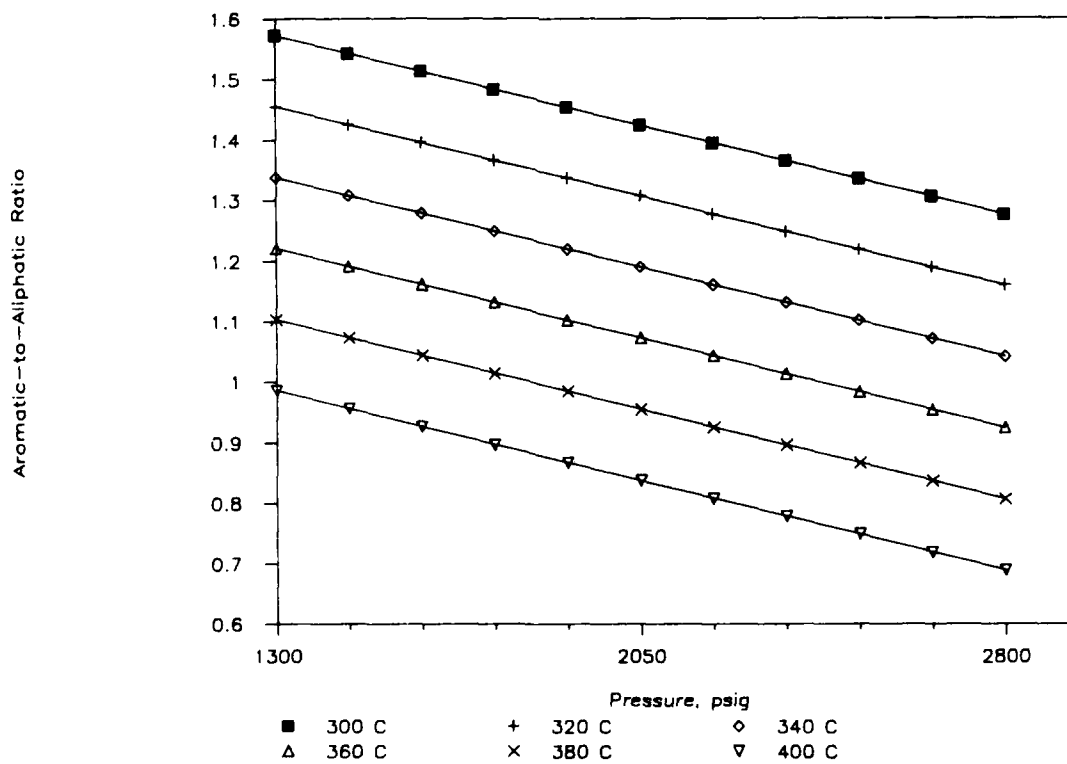


Figure 8. Effect of temperature on the ratio of aromatic content to aliphatic content over the entire pressure range tested.

Analysis of Variance

The complete results of the analysis of variance are presented as Appendix A, while the conditions and results of analyses of all runs performed as a part of the matrix or as verification runs are tabulated in Appendix B. Two criteria of the analysis of variance were used to show that the mathematical models which were derived are statistically valid. The first is the R-square value, which represents the degree of fit of the equation to the data. Generally, R-square values of 0.90 and greater are considered to represent a "good" fit to the data. As the tables in Appendix A show, the R-square values were 0.920, 0.999, 0.740, 0.908, and 0.899 for the heteroatom content, nitrogen content, sulfur content, aliphatic content, and aromatic-to-aliphatic ratio, respectively. Therefore, based upon the degree of fit, it would seem that "good" fits were obtained by all models with the exception of the sulfur content model.

The second criterion is the measure of the interdependency of the variables in the resulting equation. This was calculated for the total heteroatom content equation and can be found in the Correlation of Estimates appearing at the end of the section of Appendix A dealing with this variable. The correlation matrix presents data which show the relationship between variables; i.e., the changes in a variable caused by a change in another variable. Obviously, it is desirable to have independent variables, and a model is generally considered to be a good one if the absolute values of the correlation coefficients are less than about 0.6. Given this criterion, it can be seen that the model which was calculated for heteroatom content is probably fairly accurate.

Verification of the Predictions of Conditions

The mathematical models were used to predict "optimal" first-stage processing conditions; these conditions are summarized in Table 8. As the table shows, the higher temperatures of 380^o-400^oC are predicted to be the most successful at removing heteroatoms and increasing aliphatic content. The higher pressures of 2650-2800 psig are predicted to be the most effective in removing oxygen and increasing the aliphatic content. Intermediate pressures (relative to the matrix) are predicted to be the most successful at nitrogen removal, while lower pressures are predicted to result in the lowest sulfur content. Runs were made at fairly high temperatures of 380^o-400^oC and intermediate pressures to verify the results of the mathematical modeling and to produce feedstock for second-stage hydrotreating tests.

Two verification runs were performed: N-432 and N-433. Run N-432 was run at an average temperature of 395^oC and an average pressure of 2384 psig, while N-433 was performed at 380^oC and 2250 psig. Using the mathematical models, predictions were made with respect to nitrogen, sulfur, total heteroatom, and aliphatic contents and aromatic-to-aliphatic ratios of the products. These predictions are compared in Table 9 with the actual results of the analyses performed on the products. When comparing the predicted and actual results, the sensitivity of the analytical equipment must be taken into account. Whereas the mathematical models can predict very small values, the analytical equipment has a detectability limit of 0.01 weight percent.

TABLE 8
PREDICTED "OPTIMAL" FIRST-STAGE PROCESSING CONDITIONS
FOR GPGP TAR OILS

Parameter	Temperature (°C)	Pressure (psig)
Total Heteroatom Content	400	2650
Nitrogen Content	360 - 380	2272 - 2425
Sulfur Content	---	2050
Aliphatic Content	400	2800
Aromatic:Aliphatic	400	2800

The models indicate that Run N-432 was performed at an "optimal" pressure for nitrogen removal and fairly close to the pressures required for increased aliphatic content and total heteroatom removal. It must be kept in mind that the "optimal" pressures are different for each of the parameters, and that an intermediate pressure such as 2400 psig will probably produce the best overall results. The temperature at which the run was performed was too high for predicted complete nitrogen removal, but was very close to the "optimum" temperature for the other parameters. Therefore, it would be expected that the product of N-432 would contain small quantities of nitrogen and sulfur, but that total heteroatom content would be low and aliphatic content would be relatively high. As the results listed in Table 9 show, this was the case except that the product sulfur content was less than the sensitivity of the analytical equipment (i.e., 0.01 weight percent).

Run N-433 was performed at the "optimal" temperature of 380°C, but a slightly low pressure for nitrogen and oxygen removal or increased aliphatic content. However, it would seem that there would be virtually complete heteroatom removal in the product of this run and that the aliphatic content would be fairly high. Analysis of the product of this run proved this to be the case, as total heteroatom content was reduced to less than 0.01 weight percent.

To show that conditions which were outside of the predicted ranges would not result in products of desired composition, the product of Run N-423 was examined with respect to the predicted "optimal" conditions. This run was performed at 345°C and 1975 psig, both of which are too low for complete heteroatom removal and relatively high aliphatic content. The pressure of the run was, however, fairly close to the "optimum" pressure predicted for the lowest product sulfur content. The results of the analyses performed on the product show that, although the sulfur content was predictably low, the nitrogen and oxygen contents were unacceptably high and the aliphatic content was low.

TABLE 9

COMPARISON OF FEEDSTOCK WITH PREDICTED AND ACTUAL RESULTS OF VERIFICATION RUNS

Parameter	Feed	N-423	N-432	N-433
Avg. Temp. (°C)	NA ^a	345	395	380
Avg. Pressure (psig)	NA	1975	2384	2250
Total Heteroatom Content (O + N + S, wt %)				
Predicted	NA	4.48	0.54	1.74
Actual	7.41	5.98	1.22	-- ^b
Nitrogen Content (wt %)				
Predicted	NA	0.026	0.024	0.000
Actual	0.52	0.23	0.06	--
Sulfur Content (wt %)				
Predicted	NA	0.017	0.030	0.019
Actual	0.39	0.08	--	--
Aliphatic Content (wt %)				
Predicted	NA	46.44	54.86	52.28
Actual	31.9	45.4	ND ^c	ND
Aromatic-to-Aliphatic Ratio				
Predicted	NA	1.17	0.80	0.92
Actual	2.13	1.20	ND	ND

^a Not applicable.^b Actual values of these species are below the detectability limit of the measurement equipment.^c Not determined.

The mathematical models were successful in predicting conditions which would be the most likely to produce the desired product composition, as Run N-433 had a total heteroatom content which was below the detectability limits of the analytical equipment. The models also successfully predicted that the conditions of Run N-423 would not result in a desired product composition. The purpose of the models was not to predict exact product composition, but to identify the most appropriate conditions at which to operate the processing equipment. In this regard, the models are considered to have been successful.

INTERPRETATION OF TIME SAMPLE DATA

Time samples were taken during most runs, and the data were analyzed to provide an understanding of the reactions which took place as a function of time. Nitrogen is removed more rapidly during the higher-pressure runs than during the lower-pressure runs. The comparison of nitrogen content as a

function of time at two temperatures and two pressures is shown in Figure 9. A significant difference can be seen between the two pressures illustrated in this figure, but both show the strong pressure dependence of HDN reactions.

Figure 10 shows that sulfur was removed rapidly during the runs, especially at higher pressures. The figure shows very little difference between runs with respect to sulfur removal with time with the exception of Run N-416 which was performed at the low pressure of 1491 psig. The pressure of this run was not sufficient to remove the sulfur from the feedstock.

The effect of pressure on the hydrogen-to-carbon ratio is shown in Figure 11. As the figure shows, the hydrogen-to-carbon ratio increased the most rapidly and to a higher value when a higher pressure was used.

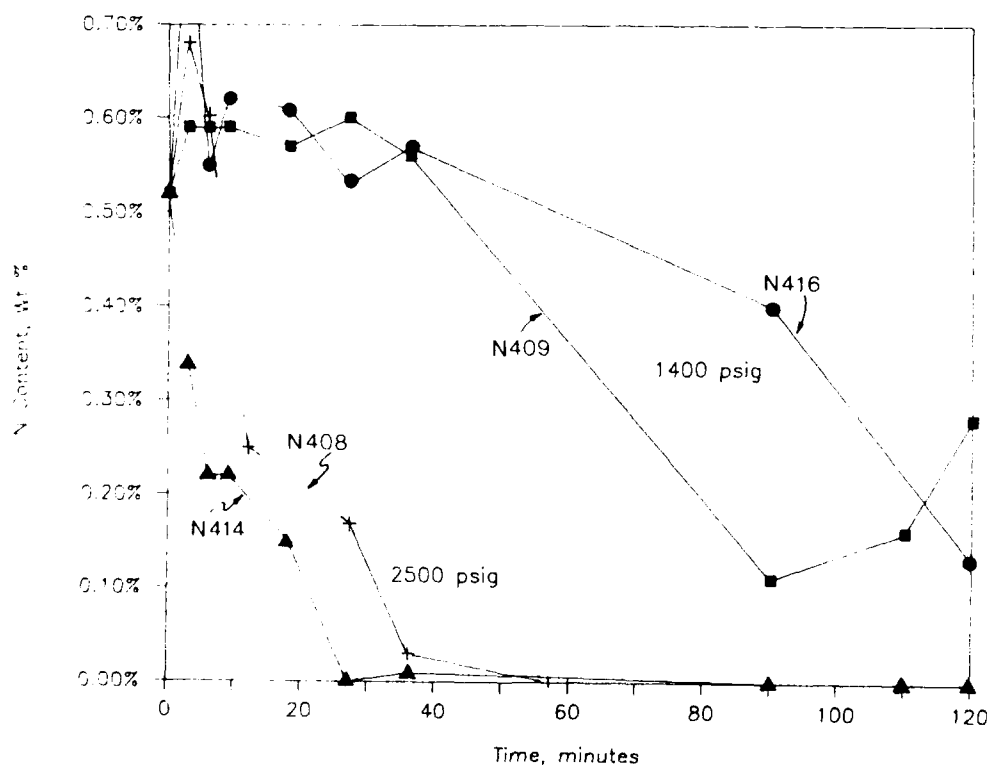


Figure 9. Nitrogen content as a function of time during first-stage processing.

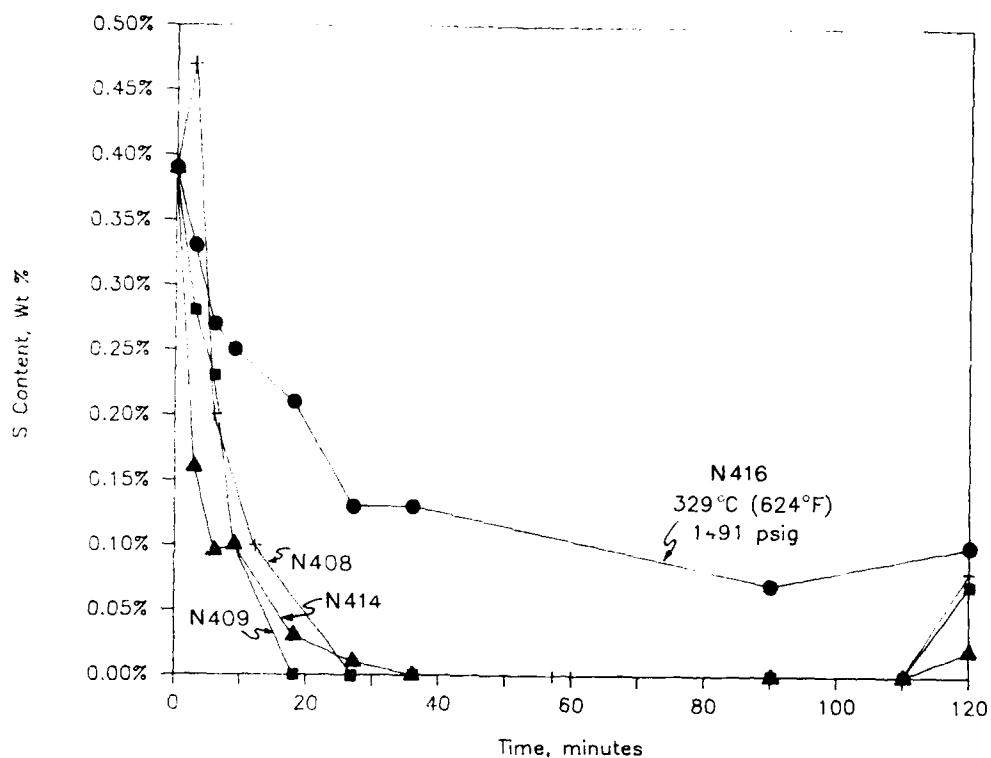


Figure 10. Sulfur content as a function of time during first-stage processing.

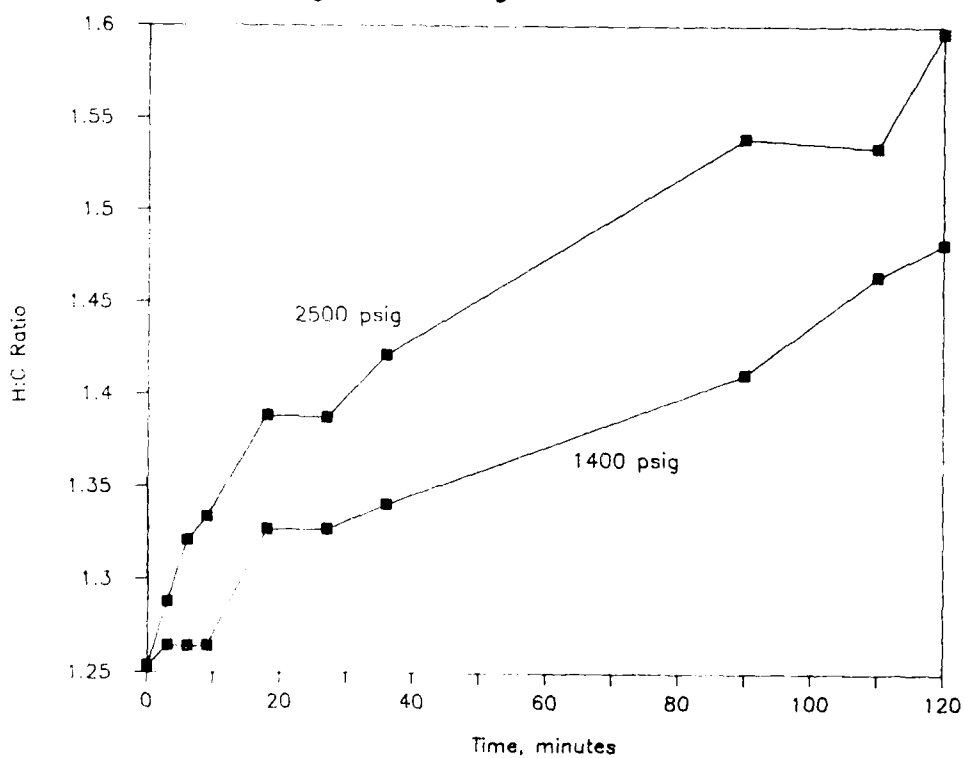


Figure 11. Hydrogen-to-carbon ratio as a function of time during first-stage processing.

MASS BALANCE

During hydrogenation, heteroatoms are usually removed in the gaseous phase in the form of H_2O , NH_3 , and H_2S . Due to the volume of hydrogen contained in the gas phase, other species were present in such small quantities that they were virtually below the detectability limits of the gas chromatograph. It was possible to ascertain the presence of these species, but their fate could not be determined in a more precise manner. To illustrate this, the gas analysis for Run N-414 is given in Table 10. This analysis is typical of the gas analyses which were performed during this processing. As the table shows, the product gas contained 98.2 weight percent hydrogen and very small quantities of other components. The error of these normalized results is larger than any of the differences that are noted, and valid judgements concerning the gas analysis cannot be made. Because good mass balances were obtained for all streams with the exception of the gas stream, it was decided to look at the liquid stream balance for information which might corroborate the heteroatom removals detected during the analytical workups.

A liquid balance should reflect the removal of heteroatoms from the liquid phase to a limit of those present in the feedstock. In other words, if all heteroatoms were removed from the feedstock, the mass of the liquid product would equal the mass of the carbon and hydrogen which were originally present in the feedstock. This assumption appears to be a valid one based upon the data. Table 11 presents heteroatom removal and liquid recovery data from three runs and compares this information with the liquid recovery which would be expected for complete heteroatom removal. As the table shows, liquid recovery decreased as the degree of heteroatom removal increased. Therefore, the liquid balance data corroborate the analytical information with respect to heteroatom removal.

SINGLE-STAGE PROCESSING

Three runs, N-418, N-419, and N-420, were performed using two other catalysts: NT550 and Katalco 660. These were nickel-tungsten catalysts on an alumina support and an experimental silicon dioxide support, respectively. It was suggested by the manufacturers of these catalysts that they might perform the equivalent functions of the two-stage processing in a single stage. An effort was made to compare the ability of these catalysts to remove heteroatoms and increase aliphatic content with that of the Shell 424 catalyst. It was not possible to directly compare results because Runs N-419 and N-420 were not made at conditions at which Shell 424 runs had been performed. Therefore, the Shell 424-based mathematical models were used to calculate the expected product compositions for runs made at those conditions using Shell 424 catalyst. Because Run N-418 was performed at the same conditions as Run N-415, a Shell 424 run, the actual results of Run N-418 were compared with the predicted results. This comparison is shown in Table 12. As the table shows, the predicted results for the conditions of Run N-418 and the actual results of Run N-415 were similar. It was therefore assumed that the predictions at the N-419 and N-420 conditions would also be similar to results which would have been obtained using Shell 424 catalyst. With this in mind, relative differences were determined between Shell 424, NT550, and Katalco 660. As the table shows, NT550 behaved in a manner similar to that of Shell 424. Katalco 660 was different, as the product had a higher oxygen

TABLE 10
RESULTS OF GAS ANALYSIS OF RUN N-414

Component	Normalized Wt%
H ₂	98.20
CO ₂	0.06
C ₃ H ₈	0.19
C ₃ H ₆	0.00
i-C ₄	0.02
COS	0.00
n-C ₄	0.15
H ₂ S	0.10
1-Butene	0.00
t-2-Butene	0.00
i-C ₅	0.04
C-2-Butene	0.00
n-C ₅	0.11
C ₂ H ₄	0.00
C ₂ H ₆	0.30
CH ₄	0.81
CO	<u>0.00</u>
Total	100.00

content and a significantly lower aliphatic content than would be predicted for a Shell 424-catalyzed product at the same conditions. Runs N-419 and N-420 were run at nominally the same conditions (see Table 6). The results indicate that NT550 was more successful in lowering the total heteroatom content and in increasing the aliphatic content than Katalco 660.

TABLE 11
LIQUID RECOVERIES DURING HETEROATOM REMOVAL

Run	Heteroatom Removal (%)	Liquid Recovery (wt%)
N-416	12.42	96.55
N-421	33.06	93.32
N-409	67.88	92.90
theoretical	100.00	92.59

TABLE 12
RESULTS OF SINGLE-STAGE PROCESSING

	HC ^a (wt%)	N ^b (wt%)	S ^c (wt%)	Aliphatic (wt%)	Aro:Ali ^d
N-418 - NT550					
Actual	3.72	0.43	0.00	45.60	1.19
Predicted	3.84	0.01	0.02	47.72	1.12
Run N-415	2.73	0.01	0.00	47.50	1.11
N-419 - NT550					
Actual	2.78	0.08	-- ^e	46.20	1.16
Predicted	1.39	0.08	0.02	52.35	0.91
N-420 - Katalco 660					
Actual	4.99	0.27	--	43.60	1.29
Predicted	1.09	0.09	0.02	52.99	0.88

^a Heteroatom content.

^b Nitrogen content.

^c Sulfur content.

^d Aromatic-to-aliphatic ratio.

^e Undetected.

SECOND-STAGE PROCESSING

Three runs were performed as second-stage hydrogenation runs. The product of Run N-423 was used as the feedstock for Runs N-424 and N-425, while the products of Runs N-432 and N-433 were sampled, combined, and used as the feedstock for Run N-435. The product of Run N-423 contained some heteroatoms and a less-than-optimal aliphatic content. It was used as a feed to determine if less-than-perfect feed could be used during the hydrogenation step to produce aviation fuel. The product of Run N-433 contained no measurable amounts of heteroatoms and was considered to be an "optimal" feedstock. Englehard S-661, a platinum catalyst, was used as the catalyst for this processing, which was performed under the mild conditions listed in Table 13. The catalyst was chosen following conversations with various catalyst manufacturers.

TABLE 13
RESULTS OF SECOND-STAGE PROCESSING

	Feed For N-424, N-425	N-424	N-425	Feed For N-435 ^a	N-435
Date		12/16/87	12/18/87		8/03/88
Temp. (°C)		150	200		205
Pressure (psig)		750	700		750
Elemental Analysis (wt%)					
C	83.74	87.25	86.78	88.13	88.56
H	10.28	10.16	10.14	11.27	11.27
N	0.23	0.29	0.29	90.03	-- ^b
S	0.08	0.04	--	--	--
O ^c	5.67	2.26	2.79	0.58	0.17
Total Heteroatom Content (wt%)	5.98	2.59	3.08	0.61	0.17
Aliphatic Content (wt%)	45.40	41.40	42.60	ND ^d	53.13
Aromatic:Aliphatic	1.20	1.42	1.35	ND	0.88

^a Values calculated as an average of the values of the products of Runs N-432 and N-433; the two feeds were combined in a 1:1 ratio.

^b Undetected.

^c By difference.

^d Not determined.

As Table 13 shows, the products of Run N-424 and N-425 did not exhibit an increase in aliphatic content. This may be due to one of three reasons: the catalyst itself was ineffective in this particular system, the conditions at which the processing was performed were not optimal for the catalyst, or the heteroatoms which were present in the N-423 product which was used as feedstock poisoned the catalyst. The results of Run N-435, which utilized the more "optimal" feedstock, were much more encouraging, as the resulting product was relatively enriched in aliphatic content compared to other samples obtained during the research. It should be noted that the specifications for jet fuel list a maximum aromatic content of 25 weight percent; i.e., 75 weight percent aliphatic content. Even the aliphatic content of Run N-435 did not approach this target, which could be due to poisoning of the catalyst by the undetectable quantities of heteroatoms that may have been present in the N-432 and N-433 products. These results indicate that, although the first-stage products appear to be excellent candidates for high-density fuels due to their high aromaticity, the second-stage catalysts which were used were not effective in producing a product with a low aromatic content.

CONCLUSIONS

- The mathematical models derived from the statistical analysis of the data appear to be statistically valid. The results of Runs N-423, N-432, and N-433 successfully verified the mathematical models' usefulness in predicting "optimal" conditions at which to perform the processing.
- During the first-stage processing, it is possible to reduce the heteroatom content of the GPGP tar oil stream to below the detectability limits of the equipment.
- The product of the first-stage processing would be a good candidate for further processing to produce specification-grade JP-8 or high-density jet fuel due to its high aromaticity.
- Generally, the higher-pressure runs removed heteroatoms and increased hydrogen-to-carbon ratio at a more rapid rate than did the lower-pressure runs.
- The liquid balances which were calculated for the runs corroborated the analytical results.
- The single-stage processing which was attempted was unsuccessful. One of the catalysts which was tested behaved similarly to the Shell 424 catalyst which was used during the first-stage testing. The other catalyst was less effective at heteroatom removal. Neither catalyst successfully increased the aliphatic content.
- The results of the second-stage testing indicate that the catalysts which were used were not effective at saturating the ring structures. This could be due to poisoning of the catalyst due to minute quantities of heteroatoms present in the second-stage feedstock, poor operating conditions relative to the catalyst, or ineffectiveness of the catalyst in this particular system.

RECOMMENDATIONS

Further second-stage testing should be performed to investigate the effectiveness of different catalysts at saturating the ring structures in order to achieve specification-grade fuels.

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LIST OF ABBREVIATIONS AND SYMBOLS

ALI CON	aliphatic content
ARO:ALI	aromatic-to-aliphatic ratio
ASTM	American Society for Testing Materials
bbl	barrel
Btu	British thermal unit
°C	degrees Celsius
g	gram
gal	gallon
GC	gas chromatograph
GPGP	Great Plains Gasification Plant
HC	heteroatom content
HDN	hydrodenitrogenation
hr	hour
JP-4	Grade 4 jet fuel
JP-8	Grade 8 jet fuel
JP-8X	high-density Grade 8 jet fuel
KF-water	water determined by Karl Fisher titration
kg	kilogram
MS	mass spectroscopy
N	nitrogen content
NMR	nuclear magnetic resonance spectroscopy
NT550	Ni-W catalyst on an alumina support
P	pressure
psig	pounds per square inch gauge
scf	standard cubic feet
SNG	synthetic natural gas
sp. gr.	specific gravity
S	sulfur content
T	temperature
THFI	tetrahydrofuran insolubles
vol%	volume percent
wt%	weight percent
X ₁	temperature factor in modeling equations
X ₂	pressure factor in modeling equations
%	percent

APPENDIX A
STATISTICAL EXPERIMENTAL DESIGN

SAS

10:15 Wednesday, January 20, 1988

1

Model: MODEL1

Dep Variable: Y

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Value	Prob>F
Model	5	25.47698	5.09540	5.895	0.1514
Error	2	1.72870	0.86435		
C Total	7	27.20569			
Root MSE		0.92971	R-Square	0.9365	
Dep Mean		2.97125	Adj R-Sq	0.7776	
C.V.		31.29005			

Parameter Estimates

Variable	DF	Parameter Estimate	Standard Error	T for H0: Parameter=0	Prob > T
INTERCEP	1	3.459163	0.65615638	5.272	0.0341
X1	1	-1.933013	1.06348806	-1.818	0.2108
X2	1	-0.814979	0.77186311	-1.056	0.4017
X3	1	0.231305	1.22190418	0.189	0.8673
X4	1	0.186708	1.11270893	0.168	0.8822
X5	1	-0.252352	0.53236120	-0.474	0.6822

Backward Elimination Procedure for Dependent Variable Y

Step 0 All Variables Entered R-square = 0.93645796 C(p) = 6.00000000

	DF	Sum of Squares	Mean Square	F	Prob>F
Regression	5	25.47698252	5.09539650	5.90	0.1514
Error	2	1.72870498	0.86435249		
Total	7	27.20568750			

Variable	Parameter Estimate	Standard Error	Type II Sum of Squares	F	Prob>F
INTERCEP	3.45916336	0.65615638	24.02250624	27.79	0.0341
X1	-1.93301320	1.06348806	2.85558628	3.30	0.2108
X2	-0.81497937	0.77186311	0.96361498	1.11	0.4017
X3	0.23130544	1.22190418	0.03097336	0.04	0.8673
X4	0.18670759	1.11270893	0.02433614	0.03	0.8822
X5	-0.25235197	0.53236120	0.19421890	0.22	0.6822

Bounds on condition number: 5.0008, 93.2912

Step 1 Variable X4 Removed R-square = 0.93556343 C(p) = 4.02615534

	DF	Sum of Squares	Mean Square	F	Prob>F
Regression	4	25.45264638	6.36316159	10.89	0.0393
Error	3	1.75304112	0.58434704		
Total	7	27.20568750			

Variable	Parameter Estimate	Standard Error	Type II Sum of Squares	F	Prob>F
INTERCEP	3.50330944	0.49423953	29.35978591	50.24	0.0058
X1	-1.80031061	0.58461727	5.54143764	9.48	0.0542
X2	-0.90471714	0.45761531	2.28399634	3.91	0.1425
X3	0.38048519	0.64510748	0.21191204	0.36	0.5895
X5	-0.29118837	0.39418657	0.31887117	0.55	0.5136

Bounds on condition number: 2.6001, 31.3515

Step 2 Variable X3 Removed R-square = 0.92777418 C(p) = 2.27332389

	DF	Sum of Squares	Mean Square	F	Prob>F
Regression	3	25.24073434	8.41357811	17.13	0.0095
Error	4	1.96495316	0.49123829		
Total	7	27.20568750			

Variable	Parameter Estimate	Standard Error	Type II Sum of Squares	F	Prob>F
----------	--------------------	----------------	------------------------	---	--------

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INTERCEP	3.52895951	0.41078771	38.33751605	78.04	0.0009
X1	-2.01394684	0.42605048	10.97655600	22.34	0.0091
X2	-0.71525683	0.30468830	2.70710238	5.51	0.0787
X5	-0.22826650	0.34849216	0.21076115	0.43	0.5482

Bounds on condition number: 1.3711, 11.2168

Step 3 Variable X5 Removed R-square = 0.92002723 C(p) = 0.51716092

	DF	Sum of Squares	Mean Square	F	Prob>F
Regression	2	25.02997319	12.51498659	28.76	0.0018
Error	5	2.17571431	0.43514286		
Total	7	27.20568750			

Variable	Parameter Estimate	Standard Error	Type III Sum of Squares	F	Prob>F
INTERCEP	3.43002277	0.26030670	75.55360503	173.63	0.0001
X1	-2.03847496	0.39943570	11.33310408	26.04	0.0038
X2	-0.67451379	0.28066521	2.51176364	5.77	0.0614

Bounds on condition number: 1.3134, 5.2536

All variables in the model are significant at the 0.1000 level.

Summary of Backward Elimination Procedure for Dependent Variable Y

Step	Variable Removed	Number In	Partial R**2	Model R**2	C(p)	F	Prob>F
1	X4	4	0.0009	0.9356	4.0282	0.0282	0.8822
2	X3	3	0.0078	0.9278	2.2733	0.3626	0.5895
3	X5	2	0.0077	0.9200	0.5172	0.4290	0.5482

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Model: MODEL1

Model Crossproducts X'X X'Y Y'Y

X'X	INTERCEP	X1	X2	X3
INTERCEP	8	2.0333333333	-0.704	2.3113333333
X1	2.0333333333	4.0988888889	2.3113333333	-1.1779244444
X2	-0.704	2.3113333333	7.3172	1.7980301333
X3	2.3113333333	-1.1779244444	1.7980301333	3.5035361867
X4	4.0988888889	1.7593703704	-1.1779244444	2.0210694815
X5	7.3172	1.7980301333	-1.677663008	2.3279697381
Y	23.77	-2.939666667	-12.06042	7.4741206667

X'X	X4	X5	Y
INTERCEP	4.0988888889	7.3172	23.77
X1	1.7593703704	1.7980301333	-2.939666667
X2	-1.1779244444	-1.677663008	-12.06042
X3	2.0210694815	2.3279697381	7.4741206667
X4	3.9759469136	3.5035361867	11.248544444
X5	3.5035361867	10.916344435	21.64088276
Y	11.248544444	21.64088276	97.8323

X'X Inverse, Parameter Estimates, and SSE

INVERSE	INTERCEP	X1	X2	Y
INTERCEP	.15571799941	-.1042672539	.04791748909	3.4300227731
X1	-.1042672539	.36665660644	-.1258506547	-2.038474962
X2	.04791748909	-.1258506547	.18102781467	-.6743137864
Y	3.4300227731	-2.038474962	-.6743137864	2.1757143105

Dep Variable: Y

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Value	Prob>F
Model	2	25.02997	12.51499	28.761	0.0018
Error	5	2.17571	0.43514		
C Total	7	27.20569			
Root MSE		0.65965	R-Square	0.9200	
Dep Mean		2.97125	Adj R-Sq	0.8880	
C.V.		22.20121			

Parameter Estimates

Variable	DF	Parameter Estimate	Standard Error	T for H0: Parameter=0	Prob > T
INTERCEP	1	3.430023	0.26030670	13.177	0.0001
X1	1	-2.038475	0.39943570	-5.103	0.0038
X2	1	-0.674314	0.28066521	-2.403	0.0614

Variable	DF	Type I SS	Type II SS	Standardized Estimate	Tolerance
INTERCEP	1	70.626612	75.553605	0.00000000	.
X1	1	22.518210	11.333104	-0.73967914	0.76138169
X2	1	2.511764	2.511764	-0.34822369	0.76138169

Variable	DF	Variance Inflation
INTERCEP	1	0.00000000
X1	1	1.31340169
X2	1	1.31340169

Covariance of Estimates

COVB	INTERCEP	X1	X2
INTERCEP	.06775957594	-.0453711513	.02085095335
X1	-.0453711513	.15954887629	-.0547630141
X2	.02085095335	-.0547630141	.07877296139

Correlation of Estimates

CORRE	INTERCEP	X1	X2
INTERCEP	1.0000	-0.4364	0.2854
X1	-0.4364	1.0000	-0.4885
X2	0.2854	-0.4885	1.0000

Obs	Y	Predict Value	Std Err Predict	Lower95% Mean	Upper95% Mean	Lower95% Predict	Upper95% Predict
1	1.1600	1.5684	0.437	0.4449	2.6919	-0.4657	3.6025
2	2.3800	2.4933	0.509	1.1637	3.8028	0.3508	4.6358
3	1.1400	0.8028	0.385	-0.1878	1.7934	-1.1610	2.7666
4	4.3100	4.5779	0.399	3.5526	5.6033	2.5963	6.5595
5	1.0600	0.9211	0.370	-0.0312	1.8733	-1.0237	2.8658
6	2.7300	3.6339	0.280	2.9140	4.3538	1.7917	5.4760
7	6.4900	6.2229	0.506	4.9227	7.5231	4.0861	8.3597
8	4.5000	3.5497	0.275	2.8423	4.2572	1.7124	5.3871

Obs	Residual	Std Err Residual	Student Residual	-2 -1 -0 1 2	Cook's D
1	-0.4084	0.494	-0.827	*	0.178
2	-0.1133	0.419	-0.270		0.036
3	0.3372	0.535	0.630	*	0.069
4	-0.2679	0.525	-0.510	*	0.050
5	0.1389	0.546	0.255		0.010
6	-0.9039	0.597	-1.513	***	0.168
7	0.2671	0.423	0.631	*	0.189
8	0.9503	0.600	1.585	***	0.176

Sum of Residuals -3.9968E-15
Sum of Squared Residuals 2.1757
Predicted Resid SS (Press) 4.0500

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NOTE: AUTOEXEC processing completed.

```
1    option ps=56;  
2    data set jetfuel;  
3        infile "b:jet.dat";  
4        input temp press n s aliph aro_ali;  
5        x1 = (temp-360)/30;  
6        x2 = (press-2000)/500;  
7        x3 = x1*x2;  
8        x4 = x1*x1;  
9        x5 = x2*x2;  
10       run;
```

NOTE: The infile "B:JET.DAT" is file B:\JET.DAT.

NOTE: 8 records were read from the infile B:\JET.DAT

The maximum record length was 32.

The minimum record length was 32.

NOTE: The data set WORK.SET has 8 observations and 11 variables.

NOTE: The data set WORK.JETFUEL has 8 observations and 11 variables.

NOTE: The DATA statement used 34.00 seconds.

```
11    proc reg;  
12        model n s aliph aro_ali = x1-x5 / r;  
13    run;  
14    proc reg;
```

NOTE: The PROCEDURE REG used 2.17 minutes.

```
15        model n s aliph aro_ali = x1-x5 / method=b r;  
16    run;  
17    quit;
```

NOTE: The PROCEDURE REG used 2.85 minutes.

```
18    proc reg;  
19        model s = x2 x5 / r;  
20    run;  
21    quit;
```

NOTE: The PROCEDURE REG used 1.00 minutes.

Model: MODEL1
Dep Variable: N

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Value	Prob>F
Model	5	0.00001	0.00000	1194.820	0.0008
Error	2	0.00000	0.00000		
C Total	7	0.00001			
Root MSE		0.00004	R-Square	0.9997	
Dep Mean		0.00086	Adj R-Sq	0.9988	
C.V.		4.39794			

Parameter Estimates

Variable	DF	Parameter Estimate	Standard Error	T for H0: Parameter=0	Prob > T
INTERCEP	1	0.000104	0.00002678	3.889	0.0602
X1	1	0.000040989	0.00004416	0.928	0.4513
X2	1	-0.000661	0.00003268	-20.217	0.0024
X3	1	-0.000722	0.00005220	-13.838	0.0052
X4	1	0.000655	0.00004682	13.982	0.0051
X5	1	0.000602	0.00002168	27.780	0.0013

Dep Variable: S

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Value	Prob>F
Model	5	0.00000	0.00000	2.366	0.3233
Error	2	0.00000	0.00000		
C Total	7	0.00000			
Root MSE		0.00032	R-Square	0.8554	
Dep Mean		0.00056	Adj R-Sq	0.4939	
C.V.		57.33974			

Parameter Estimates

Variable	DF	Parameter Estimate	Standard Error	T for H0: Parameter=0	Prob > T
INTERCEP	1	0.000014705	0.00022768	0.065	0.9544
X1	1	-0.000011615	0.00037552	-0.031	0.9781
X2	1	-0.000189	0.00027789	-0.680	0.5665
X3	1	0.000123	0.00044389	0.277	0.8077
X4	1	0.000214	0.00039809	0.537	0.6449
X5	1	0.000428	0.00018432	2.323	0.1459

Dep Variable: ALIPH

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Value	Prob>F
Model	5	144.72367	28.94473	7.021	0.1294
Error	2	8.24508	4.12254		
C Total	7	152.96875			
Root MSE		2.03040	R-Square	0.9461	
Dep Mean		49.31250	Adj R-Sq	0.8113	
C.V.		4.11742			

Parameter Estimates

Variable	DF	Parameter Estimate	Standard Error	T for H0: Parameter=0	Prob > T
INTERCEP	1	49.240984	1.43327831	34.355	0.0008
X1	1	2.199264	2.36392880	0.930	0.4504
X2	1	3.693924	1.74935358	2.112	0.1691
X3	1	-2.655819	2.79432798	-0.950	0.4422
X4	1	1.320364	2.50604090	0.527	0.6509
X5	1	-0.157338	1.16033701	-0.136	0.9046

Dep Variable: ARD_ALI

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Value	Prob>F
Model	5	0.27914	0.05583	8.689	0.1064
Error	2	0.01285	0.00643		
C Total	7	0.29199			
Root MSE		0.08016	R-Square	0.9560	
Dep Mean		1.04375	Adj R-Sq	0.8460	
C.V.		7.67979			

Parameter Estimates

Variable	DF	Parameter Estimate	Standard Error	T for H0: Parameter=0	Prob > T
INTERCEP	1	1.031494	0.05658402	18.229	0.0030
X1	1	-0.104882	0.09332493	-1.124	0.3779
X2	1	-0.155370	0.06906228	-2.250	0.1534
X3	1	0.121732	0.11031655	1.103	0.3848
X4	1	-0.041598	0.09893534	-0.420	0.7150
X5	1	0.016151	0.04580864	0.353	0.7581

Obs	N	Predict Value	Std Err Predict	Residual	Std Err Residual	Student Residual
1	0	1.623E-5	0.000	-1.62E-5	0.000	-1.378
2	0.00280	0.00279	0.000	1.13E-5	0.000	1.386
3	4E-4	4.291E-4	0.000	-2.91E-5	0.000	-1.383
4	0.00220	0.00221	0.000	-9.44E-6	0.000	-1.391
5	0	-3.75E-5	0.000	3.745E-5	0.000	1.376
6	1E-4	1.066E-4	0.000	-6.59E-6	0.000	-0.246
7	0.00130	0.00130	0.000	2.523E-6	0.000	1.411
8	1E-4	8.996E-5	0.000	1.004E-5	0.000	0.374

Obs	-2	-1	0	1	2	Cook's D
1		**				2.966
2			**			6.605
3		**				0.721
4		**				9.757
5			**			0.298
6						0.010
7			**			148.777
8						0.023

Sum of Residuals -2.81893E-18
Sum of Squared Residuals 0.0000
Predicted Resid SS (Press) 0.0000

Obs	S	Predict Value	Std Err Predict	Residual	Std Err Residual	Student Residual
1	8E-4	6.584E-4	0.000	1.416E-4	0.000	1.414
2	7E-4	7.98E-4	0.000	-9.8E-5	0.000	-1.414

Obs	S	Predict Value	Std Err Predict	Residual	Std Err Residual	Student Residual
3	6E-4	3.474E-4	0.000	2.526E-4	0.000	1.414
4	0.00120	0.00112	0.000	8.149E-5	0.000	1.412
5	2E-4	5.272E-4	0.000	-3.27E-4	0.000	-1.414
6	0	1.8E-5	0.000	-1.8E-5	0.000	-0.079
7	0.00100	0.00102	0.000	-2.05E-5	0.000	-1.350
8	0	1.194E-5	0.000	-1.19E-5	0.000	-0.052

Obs	-2-1-0 1 2	Cook's D
1	**	3.124
2	**	6.873
3	**	0.753
4	**	10.059
5	**	0.314
6		0.001
7	**	136.298
8		0.000

Sum of Residuals -4.69256E-19
Sum of Squared Residuals 0.0000
Predicted Resid SS (Press) 0.0001

Obs	ALIPH	Predict Value	Std Err Predict	Residual	Std Err Residual	Student Residual
1	54.2000	53.5817	1.930	0.6183	0.630	0.981
2	49.7000	50.1165	1.983	-0.4165	0.436	-0.954
3	54.8000	53.7161	1.691	1.0839	1.125	0.964
4	44.1000	43.7611	1.998	0.3389	0.363	0.933
5	52.0000	53.4362	1.415	-1.4362	1.457	-0.986
6	47.5000	49.0343	1.436	-1.5343	1.436	-1.069
7	41.6000	41.6611	2.028	-0.0611	0.096	-0.638
8	50.6000	49.1930	1.433	1.4070	1.438	0.978

Obs	-2-1-0 1 2	Cook's D
1	*	1.502
2	*	3.131
3	*	0.350
4	*	4.390
5	*	0.153

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Obs	-2	-1	-0	1	2	Cook's D
6		**				0.190
7		*				30.403
8		*				0.158

Sum of Residuals 0
 Sum of Squared Residuals 8.2451
 Predicted Resid SS (Press) 1025.7332

Obs	ARD_ALI	Predict Value	Std Err Predict	Residual	Std Err Residual	Student Residual
1	0.8500	0.8699	0.076	-0.0199	0.025	-0.798
2	1.0100	0.9968	0.078	0.0132	0.017	0.768
3	0.8200	0.8546	0.067	-0.0346	0.044	-0.779
4	1.2700	1.2807	0.079	-0.0107	0.014	-0.744
5	0.9200	0.8737	0.056	0.0463	0.058	0.804
6	1.1100	1.0416	0.057	0.0684	0.057	1.207
7	1.4000	1.3984	0.080	0.00159	0.004	0.420
8	0.9700	1.0344	0.057	-0.0644	0.057	-1.134

Obs	-2	-1	-0	1	2	Cook's D
1		*				0.995
2		*				2.029
3		*				0.229
4		*				2.791
5		*				0.102
6		**				0.243
7						13.168
8		**				0.213

Sum of Residuals 4.440892E-16
 Sum of Squared Residuals 0.0129
 Predicted Resid SS (Press) 0.8004

Backward Elimination Procedure for Dependent Variable N

Step 0 All Variables Entered R-square = 0.99966533 C(p) = 6.00000000

	DF	Sum of Squares	Mean Square	F	Prob>F
Regression	5	0.00000860	0.00000172	1194.82	0.0008
Error	2	0.00000000	0.00000000		
Total	7	0.00000860			

Variable	Parameter Estimate	Standard Error	Type II Sum of Squares	F	Prob>F
INTERCEP	0.00010414	0.00002678	0.00000002	15.13	0.0602
X1	0.00004099	0.00004416	0.00000000	0.86	0.4513
X2	-0.00066071	0.00003268	0.00000059	408.71	0.0024
X3	-0.00072242	0.00005220	0.00000028	191.50	0.0052
X4	0.00065459	0.00004682	0.00000028	195.48	0.0051
X5	0.00060219	0.00002168	0.00000111	771.71	0.0013

Bounds on condition number: 5.4825, 99.5

Step 1 Variable X1 Removed R-square = 0.99952119 C(p) = 4.86143709

	DF	Sum of Squares	Mean Square	F	Prob>F
Regression	4	0.00000859	0.00000215	1565.62	0.0001
Error	3	0.00000000	0.00000000		
Total	7	0.00000860			

Variable	Parameter Estimate	Standard Error	Type II Sum of Squares	F	Prob>F
INTERCEP	0.00010304	0.00002613	0.00000002	15.55	0.0291
X2	-0.00063467	0.00001636	0.00000207	1504.86	0.0001
X3	-0.00076312	0.00002766	0.00000104	761.31	0.0001
X4	0.00068736	0.00003002	0.00000072	524.12	0.0002
X5	0.00061162	0.00001870	0.00000147	1069.36	0.0001

Bounds on condition number: 1.6134, 21.3751

All variables in the model are significant at the 0.1000 level.

Summary of Backward Elimination Procedure for Dependent Variable N

Step	Variable Removed	Number In	Partial R**2	Model R**2	C(p)	F	Prob>F
1	x1	4	0.0001	0.9995	4.8614	0.8614	0.4513

Backward Elimination Procedure for Dependent Variable S

Step 0 All Variables Entered R-square = 0.85538904 C(p) = 6.00000000

	DF	Sum of Squares	Mean Square	F	Prob>F
Regression	5	0.00000123	0.00000025	2.37	0.3233
Error	2	0.00000021	0.00000010		
Total	7	0.00000144			

Variable	Parameter Estimate	Standard Error	Type II Sum of Squares	F	Prob>F
INTERCEP	0.00001470	0.00022768	0.00000000	0.00	0.9544
X1	-0.00001162	0.00037552	0.00000000	0.00	0.9761
X2	-0.00018906	0.00027789	0.00000005	0.46	0.5665
X3	0.00012298	0.00044389	0.00000001	0.08	0.8077
X4	0.00021383	0.00039809	0.00000003	0.29	0.6449
X5	0.00042812	0.00018432	0.00000056	5.39	0.1459

Bounds on condition number: 5.4825, 99.5

Step 1 Variable X1 Removed R-square = 0.85531986 C(p) = 4.00095678

	DF	Sum of Squares	Mean Square	F	Prob>F
Regression	4	0.00000123	0.00000031	4.43	0.1256
Error	3	0.00000021	0.00000007		
Total	7	0.00000144			

Variable	Parameter Estimate	Standard Error	Type II Sum of Squares	F	Prob>F
INTERCEP	0.00001502	0.00018576	0.00000000	0.01	0.9407
X2	-0.00019644	0.00011633	0.00000020	2.85	0.1899
X3	0.00013452	0.00019666	0.00000003	0.47	0.5431
X4	0.00020455	0.00021348	0.00000006	0.92	0.4087
X5	0.00042545	0.00013299	0.00000071	10.23	0.0494

Bounds on condition number: 1.6134, 21.3751

Step 2 Variable X3 Removed R-square = 0.83275584 C(p) = 2.31302193

	DF	Sum of Squares	Mean Square	F	Prob>F
Regression	3	0.00000120	0.00000040	6.64	0.0494
Error	4	0.00000024	0.00000006		
Total	7	0.00000144			

Variable	Parameter Estimate	Standard Error	Type II Sum of Squares	F	Prob>F
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INTERCEP	0.00000840	0.00017273	0.00000000	0.00	0.9636
X2	-0.00015534	0.00009275	0.00000017	2.80	0.1693
X4	0.00026735	0.00017946	0.00000013	2.22	0.2105
X5	0.00044147	0.00012189	0.00000079	13.12	0.0223

Bounds on condition number: 1.0432, 9.2712

Step 3 Variable X4 Removed R-square = 0.73996072 C(p) = 1.59639804

	DF	Sum of Squares	Mean Square	F	Prob>F
Regression	2	0.00000106	0.00000053	7.11	0.0345
Error	5	0.00000037	0.00000007		
Total	7	0.00000144			

See Pg 20

Variable	Parameter Estimate	Standard Error	Type II Sum of Squares	F	Prob>F
INTERCEP	0.00015917	0.00015611	0.00000008	1.04	0.3547
X2	-0.00015025	0.00010337	0.00000016	2.11	0.2058
X5	0.00042651	0.00013548	0.00000074	9.91	0.0254

Bounds on condition number: 1.0361, 4.1445

Step 4 Variable X2 Removed R-square = 0.63009214 C(p) = 1.11590356

	DF	Sum of Squares	Mean Square	F	Prob>F
Regression	1	0.00000091	0.00000091	10.22	0.0187
Error	6	0.00000053	0.00000009		
Total	7	0.00000144			

Variable	Parameter Estimate	Standard Error	Type II Sum of Squares	F	Prob>F
INTERCEP	0.00013875	0.00016928	0.00000006	0.67	0.4437
X5	0.00046329	0.00014492	0.00000091	10.22	0.0187

Bounds on condition number: 1.0000, 1.0000

All variables in the model are significant at the 0.1000 level.

Summary of Backward Elimination Procedure for Dependent Variable S

Step	Variable Removed	Number In	Partial R**2	Model R**2	C(p)	F	Prob>F
1	X1	4	0.0001	0.8553	4.0010	0.0010	0.9781
2	X3	3	0.0226	0.8328	2.3130	0.4679	0.5431
3	X4	2	0.0928	0.7400	1.5964	2.2194	0.2105
4	X2	1	0.1099	0.6301	1.1159	2.1125	0.2058

Backward Elimination Procedure for Dependent Variable ALIPH

Step 0 All Variables Entered R-square = 0.94609958 C(p) = 6.00000000

	DF	Sum of Squares	Mean Square	F	Prob>F
Regression	5	144.72367080	28.94473416	7.02	0.1294
Error	2	8.24507920	4.12253960		
Total	7	152.96875000			

Variable	Parameter Estimate	Standard Error	Type II Sum of Squares	F	Prob>F
INTERCEP	49.24098449	1.43327831	4865.83337841	1180.30	0.0008
X1	2.19926369	2.36392880	3.56821208	0.87	0.4504
X2	3.69392410	1.74935358	18.38169577	4.46	0.1691
X3	-2.65581867	2.79432798	3.72397637	0.90	0.4422
X4	1.32036425	2.50604090	1.14439523	0.28	0.6509
X5	-0.15733764	1.16033701	0.07579871	0.02	0.9046

Bounds on condition number: 5.4825, 99.5

Step 1 Variable X5 Removed R-square = 0.94560407 C(p) = 4.01838641

	DF	Sum of Squares	Mean Square	F	Prob>F
Regression	4	144.64787209	36.16196802	13.04	0.0307
Error	3	8.32087791	2.77362597		
Total	7	152.96875000			

Variable	Parameter Estimate	Standard Error	Type II Sum of Squares	F	Prob>F
INTERCEP	49.12061816	0.92302116	7855.10929872	2832.07	0.0001
X1	2.04907720	1.71298571	3.96878031	1.43	0.3175
X2	3.81568713	1.23141899	26.63064672	9.60	0.0534
X3	-2.83693001	2.01323182	5.50753882	1.99	0.2536
X4	1.46980135	1.84612174	1.75810378	0.63	0.4841

Bounds on condition number: 4.2299, 56.9513

Step 2 Variable X4 Removed R-square = 0.93411084 C(p) = 2.44484776

	DF	Sum of Squares	Mean Square	F	Prob>F
Regression	3	142.88976831	47.62992277	18.90	0.0080
Error	4	10.07898169	2.51974542		
Total	7	152.96875000			

Variable	Parameter Estimate	Standard Error	Type II Sum of Squares	F	Prob>F
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INTERCEP	49.24810930	0.86642291	8140.96580094	3230.87	0.0001
X1	2.99129195	1.18040876	16.18115131	6.42	0.0644
X2	3.19617882	0.90969013	31.10511656	12.34	0.0246
X3	-1.66542249	1.30962426	4.07485437	1.62	0.2724

Bounds on condition number: 2.3828, 18.8986

Step 3 Variable X3 Removed R-square = 0.90747237 C(p) = 1.43328080

	DF	Sum of Squares	Mean Square	F	Prob>F
Regression	2	138.81491394	69.40745697	24.52	0.0026
Error	5	14.15383606	2.83076721		
Total	7	152.96875000			

Variable	Parameter Estimate	Standard Error	Type II Sum of Squares	F	Prob>F
INTERCEP	48.49231385	0.66822345	14907.55924729	5266.26	0.0001
X1	3.87056715	1.01403639	41.24262371	14.57	0.0124
X2	2.40869424	0.70631551	32.92077253	11.63	0.0190

Bounds on condition number: 1.2786, 5.1145

All variables in the model are significant at the 0.1000 level.

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Summary of Backward Elimination Procedure for Dependent Variable ALIPH

Step	Variable Removed	Number In	Partial R**2	Model R**2	C(p)	F	Prob>F
1	X5	4	0.0005	0.9456	4.0184	0.0184	0.9046
2	X4	3	0.0115	0.9341	2.4448	0.6339	0.4841
3	X3	2	0.0266	0.9075	1.4333	1.6172	0.2724

Backward Elimination Procedure for Dependent Variable ARO_ALI

Step 0 All Variables Entered R-square = 0.95598942 C(p) = 6.00000000

	DF	Sum of Squares	Mean Square	F	Prob>F
Regression	5	0.27913696	0.05582739	8.69	0.1064
Error	2	0.01285054	0.00642527		
Total	7	0.29198750			

Variable	Parameter Estimate	Standard Error	Type II Sum of Squares	F	Prob>F
INTERCEP	1.03149430	0.05658402	2.13519449	332.31	0.0000
X1	-0.10488231	0.09332493	0.00811522	1.26	0.3279
X2	-0.15536987	0.06906228	0.03251945	5.06	0.1534
X3	0.12173164	0.11031655	0.00782379	1.22	0.3848
X4	-0.04159778	0.09893534	0.00113587	0.18	0.7150
X5	0.01615138	0.04580864	0.00079876	0.12	0.7581

Bounds on condition number: 5.4825, 99.5

Step 1 Variable X5 Removed R-square = 0.95325382 C(p) = 4.12431520

	DF	Sum of Squares	Mean Square	F	Prob>F
Regression	4	0.27833820	0.06958455	15.29	0.0246
Error	3	0.01364930	0.00454977		
Total	7	0.29198750			

Variable	Parameter Estimate	Standard Error	Type II Sum of Squares	F	Prob>F
INTERCEP	1.04385041	0.03738370	3.54732615	779.67	0.0001
X1	-0.08946502	0.06937841	0.00756566	1.66	0.2876
X2	-0.16786937	0.04987426	0.05154412	11.33	0.0435
X3	0.14032349	0.08153882	0.01347476	2.96	0.1837
X4	-0.05693813	0.07477061	0.00263836	0.58	0.5017

Bounds on condition number: 4.2299, 56.9513

Step 2 Variable X4 Removed R-square = 0.94421796 C(p) = 2.53493732

	DF	Sum of Squares	Mean Square	F	Prob>F
Regression	3	0.27569984	0.09189995	22.57	0.0057
Error	4	0.01628766	0.00407191		
Total	7	0.29198750			

Variable	Parameter Estimate	Standard Error	Type II Sum of Squares	F	Prob>F
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INTERCEP	1.03891158	0.03482979	3.62288025	889.72	0.0001
X1	-0.12596516	0.04745188	0.02869411	7.05	0.0567
X2	-0.14387045	0.03656912	0.06302500	15.48	0.0170
X3	0.09494086	0.05264628	0.01324249	3.25	0.1457

Bounds on condition number: 2.3828, 18.8986

Step 3 Variable X3 Removed R-square = 0.89886504 C(p) = 2.59593814

	DF	Sum of Squares	Mean Square	F	Prob>F
Regression	2	0.26245736	0.13122868	22.22	0.0033
Error	5	0.02953014	0.00590603		
Total	7	0.29198750			

Variable	Parameter Estimate	Standard Error	Type III Sum of Squares	F	Prob>F
INTERCEP	1.08199726	0.03052231	7.42186507	1256.66	0.0001
X1	-0.17609006	0.04631794	0.08536243	14.45	0.0126
X2	-0.09897826	0.03226224	0.05558867	9.41	0.0278

Bounds on condition number: 1.2786, 5.1145

All variables in the model are significant at the 0.1000 level.

Summary of Backward Elimination Procedure for Dependent Variable ARO_ALI

Step	Variable Removed	Number In	Partial R**2	Model R**2	C(p)	F	Prob > F
1	X5	4	0.0027	0.9533	4.1243	0.1243	0.7581
2	X4	3	0.0090	0.9442	2.5349	0.5799	0.5017
3	X3	2	0.0454	0.8989	2.5959	3.2522	0.1457

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Obs	N	Predict Value	Std Err Predict	Residual	Std Err Residual	Student Residual
1	0	2.984E-5	0.000	-2.98E-5	0.000	-1.625
2	0.00280	0.00280	0.000	2.867E-6	0.000	0.240
3	4E-4	4.162E-4	0.000	-1.62E-5	0.000	-0.661
4	0.00220	0.00219	0.000	9.65E-6	0.000	0.456
5	0	-5.01E-5	0.000	5.006E-5	0.000	1.685
6	1E-4	1.099E-4	0.000	-9.91E-6	0.000	-0.375
7	0.00130	0.00131	0.000	-1.42E-5	0.000	-0.803
8	1E-4	9.243E-5	0.000	7.567E-6	0.000	0.287

Obs	-2	-1	0	1	2	Cook's D
1	:	***	:	:	:	1.620
2	:	:	:	:	:	0.100
3	:	*	:	:	:	0.112
4	:	:	:	:	:	0.086
5	:	:	***	:	:	0.316
6	:	:	:	:	:	0.027
7	:	*	:	:	:	0.439
8	:	:	:	:	:	0.016

Sum of Residuals -1.43657E-18
Sum of Squared Residuals 0.0000
Predicted Resid SS (Press) 0.0000

Obs	S	Predict Value	Std Err Predict	Residual	Std Err Residual	Student Residual
1	8E-4	9.831E-4	0.000	-1.83E-4	0.000	-0.746
2	7E-4	7.303E-4	0.000	-3.03E-5	0.000	-0.111
3	6E-4	2.411E-4	0.000	3.589E-4	0.000	1.381
4	0.00120	0.00105	0.000	1.532E-4	0.000	0.655
5	2E-4	6.02E-4	0.000	-4.02E-4	0.000	-1.445
6	0	1.388E-4	0.000	-1.39E-4	0.000	-0.566
7	0.00100	6.189E-4	0.000	3.811E-4	0.000	1.371
8	0	1.39E-4	0.000	-1.39E-4	0.000	-0.567

Obs	-2	-1	0	1	2	Cook's D
1	:	*	:	:	:	0.131
2	:	:	:	:	:	0.001
3	:	:	**	:	:	0.300

Obs	-2	-1	0	1	2	Cook's D
4				*		0.134
5			**			0.151
6			*			0.077
7				**		0.139
8			*			0.077

Sum of Residuals -1.19262E-18
 Sum of Squared Residuals 0.0000
 Predicted Resid SS (Press) 0.0000

Obs	ALIPH	Predict Value	Std Err Predict	Residual	Std Err Residual	Student Residual
1	54.2000	53.5503	1.111	0.6497	1.264	0.514
2	49.7000	48.9960	1.273	0.7040	1.100	0.640
3	54.8000	54.0110	0.979	0.7890	1.368	0.577
4	44.1000	45.1201	1.026	-1.0201	1.334	-0.765
5	52.0000	54.3845	0.947	-2.3845	1.391	-1.714
6	47.5000	48.1053	0.719	-0.6053	1.521	-0.398
7	41.6000	42.0407	1.309	-0.4407	1.056	-0.417
8	50.6000	48.2921	0.707	2.3079	1.527	1.511

Obs	-2	-1	0	1	2	Cook's D
1				*		0.068
2				*		0.183
3				*		0.057
4			*			0.115
5			***			0.454
6						0.012
7						0.089
8				***		0.163

Sum of Residuals -7.10543E-15
 Sum of Squared Residuals 14.1538
 Predicted Resid SS (Press) 29.9190

Obs	ARO_ALI	Predict Value	Std Err Predict	Residual	Std Err Residual	Student Residual
1	0.8500	0.8662	0.051	-0.0162	0.058	-0.281

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Obs	ARO ALI	Predict Value	Std Err Predict	Residual	Std Err Residual	Student Residual
2	1.0100	1.0471	0.058	-0.0371	0.050	-0.738
3	0.8200	0.8359	0.045	-0.0159	0.063	-0.255
4	1.2700	1.2206	0.047	0.0494	0.061	0.811
5	0.9200	0.8245	0.043	0.0955	0.064	1.503
6	1.1100	1.0996	0.033	0.0104	0.069	0.150
7	1.4000	1.3647	0.060	0.0353	0.048	0.731
8	0.9700	1.0914	0.032	-0.1214	0.070	-1.740

Obs	-2-1-0 1 2	Cook's D
1		0.020
2	*	0.243
3		0.011
4	*	0.130
5	***	0.349
6		0.002
7	*	0.274
8	***	0.216

Sum of Residuals -1.11022E-16
Sum of Squared Residuals 0.0295
Predicted Resid SS (Press) 0.0645

Model: MODEL1
Dep Variable: S

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Value	Prob>F
Model	2	0.00000	0.00000	7.114	0.0345
Error	5	0.00000	0.00000		
C Total	7	0.00000			
Root MSE		0.00027	R-Square	0.7400	
Dep Mean		0.00056	Adj R-Sq	0.6359	
C.V.		48.63004			

Parameter Estimates

Variable	DF	Parameter Estimate	Standard Error	T for H0: Parameter=0	Prob > T
INTERCEP	1	0.000159	0.00015611	1.020	0.3547
X2	1	-0.000150	0.00010337	-1.453	0.2058
X5	1	0.000427	0.00013548	3.148	0.0254

Obs	S	Predict Value	Std Err Predict	Residual	Std Err Residual	Student Residual
1	8E-4	7.337E-4	0.000	6.635E-5	0.000	0.453
2	7E-4	8.736E-4	0.000	-1.74E-4	0.000	-0.751
3	6E-4	1.828E-4	0.000	4.172E-4	0.000	1.774
4	0.00120	0.00121	0.000	-5.48E-6	0.000	-0.030
5	2E-4	4.354E-4	0.000	-2.35E-4	0.000	-1.030
6	0	1.592E-4	0.000	-1.59E-4	0.000	-0.709
7	0.00100	7.541E-4	0.000	2.459E-4	0.000	1.034
8	0	1.558E-4	0.000	-1.56E-4	0.000	-0.693

Obs	-2	-1	0	1	2	Cook's D
1						0.171
2						0.075
3						0.369
4						0.000
5						0.153
6						0.081

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Obs	-2-1-0 1 2	Cook's D
7	**	0.115
8	*	0.077
Sum of Residuals		-1.0571E-18
Sum of Squared Residuals		0.0000
Predicted Resid SS (Press)		0.0000

APPENDIX B
DATA TABLES

CHL Data

NAME	A	H	N	S	U	U (DIT)	U (DIT)	U (DIT)	total neters
N416-1	0.8434	0.0897	0.0085	0.0033	0.0756				3
N416-2	0.8397	0.0872	0.0055	0.0027	0.0739				6
N416-3	0.8313	0.0886	0.0062	0.0025	0.0714				9
N416-4									12
N416-5									15
N416-6	0.8519	0.0920	0.0061	0.0021	0.0479				18
N416-8									24
N416-9	0.8475	0.0925	0.0053	0.0012	0.0534				27
N416-10									30
N416-11									33
N416-12	0.8499	0.0928	0.0057	0.0013	0.0503				36
N416-14									42
N416-15									45
N416-17									51
N416-18									54
N416-19									57
N416-20									60
N416-21	0.8412	0.0958	0.0040	0.0007	0.0583				70
N416-22									110
N416-110	0.8332	0.0969	0.0013	0.0010	0.0636				120
100-011	0.8376	0.0883	0.0052	0.0039	0.065				9
N417-1	0.8341	0.0880	0.0074						3
N417-2	0.8522	0.0911	0.0061						6
N417-3	0.8543	0.0931	0.0050						9
N417-4									12
N417-5									15
N417-6	0.8527	0.0954	0.0043						18
N417-8									24
N417-9	0.8497	0.0957	0.0003						27
N417-10									30
N417-11									33
N417-12	0.8630	0.1015	0.0023						36
N417-14									42
N417-15									45
N417-17									51
N417-18									54
N417-19									57
N417-20									60
N417-21	0.8615	0.1031	0.0005						70
N417-22	0.8639	0.1092	0.0000						110
N417-110	0.8454	0.1096	0.0001						120

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CHIN DATA

NAME	L	H	N	S	U (DIFF)	TIME	total hetero
N414-1	0.8481	0.0913	0.0334	0.0016	0.0256	3	0.0606
N414-2	0.8474	0.0913	0.0016	0.0010	0.0364	6	0.0529
N414-3	0.8559	0.0937	0.0078	0.0010	0.0471	9	0.0509
N414-4						12	
N414-5						15	
N414-6	0.8605	0.0939	0.0015	0.0002	0.0378	18	0.0396
N414-8						24	
N414-9	0.8512	0.0999	0.0000	0.0001	0.0688	27	0.0689
N414-10						30	
N414-11						33	
N414-12	0.8384	0.1032	0.0001	0.0000	0.0583	36	0.0584
N414-14						42	
N414-15						45	
N414-17						51	
N414-18						54	
N414-19						57	
N414-20						60	
N414-21	0.8565	0.1141	0.0000	0.0000	0.0294	90	0.0294
N414-22	0.8570	0.1138	0.0000	0.0000	0.0292	110	0.0292
N414-EP	0.8723	0.1171	0.0000	0.0002	0.0104	120	0.0106
TRK OIL	0.8376	0.0883	0.0052	0.0039	0.065	0	0.0741
N415-1	0.8486	0.0897	0.0054	0.0027	0.0536	3	0.0617
N415-2	0.8464	0.0916	0.0055	0.0018	0.0547	6	0.0637
N415-3	0.8496	0.0914	0.0064	0.0014	0.0512	9	0.0599
N415-4						12	
N415-5						15	
N415-6	0.8431	0.0938	0.0035	0.0002	0.0594	18	0.0631
N415-8						24	
N415-9	0.8502	0.0958	0.0028	0.0000	0.0512	27	0.054
N415-10						30	
N415-11						33	
N415-12	0.8586	0.0937	0.0007	0.0000	0.0420	36	0.0427
N415-14						42	
N415-15						45	
N415-17						51	
N415-18						54	
N415-19						57	
N415-20						60	
N415-21	0.8622	0.1072	0.0000	0.0000	0.0306	90	0.0306
N415-22	0.8600	0.1078	0.0000	0.0000	0.0322	110	0.0322
N415-EP	0.8631	0.1096	0.0001	0.0000	0.0272	120	0.0273

LINE DATA

NAME	L	H	N	S	U (DIFF)	TIME	total hetero
THR-01L	0.8376	0.0883	0.0052	0.0039	0.065	0	0.0741
N409-1	0.8336	0.0883	0.0065	0.0028	0.0633	3	0.0781
N409-2	0.8411	0.0889	0.0029	0.0023	0.0618	6	0.07
N409-3	0.8502	0.0892	0.0033	0.0019	0.0501	9	0.0599
N409-4						12	
N409-5						15	
N409-6	0.8362	0.0944	0.0057	0.0009	0.0637	18	0.0694
N409-8						24	
N409-9	0.8454	0.0932	0.0060	0.0009	0.0554	27	0.0614
N409-10						30	
N409-11						33	
N409-12	0.8565	0.0969	0.0056	0.0009	0.0418	36	0.0474
N409-14						42	
N409-15						45	
N409-17						51	
N409-18						54	
N409-19						57	
N409-20						60	
N409-21	0.8796	0.1038	0.0011	0.0009	0.0155	90	0.0166
N409-22	0.8794	0.1077	0.0016	0.0009	0.0113	110	0.0129
N409-23	0.8680	0.1082	0.0028	0.0007	0.0203	120	0.0238
THR-01R	0.8376	0.0883	0.0052	0.0039	0.065	0	0.0741
N413-1	0.8307	0.0862	0.0084	0.0028	0.0719	3	0.0831
N413-2	0.8366	0.0871	0.0102	0.0029	0.0632	6	0.0763
N413-3	0.8443	0.0888	0.0087	0.0019	0.0563	9	0.0669
N413-4						12	
N413-5						15	
N413-6	0.8377	0.0904	0.0058	0.0005	0.0656	18	0.0719
N413-8						24	
N413-9	0.8245	0.0901	0.0056	0.0009	0.0798	27	0.0854
N413-10						30	
N413-11						33	
N413-12	0.8026	0.0876	0.0067	0.0009	0.1031	36	0.1098
N413-13						42	
N413-14						45	
N413-17						51	
N413-18						54	
N413-19						57	
N413-20						60	
N413-21	0.8311	0.1027	0.0047	0.0009	0.0615	90	0.0662
N413-22	0.8209	0.0989	0.0042	0.0009	0.0760	110	0.0802
N413-23	0.8257	0.1017	0.0027	0.0012	0.0397	120	0.0431

LINE DATA

NAME	C	H	N	S	U (DIFF)	TIME	total netere
TRR-D11	0.8376	0.0883	0.0052	0.0039	0.065	0	0.0741
N410-1	0.8526	0.0919	0.0050	0.0011	0.0492	3	0.0553
N410-2	0.8554	0.0924	0.0043	0.0009	0.0470	6	0.0527
N410-3	0.8532	0.0945	0.0062	0.0004	0.0458	9	0.0523
N410-4						12	
N410-5						15	
N410-6	0.8632	0.0975	0.0030	0.0000	0.0323	18	0.0363
N410-8						24	
N410-9	0.8700	0.1001	0.0029	0.0000	0.0270	27	0.0292
N410-10						30	
N410-11						33	
N410-12	0.8624	0.1022	0.0018	0.0000	0.0336	36	0.0354
N410-14						42	
N410-15	0.8821	0.1049	0.0009	0.0000	0.0121	45	0.013
N410-17						51	
N410-18	0.8789	0.1060	0.0004	0.0000	0.0147	54	0.0151
N410-19						57	
N410-20						60	
N410-21	0.8796	0.1121	0.0000	0.0000	0.0083	60	0.0083
N410-22	0.8879	0.1137	0.0000	0.0000	0.0000	110	0
N410-EP	0.8745	0.1141	0.0004	0.0006	0.0104	120	0.0114
TRR-D11	0.8376	0.0883	0.0052	0.0039	0.065	0	0.0741
N408-1	0.8530	0.0888	0.0068	0.0047	0.0467	3	0.0532
N408-2	0.8601	0.0903	0.0060	0.0020	0.0416	6	0.0426
N408-3						9	
N408-4	0.8499	0.0926	0.0025	0.0010	0.0340	12	0.0373
N408-5						15	
N408-6						18	
N408-8						24	
N408-9	0.8759	0.1003	0.0017	0.0000	0.0221	27	0.0238
N408-10						30	
N408-11						33	
N408-12	0.8717	0.1043	0.0003	0.0000	0.0237	36	0.024
N408-14						42	
N408-15						45	
N408-17						51	
N408-18						54	
N408-19	0.8718	0.1056	0.0000	0.0000	0.0226	57	0.0236
N408-20	0.8786	0.1081	0.0000	0.0000	0.0133	60	0.0133
N408-21						90	
N408-22	0.8705	0.1173	0.0000	0.0000	0.0122	110	0.0122
N408-EP	0.8715	0.1169	0.0000	0.0008	0.0108	120	0.0116

CHM DATA

NAME	L	H	N	S	U (DIFF) TIME	total hetero
N418-1	0.8519	0.0900	0.0060		3	0.0581
N418-2	0.8472	0.0901	0.0056		6	0.0627
N418-3	0.8525	0.0908	0.0067		9	0.0567
N418-4					12	
N418-5					15	
N418-6	0.8420	0.0916	0.0059		18	0.0664
N418-8					24	
N418-9	0.8382	0.0917	0.0001		27	0.0701
N418-10					30	
N418-11					33	
N418-12	0.8573	0.0954	0.0040		36	0.0473
N418-14					42	
N418-15					45	
N418-17					51	
N418-18					54	
N418-19					57	
N418-20					60	
N418-21	0.8541	0.1017	0.0050		90	0.0442
N418-22					110	
N418-23	0.8586	0.1042	0.0043		120	0.0372
N418-24	0.8627	0.1095	0.0008		120	0.0278

CHM DATA

NAME	L	H	N	S	U (DIFF) TIME	total hetero	
N420-1	0.833	0.0915	0.0044			3	0.0555
N420-2	0.8379	0.0901	0.0027			6	0.052
N420-3	0.8439	0.0885	0.0036			9	0.0676
N420-4						12	
N420-5						15	
N420-6	0.8405	0.0897	0.0052			18	0.0698
N420-8						24	
N420-9	0.8431	0.0911	0.0054			27	0.0658
N420-10						30	
N420-11						33	
N420-12	0.8584	0.0953	0.0041			36	0.0463
N420-14						42	
N420-15						45	
N420-17						51	
N420-18						54	
N420-19						57	
N420-20						60	
N420-21	0.8332	0.0934	0.003			90	0.0674
N420-22	0.8286	0.0982	0.0026			120	0.0732
N420-23	0.846	0.1041	0.0027			120	0.0499
FOR DIFF	0.8376	0.0883	0.0052	0.0039	0.065	0	0.0741
N420-24	0.8374	0.1028	0.0023	0.0008	0.0567	120	0.0598
N420-25	0.8725	0.1016	0.0029	0.00036	0.0226	120	0.0259
N420-26	0.8678	0.1014	0.0029	0	0.0279	120	0.0308

NAME	AROMATICS DATA			
	Aromatic 9.0-5.9ppm	Phenolic OH 5.2-4.4ppm	Methoxy/Fluor 4.4-3.5ppm	Acenaph. 3.5-3.3pp
TARPHEN PROD JET A TAR OIL	25.8	1.5	2.6	0.8
TAR OIL	25.8	1.5	2.6	0.8
N410-1				
N410-2	18.5	2.1	2.6	0.8
N410-3				
N410-4				
N410-5				
N410-6	19.6	1.4	1.8	0.6
N410-8				
N410-9				
N410-10				
N410-11				
N410-12	16.1	1.3	2	0.7
N410-14				
N410-15				
N410-17				
N410-18	14.8	0.8	1.3	0.5
N410-19				
N410-20				
N410-21				
N410-22				
N410-EP	11.1	1	1.1	0.3
TAR OIL	25.8	1.5	2.6	0.8
N408-1				
N408-2	20.3	0.7	2.2	0.7
N408-3				
N408-4				
N408-5	13.7	1.5	2.2	0.7
N408-6				
N408-8				
N408-9				
N408-10				
N408-11				
N408-12	13.4	1.6	2	0.6
N408-14				
N408-15				
N408-17				
N408-18				
N408-19	12.4	1	1.6	0.6
N408-20				
N408-21				
N408-22				
N408-EP	10.5	0.9	1.2	0.3

NAME	AROMATICS DATA			
	Aromatic 9.0-5.9ppm	Phenolic OH 5.2-4.4ppm	Methoxy/Fluor 4.4-3.5ppm	Acenaph. 3.5-3.3pp
TAR OIL	25.8	1.5	2.6	0.8
N409-1				
N409-2	22.1	0.6	1.3	0.4
N409-3				
N409-4				
N409-5				
N409-6	19.4	1.2	1.7	0.4
N409-8				
N409-9				
N409-10				
N409-11				
N409-12	18.2	1.8	2.1	0.7
N409-14				
N409-15				
N409-17				
N409-18	18.5	1.2	1.8	0.6
N409-19				
N409-20				
N409-21				
N409-22				
N409-EP	14.2	0.5	1	0.4
TAR OIL	25.8	1.5	2.6	0.8
N413-1				
N413-2	21.6	2.6	2.4	0.7
N413-3				
N413-4				
N413-5	21.2	1.6	2.1	
N413-6	20.6	1.9	2	0.7
N413-8				
N413-9				
N413-10				
N413-11				
N413-12	18.7	2	2.3	0.8
N413-14				
N413-15				
N413-17				
N413-18				
N413-19				
N413-20				
N413-21				
N413-22				
N413-EP	16.3	1.3	2.5	0.7
TAR OIL	25.8	1.5	2.6	0.8
N414-1				
N414-2				
N414-3	18.7	1.4	2.3	
N414-4				
N414-5	17.2	1	1.3	
N414-6				
N414-8	13.2	1.5	1.7	
N414-9				
N414-10				

NAME	AROMATICS DATA			
	Aromatic 9.0-5.9ppm	Phenolic OH 5.2-4.4ppm	Methoxy/Fluor 4.4-3.5ppm	Acenaph. 3.5-3.3pp
N414-11	12.4	1.4	2.1	
N414-12				
N414-14				
N414-15				
N414-17				
N414-18	11.7	1	2	
N414-19				
N414-20				
N414-21				
N414-22				
N414-EP	10.1	0.6	1.3	0.4
TAR OIL				
N415-1				
N415-2				
N415-3	20.2	1.6	2.2	
N415-4				
N415-5	19.4	1.6	2.2	
N415-6				
N415-8	18.9	1.5	2.2	
N415-9				
N415-10				
N415-11	16.7	1.5	2.2	
N415-12				
N415-14				
N415-15				
N415-17				
N415-18	15	1	1.2	
N415-19				
N415-20				
N415-21				
N415-22				
N415-EP	12.8	1.1	2.1	
TAR OIL				
N416-1				
N416-2				
N416-3				
N416-4				
N416-5				
N416-6				
N416-8	21.4	1.7	2	
N416-9				
N416-10				
N416-11	20.3	1.8	2.2	
N416-12				
N416-14				
N416-15				
N416-17				
N416-18	18.9	1.6	2.2	
N416-19				
N416-20	17.3	2	2.3	
N416-21				
N416-22				

NAME	AROMATICS DATA			
	Aromatic 9.0-5.9ppm	Phenolic OH 5.2-4.4ppm	Methoxy/Fluor 4.4-3.5ppm	Acenaph. 3.5-3.3pp
N416-EP	18.4	1.9	2.6	
TAR OIL				
N417-1				
N417-2				
N417-3				
N417-4	19.8	1.6	2.1	
N417-5				
N417-6				
N417-8	18.1	1.4	1.9	
N417-9				
N417-10	16.3	1.3	1.7	
N417-11	16.7	1.1	1.2	
N417-12				
N417-14				
N417-15				
N417-17	14.9	1	1.4	
N417-18	14.7	1.5	2.3	
N417-19				
N417-20				
N417-21				
N417-22				
N417-EP	11.1	1.4	2.6	
TAR OIL				
N418-1				
N418-2				
N418-3				
N418-4	22.2	1.6	2.4	
N418-5				
N418-6				
N418-8				
N418-9				
N418-10	20.7	1.3	1.8	
N418-11				
N418-12				
N418-14				
N418-15				
N418-17				
N418-18	18	1.4	1.8	
N418-19				
N418-20				
N418-21				
N418-22				
N418-EP	16.9	2.3	1.3	
TAR OIL				
N419-1				
N419-2				
N419-3				
N419-4				
N419-5				
N419-6				
N419-8	18.4	1.8	2.1	
N419-9				

NAME	AROMATICS DATA			
	Aromatic 9.0-5.9ppm	Phenolic OH 5.2-4.4ppm	Methoxy/Fluor 4.4-3.5ppm	Acenaph. 3.5-3.3pp
N419-10				
N419-11				
N419-12	18	1.4	2.4	
N419-14				
N419-15				
N419-17				
N419-18	15.8	1	1.8	
N419-19				
N419-20				
N419-21				
N419-22				
N419-EP	13.9	1	2.4	
TAR OIL				
N420-1				
N420-2				
N420-3				
N420-4	23.1	1.7	1.9	
N420-5				
N420-6				
N420-8				
N420-9				
N420-10	20.1	1.5	1.9	
N420-11				
N420-12				
N420-14	18.8	1.3	1.7	
N420-15				
N420-17				
N420-18				
N420-19				
N420-20				
N420-21				
N420-22				
N420-EP	16.2	1	1.9	
TAR OIL				
N421-1				
N421-2				
N421-3				
N421-4				
N421-5	20.6	1.6	1.9	
N421-6				
N421-8				
N421-9				
N421-10	18.6	1.7	2.3	
N421-11				
N421-12				
N421-14				
N421-15				
N421-17				
N421-18	15.4	1.6	2.2	
N421-19				
N421-20				
N421-21				

NAME	AROMATICS DATA Aromatic 9.0-5.9ppm	Phenolic OH 5.2-4.4ppm	Methoxy/Fluor 4.4-3.5ppm	Acenaph. 3.5-3.3pp
N421-22	14.9	1.7	2.2	
N421-EP				

NAME	m	Alpha to Aromatic 3.3-1.9ppm	Beta to Aromatic 1.9-1.5ppm	Cyclohexane 1.43ppm
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CHN DATA

NAME	m	Alpha to Aromatic 3.3-1.9ppm	Beta to Aromatic 1.9-1.5ppm	Cyclohexane 1.43ppm
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TARPHEN

PROD

JET A

TAR OIL

30.9	6.5	0
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TAR OIL

30.9	6.5	0
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N410-1

N410-2

28	6.7	0
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N410-3

N410-4

N410-5

N410-6

25.1	8.3	0
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N410-8

N410-9

N410-10

N410-11

N410-12

24	9.5	0
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N410-14

N410-15

N410-17

N410-18

22.4	10.1	2.3
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N410-19

N410-20

N410-21

N410-22

N410-EP

19	12.7	3.3
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TAR OIL

30.9	6.5	0
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N408-1

N408-2

24.6	7.2	0
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N408-3

N408-4

N408-5

24	7.8	0
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N408-6

N408-8

N408-9

N408-10

N408-11

N408-12

24	11	0
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N408-14

N408-15

N408-17

N408-18

N408-19

22.8	13.2	0
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N408-20

N408-21

N408-22

N408-EP

18.6	14.3	4
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NAME	m	Alpha to Aromatic 3.3-1.9ppm	Beta to Aromatic 1.9-1.5ppm	Cyclohexane 1.43ppm
TAR OIL		30.9	6.5	0
N409-1				
N409-2		28.2	6.2	0
N409-3				
N409-4				
N409-5				
N409-6		26.9	5.1	0
N409-8				
N409-9				
N409-10				
N409-11				
N409-12		26.7	7.3	0
N409-14				
N409-15				
N409-17				
N409-18		25	9.2	0
N409-19				
N409-20				
N409-21				
N409-22				
N409-EP		22.4	11.9	3
TAR OIL		30.9	6.5	0
N413-1				
N413-2		28.8	6.5	0
N413-3				
N413-4				
N413-5		27.8	7.6	0
N413-6		26.7	7.2	0
N413-8				
N413-9				
N413-10				
N413-11				
N413-12		25.9	8.4	0
N413-14				
N413-15				
N413-17				
N413-18				
N413-19				
N413-20				
N413-21				
N413-22				
N413-EP		24.2	10.9	2.8
TAR OIL		30.9	6.5	0
N414-1				
N414-2				
N414-3		26.3	9.6	0
N414-4				
N414-5		24.9	9.8	0
N414-6				
N414-8		23.2	10.1	0
N414-9				
N414-10				

NAME	m	Alpha to Aromatic 3.3-1.9ppm	Beta to Aromatic 1.9-1.5ppm	Cyclohexane 1.43ppm
N414-11		23.3	11.4	0
N414-12				
N414-14				
N414-15				
N414-17				
N414-18		22	12.4	0
N414-19				
N414-20				
N414-21				
N414-22				
N414-EP		19.3	16.2	3.8
TAR OIL				
N415-1				
N415-2				
N415-3		27.1	8.1	
N415-4				
N415-5		27.7	8.2	
N415-6				
N415-8		26.3	9.3	
N415-9				
N415-10				
N415-11		25.9	9.7	
N415-12				
N415-14				
N415-15				
N415-17				
N415-18		24.1	10.8	
N415-19				
N415-20				
N415-21				
N415-22				
N415-EP		23.1	13.4	
TAR OIL				
N416-1				
N416-2				
N416-3				
N416-4				
N416-5				
N416-6				
N416-8		27	7.8	
N416-9				
N416-10				
N416-11		27.4	7.9	
N416-12				
N416-14				
N416-15				
N416-17				
N416-18		26.5	9	
N416-19				
N416-20		26.1	8.1	
N416-21				
N416-22				

NAME	m	Alpha to Aromatic 3.3-1.9ppm	Beta to Aromatic 1.9-1.5ppm	Cyclohexane 1.43ppm
N416-EP		25.9	9.5	
TAR OIL				
N417-1				
N417-2				
N417-3				
N417-4		27.5	8.1	
N417-5				
N417-6				
N417-8		26.1	9.5	
N417-9				
N417-10		25.1	9.7	
N417-11		24.5	10	
N417-12				
N417-14				
N417-15				
N417-17		24	10.9	
N417-18		24.5	10.9	
N417-19				
N417-20				
N417-21				
N417-22				
N417-EP		21.9	12.3	
TAR OIL				
N418-1				
N418-2				
N418-3				
N418-4		28.2	7.6	
N418-5				
N418-6				
N418-8				
N418-9				
N418-10		26.6	8.4	
N418-11				
N418-12				
N418-14				
N418-15				
N418-17				
N418-18		25.9	9.1	
N418-19				
N418-20				
N418-21				
N418-22				
N418-EP		24.1	9.8	
TAR OIL				
N419-1				
N419-2				
N419-3				
N419-4				
N419-5				
N419-6				
N419-8		26	9.3	
N419-9				

NAME	m	Alpha to Aromatic 3.3-1.9ppm	Beta to Aromatic 1.9-1.5ppm	Cyclohexane 1.43ppm
N419-10				
N419-11				
N419-12		26.6	9.9	
N419-14				
N419-15				
N419-17				
N419-18		24.9	10.5	
N419-19				
N419-20				
N419-21				
N419-22				
N419-EP		24.1	12.3	
TAR OIL				
N420-1				
N420-2				
N420-3				
N420-4		28.3	7.2	
N420-5				
N420-6				
N420-8				
N420-9				
N420-10		27.4	8.6	
N420-11				
N420-12				
N420-14		27	9.2	
N420-15				
N420-17				
N420-18				
N420-19				
N420-20				
N420-21				
N420-22				
N420-EP		25.7	11.5	
TAR OIL				
N421-1				
N421-2				
N421-3				
N421-4				
N421-5		27.4	7.6	
N421-6				
N421-8				
N421-9				
N421-10		26.7	9	
N421-11				
N421-12				
N421-14				
N421-15				
N421-17				
N421-18		25.3	9.5	
N421-19				
N421-20				
N421-21				

NAME	m	Alpha to Aromatic 3.3-1.9ppm	Beta to Aromatic 1.9-1.5ppm	Cyclohexane 1.43ppm
N421-22				
N421-EP		23.8	12	

NAME	Methylene 1.5-1.0ppm	Methyl 1.0-0.2ppm	Aromatic Aliphatic H		
CHN DATA					
NAME	Methylene 1.5-1.0ppm	Methyl 1.0-0.2ppm	Aromatic Aliphatic H		
TARPHEN					
PROD					
JET A					
TAR OIL	22.4	9.5	68.1	31.9	
					Aro:Ali
TAR OIL	22.4	9.5	68.1	31.9	2.13
N410-1					
N410-2	29.1	12.3	58.7	41.4	1.42
N410-3					
N410-4					
N410-5					
N410-6	29.3	13.8	56.8	43.1	1.32
N410-8					
N410-9					
N410-10					
N410-11					
N410-12	31.8	14.5	53.6	46.3	1.16
N410-14					
N410-15					
N410-17					
N410-18	30.8	17	49.9	50.1	1.00
N410-19					
N410-20					
N410-21					
N410-22					
N410-EP	30.4	21.1	45.2	54.8	0.82
TAR OIL	22.4	9.5	68.1	31.9	2.13
N408-1					
N408-2	31	13.4	55.7	44.4	1.25
N408-3					
N408-4					
N408-5	35.2	15	49.9	50.2	0.99
N408-6					
N408-8					
N408-9					
N408-10					
N408-11					
N408-12	32.8	14.6	52.6	47.4	1.11
N408-14					
N408-15					
N408-17					
N408-18					
N408-19	32	16.3	51.6	48.3	1.07
N408-20					
N408-21					
N408-22					
N408-EP	28.7	21.5	45.8	54.2	0.85

NAME	Methylene 1.5-1.0ppm	Methyl 1.0-0.2ppm	Aromatic	Aliphatic H	Aro:Ali
TAR OIL	22.4	9.5	68.1	31.9	2.13
N409-1					
N409-2	27.9	13.3	58.8	41.2	1.43
N409-3					
N409-4					
N409-5					
N409-6	30.9	14.7	54.7	45.6	1.20
N409-8					
N409-9					
N409-10					
N409-11					
N409-12	30.1	13.1	56.8	43.2	1.31
N409-14					
N409-15					
N409-17					
N409-18	29.7	14	56.3	43.7	1.29
N409-19					
N409-20					
N409-21					
N409-22					
N409-EP	28	18.7	50.4	49.7	1.01
TAR OIL	22.4	9.5	68.1	31.9	2.13
N413-1					
N413-2	26.1	11.3	62.6	37.4	1.67
N413-3					
N413-4					
N413-5	27.2	12.6	60.3	39.8	
N413-6	28.2	12.7	59.1	40.9	1.44
N413-8					
N413-9					
N413-10					
N413-11					
N413-12	28.9	13	58.1	41.9	1.39
N413-14					
N413-15					
N413-17					
N413-18					
N413-19					
N413-20					
N413-21					
N413-22					
N413-EP	25.5	15.8	55.9	44.1	1.27
TAR OIL	22.4	9.5	68.1	31.9	2.13
N414-1					
N414-2					
N414-3	28.2	13.4	58.3	41.6	1.40
N414-4					
N414-5	30.6	15.2	54.2	45.8	1.18
N414-6					
N414-8	33.5	16.9	49.7	50.4	0.99
N414-9					
N414-10					

NAME	Methylene 1.5-1.3ppm	Methyl 1.0-0.2ppm	Aromatic	Aliphatic H	Aro:Ali
N414-11	33.8	15.7	50.6	49.5	1.02
N414-12					
N414-14					
N414-15					
N414-17					
N414-18	33.2	17.7	49.1	50.9	0.96
N414-19					
N414-20					
N414-21					
N414-22					
N414-EP	27.9	20.3	47.9	52	0.92
TAR OIL					
N415-1					
N415-2					
N415-3	27.9	13	59.2	40.9	1.45
N415-4					
N415-5	28	12.9	59.1	40.9	1.44
N415-6					
N415-8	28.1	13.6	58.2	41.7	1.40
N415-9					
N415-10					
N415-11	29.5	14.4	56	43.9	1.28
N415-12					
N415-14					
N415-15					
N415-17					
N415-18	31.3	16.7	52.1	48	1.09
N415-19					
N415-20					
N415-21					
N415-22					
N415-EP	30	17.5	52.5	47.5	1.11
TAR OIL					
N416-1					
N416-2					
N416-3					
N416-4					
N416-5					
N416-6					
N416-8	27.1	13.1	59.9	40.2	1.49
N416-9					
N416-10					
N416-11	27.1	13.2	59.6	40.3	1.48
N416-12					
N416-14					
N416-15					
N416-17					
N416-18	28.2	13.6	58.2	41.8	1.39
N416-19					
N416-20	30.1	14.1	55.8	44.2	1.26
N416-21					
N416-22					

NAME	Methylene 1.5-1.0ppm	Methyl 1.0-0.2ppm	Aromatic Aliphatic H		Aro:Ali
N416-EP TAR OIL	27.4	14.2	58.3	41.6	1.40
N417-1					
N417-2					
N417-3					
N417-4	27.5	13.4	59.1	40.9	1.44
N417-5					
N417-6					
N417-8	28.9	14.1	57	43	1.33
N417-9					
N417-10	30.4	15.5	54.1	45.9	1.18
N417-11	30.6	15.8	53.5	46.4	1.15
N417-12					
N417-14					
N417-15					
N417-17	31.2	16.6	52.2	47.8	1.09
N417-18	30.6	15.5	53.9	46.1	1.17
N417-19					
N417-20					
N417-21					
N417-22					
N417-EP TAR OIL	32.1	18.5	49.3	50.6	0.97
N418-1					
N418-2					
N418-3					
N418-4	26	12.1	62	38.1	1.63
N418-5					
N418-6					
N418-8					
N418-9					
N418-10	27.9	13.4	58.8	41.3	1.42
N418-11					
N418-12					
N418-14					
N418-15					
N418-17					
N418-18	29.4	14.3	56.2	43.7	1.29
N418-19					
N418-20					
N418-21					
N418-22					
N418-EP TAR OIL	29.5	16.1	54.4	45.6	1.19
N419-1					
N419-2					
N419-3					
N419-4					
N419-5					
N419-6					
N419-8	28.7	13.7	57.6	42.4	1.36
N419-9					

NAME	Methylene 1.5-1.0ppm	Methyl 1.0-0.2ppm	Aromatic Aliphatic H		Aro:Ali
N419-10					
N419-11					
N419-12	28.7	13.1	58.3	41.8	1.39
N419-14					
N419-15					
N419-17					
N419-18	31	15.1	54	46.1	1.17
N419-19					
N419-20					
N419-21					
N419-22					
N419-EP	29.7	16.5	53.7	46.2	1.16
TAR OIL					
N420-1					
N420-2					
N420-3					
N420-4	26.1	11.6	62.2	37.7	1.65
N420-5					
N420-6					
N420-8					
N420-9					
N420-10	27.4	13.1	59.5	40.5	1.47
N420-11					
N420-12					
N420-14	28.3	13.7	58	42	1.38
N420-15					
N420-17					
N420-18					
N420-19					
N420-20					
N420-21					
N420-22					
N420-EP	28.2	15.4	56.3	43.6	1.29
TAR OIL					
N421-1					
N421-2					
N421-3					
N421-4					
N421-5	27.5	13.5	59.1	41	1.44
N421-6					
N421-8					
N421-9					
N421-10	28.6	13.2	58.3	41.8	1.39
N421-11					
N421-12					
N421-14					
N421-15					
N421-17					
N421-18	31	15.1	54	46.1	1.17
N421-19					
N421-20					
N421-21					

NAME	Methylene 1.5-1.0ppm	Methyl 1.0-0.2ppm	Aromatic	Aliphatic H	Aro:Ali
N421-22					
N421-EP	29.2	16.3	54.6	45.5	1.20

Jet Fuels Data - initial program work

DISTILLATION DATA

NAME	START	IBP	Time, minutes					
			5 vol%	10 vol%	20 vol%	30 vol%	40 vol%	
JET A	0	30	33	35.5	39.33	42.92	46.12	
JET A	0	16	18.16	20	23.08	26	28.66	
JP4	0	8	9.58	10.5	11.92	13.25	14.58	
TARPHEN	0	10.16	16.33	20.83	24.42	27.66	30.92	
TARLITE	0	10.66	15.83	20.33	23.17	25.83	28.58	
PRODUCT	0	8	9.66	10.66	12.66	14.91	17.33	
PHENBUT	0	17.17	18.92	20	22.08	24.33	26.66	
CRUDEPHEN	0	9	12.5	20.5	22.66	24.83	26.66	
N423EP	0	6	8.65	11.66	19.42	21.83	24.08	
N424EP	0	11.2	13.75	15.33	17.81	20	22.16	
N425EP	0	8.5	13.16	14.66	17.16	19.5	22	
Jet Fuels								

DISTILLAT

NAME	50 vol%	60 vol%	70 vol%	80 vol%	90 vol%	95 vol%	MAX	
JET A	49.5	52.25	55	58.16	60.66	62.33	66.66	
JET A	31.33	34	36.66	39.33	42.53	45.16	46	
JP4	16	17.5	19.42	21.33	23.33	24.83	26	
TARPHEN	34.08	37	40.16	43.83	49.5		51.33	
TARLITE	31.58	34.66	38.08	42.5			46.17	
PRODUCT	19.58	21.63	23.75	26.33	31.33	35.33	35.33	
PHENBUT	28.91	31.16	33.43	35.83			37.66	
CRUDEPHEN	28.66	30.83	33.25	37	42	49.5	49.5	
N423EP	26.5	29	31.92	35.25			45	
N424EP	24.66	27.16	30.33				39	
N425EP	24.66	27.33	30.42				40	
Jet Fuels								

DISTILLAT

NAME	START	IBP	5 vol%	10 vol%	20 vol%	30 vol%	Temperature	
							40 vol%	
JET A	23							
JET A	24							
JP4	23	50	96	102	108	114	118	
TARPHEN	24	90	93	183	201	214	225	
TARLITE	24	84	89	177	200	214	228	
PRODUCT	24	58	102	113	124	140	160	
PHENBUT	24	115	205	212	220	228	238	
CRUDEPHEN	25	97	101	184	188	194	195	
N423EP	26	78	95	98	188	213	235	
N424EP	26	80	150	183	207	227	240	
N425EP	25	74	147	170	204	227	247	

Jet Fuel:

DISTILLAT

NAME	re, C						Max
	50 vol%	60 vol%	70 vol%	80 vol%	90 vol%	95 vol%	
JET A				245	260	268	274
JET B				253	264	281	285
JP4	123	130	140	150	163	177	179
TARPHEN	241	258	278	304	330		332
TARLITE	243	264	287	300			320
PRODUC T	185	217	240	269	314	317	317
PHENBUT	253	266	278	290			291
CRUDEPHEN	198	205	213	244	260	265	265
N423EP	256	285	323	355			355
N424EP	272	300	335	355			355
N425EP	273	303	338				360

Jet Fuel:

DISTILLAT

NAME	Res	Dist	Loss
JET A	0.022	0.962	0.0159
JET B	0.0331	0.9583	0.0086
JP4	0.0146	0.9747	0.0106
TARPHEN	0.081	0.913	0.006 GRAMS
TARLITE	0.1514	0.8476	0.001
PRODUC T	0.0477	0.944	0.0119
PHENBUT	0.1312	0.8624	0.007
CRUDEPHEN	0.0545	0.9371	0.0085
N423EP	0.1782	0.8176	0.0042 wt%
N424EP	0.2128	0.782	0.0052 wt%
N425EP	0.2432	0.7526	0.0042 wt%

AVE PRESS 2ND STAGE	MAX PRESS 1ST STAGE	MAX PRESS 2ND STAGE	FEED GAS 1ST STAGE	GAS IN 1ST STAGE	H2S 1ST STAGE	FEED GAS 2ND STAGE
-----	750	-----	100	29.6	0	-----
-----	700	-----	100	25.0	0	-----
-----	2033	-----	100	30.8	0	-----
-----	2077	-----	100	40.1	0	-----
-----	2020	-----	100	27.4	0	-----
-----	2250	-----	100	100.8	0	-----
-----	2235	-----	100	31.5	0	-----

RUN #	COAL	SOLVENT	ADD1	ADD2	DATE	RES TIME 1ST STAGE
N424	NONE	TAR OIL (PROD N423)	NONE	ENGLEHARD S-661	12/16/87	60
N425	NONE	TAR OIL (PROD N423)	NONE	ENGLEHARD S-661	12/18/87	60
N420	NONE	TAR OIL	NONE	KATALCO 660	09/15/87	60
N419	NONE	TAR OIL	NONE	NT 550	09/11/87	60
N418	NONE	TAR OIL	NONE	NT 550	09/09/87	60
N433	NONE	TAR OIL	NONE	SHELL 424	06/09/88	60
N410	NONE	TAR OIL	NONE	SHELL 424	08/13/87	60
N432	NONE	TAR OIL	NONE	SHELL 424	06/02/88	60
N414	NONE	TAR OIL	NONE	SHELL 424	09/01/87	60
N408	NONE	TAR OIL	NONE	SHELL 424	08/05/87	60
N409	NONE	TAR OIL	NONE	SHELL 424	08/11/87	60
N415	NONE	TAR OIL	NONE	SHELL 424	09/02/87	60
N413	NONE	TAR OIL	NONE	SHELL 424	08/28/87	60
N421	NONE	TAR OIL	NONE	SHELL 424	09/18/87	60
N417	NONE	TAR OIL	NONE	SHELL 424	09/04/87	60
N416	NONE	TAR OIL	NONE	SHELL 424	09/03/87	60
N435	NONE	TAR OIL (PROD N433)	NONE	ENGLEHARD S-661	08/03/88	60

RES TIME 2ND STAGE	TIME SAMPLE	AVE TEMP 1ST STAGE	AVE TEMP 2ND STAGE	MAX TEMP 1ST STAGE	MAX TEMP 2ND STAGE	AVE PRES 1ST STAGE
-----	NO	150	-----	150	-----	750
-----	NO	200	-----	200	-----	700
-----	YES	394	-----	395	-----	2023
-----	YES	390	-----	395	-----	1997
-----	YES	354	-----	356	-----	2000
-----	NO	380	-----	395	-----	2250
-----	YES	394	-----	394	-----	2235
-----	NO	395	-----	395	-----	2384
-----	YES	387	-----	387	-----	2500
-----	YES	420	-----	420	-----	2675
-----	YES	385	-----	387	-----	1435
-----	YES	357	-----	357	-----	2000
-----	YES	357	-----	357	-----	1300
-----	YES	367	-----	367	-----	1500
-----	YES	358	-----	363	-----	2012
-----	YES	329	-----	331	-----	1491
-----	NO	203	-----	205	-----	700

RUN #	COAL	SOLVENT	ADD1	ADD2	DATE	RES TIME
						1ST STAGE
N424	NONE	TAR OIL (PROD N423)	NONE	ENGLEHARD S-661	12/16/87	60
N425	NONE	TAR OIL (PROD N423)	NONE	ENGLEHARD S-661	12/18/87	60
N420	NONE	TAR OIL	NONE	KATALCO 660	09/15/87	60
N419	NONE	TAR OIL	NONE	NT 550	09/11/87	60
N418	NONE	TAR OIL	NONE	NT 550	09/09/87	60
N433	NONE	TAR OIL	NONE	SHELL 424	06/09/88	60
N410	NONE	TAR OIL	NONE	SHELL 424	08/13/87	60
N432	NONE	TAR OIL	NONE	SHELL 424	06/02/88	60
N414	NONE	TAR OIL	NONE	SHELL 424	09/01/87	60
N408	NONE	TAR OIL	NONE	SHELL 424	08/05/87	60
N409	NONE	TAR OIL	NONE	SHELL 424	08/11/87	60
N415	NONE	TAR OIL	NONE	SHELL 424	09/02/87	60
N413	NONE	TAR OIL	NONE	SHELL 424	08/28/87	60
N421	NONE	TAR OIL	NONE	SHELL 424	09/18/87	60
N417	NONE	TAR OIL	NONE	SHELL 424	09/04/87	60
N416	NONE	TAR OIL	NONE	SHELL 424	09/03/87	60
N435	NONE	TAR OIL (PROD N433)	NONE	ENGLEHARD S-661	08/03/88	60

RES TIME	TIME	AVE TEMP	AVE TEMP	MAX TEMP	MAX TEMP	AVE PRES
END STAGE	SAMPLE	1ST STAGE	2ND STAGE	1ST STAGE	2ND STAGE	1ST STAGE
-----	NO	150	-----	150	-----	750
-----	NO	200	-----	200	-----	700
-----	YES	394	-----	395	-----	2023
-----	YES	390	-----	395	-----	1997
-----	YES	354	-----	356	-----	2000
-----	NO	380	-----	395	-----	2250
-----	YES	394	-----	394	-----	2235
-----	NO	395	-----	395	-----	2384
-----	YES	387	-----	387	-----	2500
-----	YES	420	-----	420	-----	2675
-----	YES	385	-----	387	-----	1435
-----	YES	357	-----	357	-----	2000
-----	YES	357	-----	357	-----	1300
-----	YES	367	-----	367	-----	1500
-----	YES	358	-----	363	-----	2012
-----	YLS	329	-----	331	-----	1491
-----	NO	203	-----	205	-----	700

AVE PRESS END STAGE	MAX PRESS 1ST STAGE	MAX PRESS 2ND STAGE	FEED GAS 1ST STAGE	GAS IN 1ST STAGE	H2S 1ST STAGE	FEED GAS 2ND STAGE
-----	750	-----	100	29.6	0	-----
-----	700	-----	100	25.0	0	-----
-----	2033	-----	100	30.8	0	-----
-----	2077	-----	100	40.1	0	-----
-----	2020	-----	100	27.4	0	-----
-----	2250	-----	100	100.8	0	-----
-----	2235	-----	100	31.5	0	-----
-----	2484	-----	100	113.6	0	-----
-----	2500	-----	100	45.0	0	-----
-----	2675	-----	100	40.0	0	-----
-----	1570	-----	100	35.9	0	-----
-----	2000	-----	100	39.6	0	-----
-----	1300	-----	100	16.2	0	-----
-----	1500	-----	100	8.7	0	-----
-----	2022	-----	100	33.8	0	-----
-----	1491	-----	100	23.1	0	-----
-----	750	-----	100	48.1		

GAS IN END STAGE	H2S END STAGE	AR COAL	MAF COAL	% H2O COAL	% ASH COAL	WATER ADDED	SOLVENT IN
0	0	0	0	0	0	0	1016.9
0	0	0	0	0	0	0	964.4
0	0	0	0	0	0	0	1029.2
0	0	0	0	0	0	0	1028.1
0	0	0	0	0	0	0	1024.3
0	0	0	0	0	0	0	1031.2
0	0	0	0	0	0	0	1010.1
0	0	0	0	0	0	0	1191.7
0	0	0	0	0	0	0	1015.5
0	0	0	0	0	0	0	1003.5
0	0	0	0	0	0	0	1008.1
0	0	0	0	0	0	0	1018.7
0	0	0	0	0	0	0	1013.3
0	0	0	0	0	0	0	1027.6
0	0	0	0	0	0	0	1017.1
0	0	0	0	0	0	0	1026.6
							1052.3

ADDE WT IN	SLURRY CHARGED	LIQUID PROD	LIGHT OILS	MOLES GAS OUT	MOLES H2 LEFT	MOLES CO LEFT
150	1145.6	1103.9	0	31.24592	0	0
150	1106.1	1053.7	0	17.09483	0	0
150	1159.3	1087.8	90.6	44.34515	0	0
150	1156	1103.1	81.5	27.41405	0	0
150	1154.5	1120.69	82.1	18.73569	0	0
150	1163.96	1100.8	0	8.344069	0	0
150	1116.9	1003	60	18.06333	0	0
149	1326	1242.1	70.2	30.66688	0	0
150	1144.1	1027.8	72	27.43653	0	0
150	1126.4	994.4	72	17.42364	0	0
150	1115.4	1036.2	85.1	9.481692	0	0
150	1149	1041.8	92.2	26.85358	0	0
150	1139.6	1100.3	72	7.566258	0	0
150	1169.9	1091.8	73.2	12.70832	0	0
150	1146.6	1082.3	48.6	19.44187	0	0
150	1158	1118	47.8	17.04600	0	0
149.4	1185.1	1150.7	1.8	13.656		

RUN #	CARBON	END PRODUCT			BY DIFF OXYGEN	TOTAL HETERO	H:C RATIO
		HYDROGEN	NITROGEN	SULFUR			
N424-EP	0.8725	0.1016	0.0029	0.0004	0.0226	0.0259	1.3847
N425-EP	0.8678	0.1014	0.0029	0.0000	0.0279	0.0308	1.3894
N420-EP	0.846	0.1041	0.0027	0.0000	0.0472	0.0499	1.4632
N419-EP	0.8627	0.1095	0.0008	0.0000	0.0270	0.0278	1.5093
N418-EP	0.8586	0.1042	0.0043	0.0000	0.0329	0.0372	1.4431
N433-EP	0.8863	0.1137	0	0.0000	0.0000	0	1.5255
N410-EP	0.8745	0.1141	0.0004	0.0006	0.0104	0.0114	1.5515
N432-EP	0.8772	0.1123	0.0006	0.0000	0.0099	0.0105	1.5223
N414-EP	0.8723	0.1171	0.0000	0.0002	0.0104	0.0106	1.5963
N408-EP	0.8715	0.1169	0.0000	0.0008	0.0108	0.0116	1.5950
N409-EP	0.8680	0.1082	0.0028	0.0007	0.0203	0.0238	1.4823
N415-EP	0.8631	0.1096	0.0001	0.0000	0.0272	0.0273	1.5100
N413-EP	0.8557	0.1012	0.0022	0.0012	0.0397	0.0431	1.4063
N421-EP	0.8433	0.1071	0.0056	0.0000	0.0440	0.0496	1.5102
N417-EP	0.8454	0.1096	0.0001	0.0000	0.0449	0.045	1.5416
N416-EP	0.8382	0.0969	0.0013	0.0010	0.0626	0.0649	1.3747
	0.8856	0.1127	0	0	0.0017	0.0017	1.5132

17.8	1.8	2.8		26.6	9.7		27.9
18.3	1.5	2.4		25.8	9.4		27.9
16.2	1	1.9		25.7	11.5		28.2
13.9	1	2.4		24.1	12.3		29.7
16.9	2.3	1.3		24.1	9.8		29.5
11.1	1	1.1	0.3	19	12.7	3.3	30.4
10.1	0.6	1.3	0.4	19.3	16.2	3.8	27.9
10.5	0.9	1.2	0.3	18.6	14.3	4	28.7
14.2	0.5	1	0.4	22.4	11.9	3	28
12.8	1.1	2.1		23.1	13.4		30
16.3	1.3	1.5	0.7	24.2	10.9	2.8	25.5
14.9	1.7	2.2		23.8	12		29.2
11.1	1.4	2.6		21.9	12.3		32.1
18.4	1.9	2.6		25.9	9.5		27.4
9.85	1.76	0.62		19.72	14.96	1.25	29.78

				LIQUID LOSS	LIQUID RECOVERY	CARBON BAL	HYDROGEN BAL
13.5	58.7	41.4	1.42	41.7	96.36%	100.40%	95.24%
14.7	57.4	42.6	1.35	52.4	95.26%	98.72%	93.97%
15.6	56.3	43.6	1.29	71.5	101.65%	102.67%	119.84%
16.5	53.7	46.2	1.16	52.9	102.47%	105.54%	127.08%
16.1	54.4	45.6	1.19	33.81	104.18%	106.79%	122.94%
				63.16	94.57%	100.07%	121.78%
21.1	45.2	54.8	0.82	113.9	95.17%	99.37%	122.98%
				83.9	93.97%	103.65%	125.87%
20.3	47.9	52	0.92	116.3	96.13%	100.11%	127.48%
21.5	45.8	54.2	0.85	132	94.67%	98.50%	125.34%
18.7	50.4	49.7	1.01	79.2	100.53%	104.18%	123.18%
17.5	52.5	47.5	1.11	107.2	98.69%	101.70%	122.50%
15.8	55.9	44.1	1.27	39.3	102.87%	105.03%	117.90%
16.3	54.6	45.5	1.29	78.1	99.58%	100.26%	120.78%
18.5	49.3	50.6	0.97	64.3	98.63%	99.55%	122.42%
14.2	58.3	41.6	1.40	40	100.67%	100.75%	110.48%
17.52	46.87	53.13		34.4	97.25%	99.22%	101.29%

NITROGEN BAL	SULFUR BAL	OXYGEN BAL
121.50%	43.36%	38.48%
120.11%	0.00%	46.88%
52.78%	0.00%	73.81%
15.77%	0.00%	42.57%
86.15%	0.00%	52.73%
0.00%	0.00%	0.00%
7.32%	14.64%	15.23%
11.42%	0.00%	15.07%
0.00%	4.93%	15.38%
0.00%	19.42%	15.73%
54.13%	18.04%	31.40%
1.90%	0.00%	41.30%
43.52%	31.65%	62.83%
107.24%	0.00%	67.41%
1.90%	0.00%	68.13%
25.17%	25.81%	96.96%
0.00%	0.00%	0.00%

RUN #	CARBON	END PRODUCT			BY DIFF OXYGEN	TOTAL HETERO	H:C RATIO
		HYDROGEN	NITROGEN	SULFUR			
N408-EP	0.8715	0.1169	0.0000	0.0008	0.0108	0.0116	1.5950
N409-EP	0.8680	0.1082	0.0028	0.0007	0.0203	0.0238	1.4823
N410-EP	0.8745	0.1141	0.0004	0.0006	0.0104	0.0114	1.5515
N413-EP	0.8557	0.1012	0.0022	0.0012	0.0397	0.0431	1.4063
N414-EP	0.8723	0.1171	0.0000	0.0002	0.0104	0.0106	1.5963
N415-EP	0.8631	0.1096	0.0001	0.0000	0.0272	0.0273	1.5100
N416-EP	0.8382	0.0969	0.0013	0.0010	0.0626	0.0649	1.3747
N417-EP	0.8454	0.1096	0.0001	0.0000	0.0449	0.045	1.5416
N418-EP	0.8586	0.1042	0.0043	0.0000	0.0329	0.0372	1.4431
N419-EP	0.8627	0.1095	0.0008	0.0000	0.0270	0.0278	1.5093
N420-EP	0.846	0.1041	0.0027	0.0000	0.0472	0.0499	1.4632
N421-EP	0.8433	0.1071	0.0056	0.0000	0.0440	0.0496	1.5102

RUN #	CARBON	END PRODUCT			BY DIFF OXYGEN	TOTAL HETERO	H:C RATIO
		HYDROGEN	NITROGEN	SULFUR			
N424-EP	0.8725	0.1016	0.0029	0.0004	0.0226	0.0259	1.3847
N425-EP	0.8678	0.1014	0.0029	0.0000	0.0279	0.0308	1.3894
N432-EP	0.8772	0.1123	0.0006	0.0000	0.0099	0.0105	1.5223
N433-EP	0.8853	0.1137	0	0.0000	0.0000	0	1.5255
N435-EP	0.8856	0.1127	0	0	0.0017	0.0017	1.5132

PROD Aromatic Phenolic Methoxy/FAcenaph. Alpha to Beta to ACyclohex
JET A 9.0-5.9pp5.2-4.4pp4.4-3.5pp3.5-3.3pp3.3-1.9pp1.9-1.5pp1.43ppm

N408-EP	10.5	0.9	1.2	0.3	18.6	14.3	4
N409-EP	14.2	0.5	1	0.4	22.4	11.9	3
N410-EP	11.1	1	1.1	0.3	19	12.7	3.3
N413-EP	16.3	1.3	2.5	0.7	24.2	10.9	2.8
N414-EP	10.1	0.6	1.3	0.4	19.3	16.2	3.8
N415-EP	12.8	1.1	2.1		23.1	13.4	
N416-EP	18.4	1.9	2.6		25.9	9.5	
N417-EP	11.1	1.4	2.6		21.9	12.3	
N418-EP	16.9	2.3	1.3		24.1	9.8	
N419-EP	13.9	1	2.4		24.1	12.3	
N420-EP	16.2	1	1.9		25.7	11.5	
N421-EP	14.9	1.7	2.2		23.8	12	
N424-EP	17.8	1.8	2.8		26.6	9.7	
N425-EP	18.3	1.5	2.4		25.8	9.4	
N432-EP							
N433-EP							
N435-EP	9.85	1.76	0.62		19.72	14.96	1.25

PROD	MethyleneMethyl				
JE1 A	1.5-1.0pp1.0-0.2ppAro	H2	Al1	H2	Aro:Al1
N408-EP	28.7	21.5	45.8	54.2	0.85
N409-EP	28	18.7	50.4	49.7	1.01
N410-EP	30.4	21.1	45.2	54.8	0.82
N413-EP	25.5	15.8	55.9	44.1	1.27
N414-EP	27.9	20.3	47.9	52	0.92

PROD	MethyleneMethyl				
JE1 A	1.5-1.0pp1.0-0.2ppAro	H2	Al1	H2	Aro:Al1
N415-EP	30	17.5	52.5	47.5	1.11
N416-EP	27.4	14.2	58.3	41.6	1.40
N417-EP	32.1	18.5	49.3	50.6	0.97
N418-EP	29.5	16.1	54.4	45.6	1.19
N419-EP	29.7	16.5	53.7	46.2	1.16
N420-EP	28.2	15.4	56.3	43.6	1.29
N421-EP	29.2	16.3	54.6	45.5	1.20
N424-EP	27.9	13.5	58.7	41.4	1.42
N425-EP	27.9	14.7	57.4	42.6	1.35
N432-EP					
N433-EP					
N435-EP	29.78	17.52	46.87	53.13	0.98
N423-EP	WITH ADD2 IN LIQUID STREAM				

RUN #	LIQUID LOSS	LIQUID RECOVERY	CARBON BAL	HYDROGEN BAL	NITROGEN BAL	SULFUR BAL	OXYGEN BAL
N408-EP	132	94.67%	98.50%	125.34%	0.00%	19.42%	15.73%
N409-EP	79.2	100.53%	104.18%	123.18%	54.13%	18.04%	31.40%
N410-EP	113.9	95.17%	99.37%	122.98%	7.32%	14.64%	15.23%
N413-EP	39.3	102.87%	105.09%	117.90%	43.52%	31.65%	62.83%
N414-EP	116.3	96.13%	100.11%	127.48%	0.00%	4.93%	15.38%
N415-EP	107.2	98.69%	101.70%	122.50%	1.90%	0.00%	41.30%
N416-EP	40	100.67%	100.75%	110.48%	25.17%	25.81%	96.96%
N417-EP	64.3	98.63%	99.55%	122.42%	1.90%	0.00%	68.13%
N418-EP	33.81	104.18%	106.79%	122.94%	86.15%	0.00%	52.73%
N419-EP	52.9	102.47%	105.54%	127.08%	15.77%	0.00%	42.57%
N420-EP	71.5	101.65%	102.67%	119.84%	52.78%	0.00%	73.81%
N421-EP	78.1	99.58%	100.26%	120.78%	107.24%	0.00%	67.41%
N424-EP	41.7	96.36%	100.40%	95.24%	121.50%	43.36%	38.48%
N425-EP	52.4	95.26%	98.72%	93.97%	120.11%	0.00%	46.88%
N432-EP	83.9	98.97%	103.65%	125.87%	11.42%	0.00%	15.07%
N423-EP	WITH ADD2 IN LIQUID STREAM						

RUN #	LIQUID LOSS	LIQUID RECOVERY	CARBON BAL	HYDROGEN BAL	NITROGEN BAL	SULFUR BAL	OXYGEN BAL
N433-EP	63.16	94.57%	100.07%	121.78%	0.00%	0.00%	0.00%
N435-EP	34.4	97.25%	102.13%	102.33%	0.00%	0.00%	0.00%