N78-19326

Gordian Associates, Inc.
New York, Washington, London

54

COMPUTER MODEL FOR REFINERY OPERATIONS WITH EMPHASIS ON JET FUEL PRODUCTION. VOLUME II DATA AND TECHNICAL BASES

NASA CR-135334

February 21, 1978

(NASA-CR-135334) COMPUTER MODEL FOR REFINERY OPERATIONS WITH EMPHASIS ON JET FUEL PRODUCTION. VOLUME 2: DATA AND TECHNICAL BASES Final Report (Gordian Associates, Inc., New York.) 55 p
N78-19326
HC A04/MF A01
Unclas
G3/28 09436

Prepared for:

NASA Lewis Research Center
Cleveland, Ohio 44135

Prepared by:

Daniel N. Dunbar
Barry G. Tunnah

Gordian Associates Incorporated
711 Third Avenue
New York, New York 10017

(212) 697-9023

1. Report No.	2. Government Accession No.	3. Recipient's Catalog No.
NASA CR-135334		

4. Title and Subtitle	5. Report Date
Computer Model for Refinery Operations with Emphasis on Jet Fuel Production. Volume II. Data nd Technical Bases	February 21, 1978
	6. Performing Organization Code
7. Author(s) Daniel N. Dunbar Barry G. Tunnah	8. Performing Organization Report No. 1099-1
	10. Work Unit No.
9. Performing Organization Name and Address Gordian Associates Incorporated 711 Third Avenue New York, New York 10017	11. Contract or Grant No. NASA3-20620
	13. Type of Report and Period Covered Final
12. Sponsoring Agency Name and Address National Aeronautics & Space Administration Washington, D.C. 20546	14. Sponsoring Agency Code

15. Supplementary Notes

Project Manager, Thaine W. Reynolds, Airbreathing Engines Div., NASA Lewis Research Center, Cleveland, Ohio 44135

16. Abstract

The Fortran computing program will predict the flow streams and material, energy, and economic balances of a typical petroleum refinery, with particular emphasis on production of aviation turbine fuel of varying end point and hydrogen content specifications. The program has provision for shale oil and coal oil in addition to petroleum crudes. A case study feature permits dependent cases to be run for parametric or optimization studies by input of only the variables which are changed from the base case. The report has sufficient detail for the information of most readers. However, one subsequent volume contains the mathematic details and the program listing.

17. Key Words (Suggested by Author(s))	18. Distribution Statement
Jet fuel, turbine fuel, petroleum refinery, hydrotreating, fuel oil, refinery efficiency, refinery computing program, shale oil, coal liquid, fuels blending.	

19. Security Classif. (of this report)	20 Security Classif. (of this page)	21. No. of Pages	22. Price*
Unclassified	Unclassified	51	

* For sale by the National Technical Information Service, Springfield, Virginia 22161

NASA-C-168 (Rev. 10-75)

COMPUTER MODEL FOR REFINERY OPERATIONS WITH EMPHASIS ON JET FUEL PRODUCTION. VOLUME II DATA AND TECHNICAL BASES

SUMMARY

This volume of the reports on the Gordian Refinery Simulation Model contains the correlations and data bases used in the computer program and the sources of those information. The program predicts the flow streams, material, energy and economic balances of a refinery processing shale oil, coal oil, and petroleum crudes with emphasis on the production of jet fuel of varying end point and hydrogen content specifications. The data base includes crude assays (distillation cuts and their properties), process unit yields and economic data. The correlations are used for estimating and blending heat of combustion, smoke point and freezing point for jet fuel. Also included are the blending criteria for sulfur, nitrogen, hydrogen, and paraffin, naphthene, and aromatics (PNA) content.

1.0 INTRODUCTION

Major price increases and the impending shortage of petroleum reserves with respect to increasing product demand has brought about a serious examination of possible changes in jet fuel composition. Specification aviation turbine fuel (ASTM D-1655) is produced from mid-distillate petroleum fractions, which compete with ever growing demands for diesel, fuel oil, and petrochemical feedstocks. Increased distillate production from present crudes is feasible, but conversion of gas oils and residuals increases the aromatic content of the mid-distillate pool. Moreover, promising alternate crude sources, such as shale oil, tar sands, and coal liquids yield distillates also with increased aromatic, nitrogen and sulfur contents. Special processing would be required to produce present specification aviation turbine fuel from these sources.

This view of the future has stimulated a reexamination of the optimum combination of jet fuel specifications, with respect to the refinery processing, the supply distribution system, the aircraft fuel system, and the fuel combustion qualities. The goals of current studies are assessing the suitability of jet fuels produced from cracked petroleum and alternate crude sources and developing a data base which will allow optimization of future fuel characteristics. Future aviation turbine fuel specifications must represent a trade-off betweeen energy and cost efficiency of manufacture and aircraft and engine design and performance.

This report deals with the refinery portion of the overall program. In order to have a systematic way of determining the energy efficiency of the production of various product slates involving different crude sources and different processing schemes, the Lewis Research Center of NASA has supported the development of this computer model for petroleum refinery operation. The primary objectives of this model are:

1. the flexibility to configure a refinery involving any or all of the process units commonly employed in the production of gasoline, jet fuels, and mid-distillates;

2. the ability to produce jet fuel blends of varying end-point specification and varying specified hydrogen content as part of the total slate of products;

3. the ability to handle synthetic crudes (shale and coal derived) with varying severities of hydroprocessing;

4. the determination of overall refinery energy efficiency;

5. the determination of sulfur, nitrogen, and hydrogen material balances for each process unit and for the overall refinery; and

6. the capability of carrying out economic calculations.

The Gordian Refinery Simulation Model, presented herein, has all the above capabilities. This report is the second of three volumes. Volume I (NASA CR-135333) is a detailed description of the program, input data, and sample output; and Volume III (NASA CR-135335) contains programming documentation. The complete documentation and program tape are available through the Computing Software and Management Information Office (COSMIC) under the number LEW-13047.

The purpose of this report is to support the Gordian Refinery Simulation Model by providing a record of data sources and an explanation of the correlations employed in the model. This encompasses crude oil assay data, refinery process unit yields, product blending data and correlations, and data used in the calculations of refinery economics (investment costs, fixed and variable processing costs, etc.).

While all of the data and correlation specifics may be obtained from the program Fortran listing, this manual provides data in a format which should allow for easier reference and understanding. Although many of the crude oil assays involve estimated properties, they are all considered to be adequate for the purpose of estimating refinery production volumes and properties with the exception of Elk Hills for which insufficient assay data was uncovered to make intelligent estimates.

2.0 CRUDE ASSAY DATA BASE

The assays on the following pages refer to the following ASTM D-86 cut points:

Light Straight run gasoline	IBP-250°F
Heavy Naphtha	250-400°
Light Kerosene	400-525°
Heavy Kerosene	525-650°
Vacuum Gas Oil	650-1050°
Vacuum Bottoms	1050°F plus

The above cut points may be redefined, either by making alterations to the crude oil data base subroutine (CBASE) or by redefining the crude oil assay through input variables.

There is storage capability within the model to include up to 35 crude assays. The 26 crude oils for which assays are currently stored within the program are:

		API's	Source	Date
1.	Tigre - Venezuela	24.7°	*	June,1968
2.	Lot 17 - Venezuela,	36.1°	Phillips Petr. Co.	1963
3.	Bachaquero - Venezuela,	16.8°	Oil & Gas Journal	April, 1976
4.	Nigerian Light,	34.7°	*	Feb. 1972
5.	Amal - Libya,	35.8°	*	Aug. 1966
6.	Arzew - Algeria,	44.1°	*	Feb. 1972
7.	Bakr - Egypt,	19.6°	*	1972
8.	Arabian Light,	34.2°	Esso Intl. Inc.	Oct. 1970
9.	Agha Jari - Iran,	34.3°	Esso Intl. Inc.	Aug. 1966
10.	Kuwait	31.4°	Esso Intl. Inc.	Sept. 1966
11.	Paraho Shale Oil	19.3°	Exxon Res. & Eng. Co.	July 1975
12.	Tosco Shale Oil,	21.0°	"	Oct. 1975
13.	Garett Shale Oil,	25.0°	"	Oct. 1975
14.	Synthoil (from Kentucky Coal),	5.9°	"	June 1976
15.	Alaskan, North Slope,	26.8°	Oil & Gas Journal	June 1976
16.	Ekofisk, North Sea - Norway	35.6°	Evaluation of World's Important Crudes (Oil & Gas Journal)	1973
17.	West Texas Sour,	34.0°	"	"
18.	South Louisiana - Ostrica	32.3°	"	"
19.	Louisiana Delta,	30.6°	"	"
20.	East Texas,	38.0°	"	"
21.	Aneth - Utah,	40.9°	"	"
22.	Wyoming Sour,	24.9°	"	"
23.	Oklahoma - Golden Trend,	39.9°	Petroleum Processing	Sept. 1951
24.	Elk Hills - California,	26.6°	US Bur. of Mines (IC8452)	1972
25.	Wilmington - California,	21.7°	Evaulation of Worlds Important Crudes	1973
26.	Pembina - Canada,	32.7°	(Oil and Gas Journal)	"

* In House Confidential Information.

The data for crude assays was collected from crude assays published periodically by The Oil and Gas Journal and Gordian in-house crude assay reports obtained from crude oil vendors. All of the information contained in the crude oil data base are presented in the following 26 tables. Wherever an estimate of a crude oil property was used, or a correlation was applied to derive a crude oil property, this is noted by a subscript (letters A through H). This letter corresponds to an explanatory note, which is contained in the pages immediately following the crude oil assay tables.

Crude Oil Name: TIGRE (Venezuela) No: 1

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N [A]	%H [B]	Viscosity 210°F (Linear Scale)	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion [G] (Net) (Btu/lb)
Light Straight Run (IBP-250°F)	0.0707	59.9	0.00	0.0005	14.3					
Heavy Naphtha (250°F-400°F)	0.0900	49.0	0.05	0.001	14.0					
Light Kerosene (400°F-525°F)	0.1200	36.0	0.30	0.004	13.0	0.0	P 38.0[D] N 41.0 A 21.0	-46.0	20.0	18400.0
Heavy Kerosene (525°F-650°F)	0.1800	28.0	1.02	0.010	12.1	6.0	P 38.0[D] N 41.0 A 21.0	8.0[E]	17.0	18180.0
Vacuum Gas Oil (650°F-1050°F)	0.2900	20.0	1.60	0.146	11.6	19.4				
Vacuum Bottoms (1050°F +)	0.2200	8.0	3.28	0.342	10.0	33.9				

Crude Oil Data

°API : 24.7

%S : 1.57

%N : 0.12[A]

%H : 12.0[B]

Heat of Combustion : 17890.0[G]

Light End Yield (Vol. Fraction)

Refinery Gas	0.0008
LPG	0.0041
Iso-Butane	0.0046
N-Butane	0.0086
Pentanes	0.0112
	0.0293

Crude Oil Name: Lot 17 (Venezuela) No: 2

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N [A]	%H [B]	Viscosity [C] 210°F (Linear Scale)	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion [G] (Net) (Btu/lb)
Light Straight Run (IBP-250°F)	0.1170	61.0	0.0	0.0005	14.7					
Heavy Naphtha (250°F-400°F)	0.1900	50.5	0.012	0.001	14.2					
Light Kerosene (400°F-525°F)	0.1350	41.0	0.23	0.005	13.7	0.0	P 56.3[D] N 30.0 A 13.7	-36.0	21.0	18530.0
Heavy Kerosene (525°F-650°F)	0.1150	35.0	0.66	0.020	13.2	8.0	P 56.3[D] N 30.0 A 13.7	10.0[E]	18.0[F]	18380.0
Vacuum Gas Oil (650°F-1050°F)	0.2750	25.0	1.52	0.21	12.4	16.0				
Vacuum Bottoms (1050°F +)	0.1250	10.2	2.90	0.77	10.2	31.2				

Crude Oil Data

°API : 36.1

%S : 0.98

%N : 0.16[A2]

%H : 13.2[B]

Heat of Combustion : 18400.0[G]

Light End Yield (Vol. Fraction)

Refinery Gas	0.0000
LPG	0.0070
Iso-Butane	0.0030
N-Butane	0.0100
Pentanes	0.0230
	0.0430

Crude Oil Name: Bachaquero (Venezuela) No: 3

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N [A]	%H [B]	Viscosity [C] 210°F (Linear Scale)	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion [G] (Net) (Btu/lb)
Light Straight Run (IBP-250°F)	0.0386	64.0	0.015	0.0005	14.8					
Heavy Naphtha (250°F-400°F)	0.0600	43.0	0.10	0.001	13.3					
Light Kerosene (400°F-525°F)	0.0700	34.0	0.60	0.023	12.6	0.0	P 19.2 N 54.8 A 26.0	-65.0	16.0	18420.0
Heavy Kerosene (525°F-650°F)	0.1200	27.0	1.25	0.049	11.9	8.0	P 19.2 [D1] N 54.8 A 26.0	-35.0 [E]	15.0	18100.0
Vacuum Gas Oil (650°F-1050°F)	0.3700	17.0	2.30	0.363	11.0	24.0				
Vacuum Bottoms (1050°F +)	0.3300	6.6	3.69	0.722	9.7	36.7				

Crude Oil Data

°API : 16.8

%S : 2.40

%N : 0.38

%H : 11.0 [B]

Heat of Combustion : 17610.0 [C]

Light End Yield (Vol. Fraction)

Refinery Gas	0.0012
LPG	0.0015
Iso-Butane	0.0013
N-Butane	0.0025
Pentanes	0.0049
	0.0114

Crude Oil Name: Nigerian Light

No: 4

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N[A]	%H[B]	Viscosity[C] 210°F (Linear Scale)	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion (Net) (Btu/lb)[G]
Light Straight Run (IBP-250°F)	0.1311	64.0	0.01	0.0005	14.9					
Heavy Naphtha (250°F-400°F)	0.1700	44.0	0.02	0.001	13.4					
Light Kerosene (400°F-525°F)	0.1900	37.0	0.09	0.00135	13.1	0.0	P 35.5[D] N 48.5 A 16.0	-47.0	23.0	19440.0
Heavy Kerosene (525°F-650°F)	0.1300	31.0	0.17	0.0124	12.8	8.0	P 35.5[D] N 48.5 A 16.0	-10.0[E]	20.0	18250.0
Vacuum Gas Oil (650°F-1050°F)	0.2550	22.0	0.28	0.170	12.0	19.6				
Vacuum Bottoms (1050°F +)	0.0950	15.0	0.60	0.792	11.3	28.3				

Crude Oil Data

°API : 34.7

%S : 0.14

%N : 0.12[A1]

%H : 13.0[B]

Heat of Combustion : 18370.0

Light End Yield (Vol. Fraction)

Refinery Gas	0.0003
LPG	0.0023
Iso-Butane	0.0033
N-Butane	0.0066
Pentanes	0.0164
	0.0289

Crude Oil Name: AMAL (Libya) No: 5

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N[A]	%H[B]	Viscosity[C] 210°F (Linear Scale)	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion[G] (Net) (Btu/lb)
Light Straight Run (IBP-250°F)	0.0805	75.2	0.01	0.0005	16.1					
Heavy Naphtha (250°F-400°F)	0.1320	64.0	0.01	0.001	15.9					
Light Kerosene (400°F-525°F)	0.0770	46.5	0.01	0.006	14.4	0.0	P 61.0 N 30.0 A 9.0	-20.0[E]	33.0	18650.0
Heavy Kerosene (525°F-650°F)	0.0980	42.9	0.03	0.02	14.3	8.0	P 61.0[D] N 30.0 A 9.0	25.0[E]	29.0	18570.0
Vacuum Gas Oil (650°F-1050°F)	0.3270	29.1	0.20	0.06	13.5	20.0				
Vacuum Bottoms (1050°F +)	0.2800	16.3	0.20	0.27	11.6	28.5				

Crude Oil Data

°API : 35.8

%S : 0.10

%N : 0.12

%H : 13.8[B]

Heat of Combustion : 18400.0[G]

Light End Yield (Vol. Fraction)

Refinery Gas	0.0000
LPG	0.0008
Iso-Butane	0.0002
N-Butane	0.0045
Pentanes	0.0000
	0.0055

Crude Oil Name: Arzew (Algeria) No: 6

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N [A]	%H [B]	Viscosity [C] 210°F (Linear Scale)	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion [G] (Net) (Btu/lb)
Light Straight Run (IBP-250°F)	0.1601	80.3	0.00	0.0005	16.4					
Heavy Naphtha (250°F-400°F)	0.1650	64.2	0.00	0.001	16.0					
Light Kerosene (400°F-525°F)	0.1150	49.5	0.03	0.004	14.7	0.0	P 59.0[D] N 29.0 A 12.0	20.0[E]	45.0[F]	18710.0
Heavy Kerosene (525°F-650°F)	0.1500	40.0	0.07	0.013	14.1	8.0	P 59.0[D] N 29.0 A 12.0	70.0[E]	42.0[F]	18500.0
Vacuum Gas Oil (650°F-1050°F)	0.2900	28.4	0.20	0.146	13.3	20.0				
Vacuum Bottoms (1050°F +)	0.0900	17.0	0.40	0.836	11.7	27.2				

Crude Oil Data

°API : 44.1

%S : 0.10

%N : 0.12[A1]

%H : 14.4[B]

Heat of Combustion : 18600.0[G]

Light End Yield (Vol. Fraction)

Refinery Gas	0.0013
LPG	0.0087
Iso-Butane	0.0065
N-Butane	0.0134
Pentanes	0.0000
	0.0299

Crude Oil Name: Bakr (Egypt) No:7

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N [A]	%H [B]	Viscosity 210°F (Linear Scale) [C]	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion (Net) (Btu/lb) [G]
Light Straight Run (IBP-250°F)	0.0202	65.0	0.05	0.0005	14.8					
Heavy Naphtha (250°F-400°F)	0.0814	56.0	0.10	0.0010	14.7					
Light Kerosene (400°F-525°F)	0.0610	44.0	1.20	0.008	13.9	0.0	P 39.0[D] N 44.0 A 17.0	-10.0[E]	27.0	18650.0
Heavy Kerosene (525°F-650°F)	0.0550	37.5	1.80	0.034	13.5	8.0	P 39.0[D] N 44.0 A 17.0	35.0[E]	25.0	18440.0
Vacuum Gas Oil (650°F-1050°F)	0.5070	25.0	4.50	0.084	12.1	20.0				
Vacuum Bottoms (1050°F +)	0.2730	5.0	6.50	0.276	9.2	34.0				

Crude Oil Data

°API : 19.6

%S : 4.40

%N : 0.12[A1]

%H : 10.9[B]

Heat of Combustion : 17760.0[G]

Light End Yield (Vol. Fraction)

Refinery Gas	0.0000
LPG	0.0010
Iso-Butane	0.0003
N-Butane	0.0011
Pentanes	0.0000
	0.0024

Crude Oil Name: Arabian Light (Saudi Arabia) No: 8

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N	%H[B]	Viscosity[C] 210°F (Linear Scale)	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion[G] (Net) (Btu/lb)
Light Straight Run (IBP-250°F)	0.1073	69.0	0.02	0.0005	15.1					
Heavy Naphtha (250°F-400°F)	0.1500	52.0	0.04	0.0010	14.3					
Light Kerosene (400°F-525°F)	0.1300	43.0	0.28	0.0016	13.9	0.0	P 67.0 N 20.0 A 13.0	-30.0	22.0	18580.0
Heavy Kerosene (525°F-650°F)	0.1200	35.0	1.05	0.0065	13.2	8.0	P 64.0 N 30.0 A 6.0	1.0[E]	18.0	18380.0
Vacuum Gas Oil (650°F-1050°F)	0.3250	23.1	2.27	0.080	12.0	17.2				
Vacuum Bottoms (1050°F +)	0.1250	6.5	4.29	0.340	9.6	32.8				

Crude Oil Data

°API : 34.2

%S : 1.65

%N : 0.05

%H : 13.1[B]

Heat of Combustion : 18350.0[G]

Light End Yield (Vol. Fraction)

Refinery Gas	0.0001
LPG	0.0014
Iso-Butane	0.0016
N-Butane	0.0127
Pentanes	0.0269
	0.0427

Crude Oil Name: Agha Jari (Iran)

No: 9

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N[A]	%H[B]	Viscosity[C] 210°F (Linear Scale)	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion[G] (Net) (Btu/lb)
Light Straight Run (IBP-250°F)	0.1082	-65.0	0.02	0.0005	14.9					
Heavy Naphtha (250°F-400°F)	0.1550	51.0	0.04	0.001	14.3					
Light Kerosene (400°F-525°F)	0.1300	41.0	0.40	0.004	13.6	0.0	P 47.7 N 26.3 A 26.0	-21.0	23.0	18480.0
Heavy Kerosene (525°F-650°F)	0.1250	34.0	0.95	0.010	13.1	8.0	P 47.7[D] N 26.3 A 26.0	25.0[E]	20.0	18350.0
Vacuum Gas Oil (650°F-1050°F)	0.2950	23.0	1.77	0.105	12.2	17.8				
Vacuum Bottoms (1050°F +)	0.1350	6.8	3.67	0.580	10.8	33.0				

Crude Oil Data

°API : 34.3

%S : 1.34

%N : 0.13[A2]

%H : 13.0[B]

Heat of Combustion : 18360.0[G]

Light End Yield (Vol. Fraction)

Refinery Gas	0.0011
LPG	0.0062
Iso-Butane	0.0035
N-Butane	0.0135
Pentanes	0.0275
	0.0518

Crude Oil Name: Kuwait

No: 10

Cut \ Property	Yield (Vol. Fraction)	°API	%S	%N[A]	%H[B]	Viscosity 210°F (Linear Scale)[C]	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion (Net) (Btu/lb)[G]
Light Straight Run (IBP-250°F)	0.0955	69.0	0.05	0.0005	15.4					
Heavy Naphtha (250°F-400°F)	0.1300	52.0	0.10	0.001	14.2					
Light Kerosene (400°F-525°F)	0.1100	42.5	0.45	0.092	13.8	0.0	P 80.0[D] N 17.0 A 3.0	-13.0	23.0	18560.0
Heavy Kerosene (525°F-650°F)	0.1050	34.5	1.52	0.10	13.1	8.0	P 80.0[D] N 17.0 A 3.0	28.0[E]	20.0	18360.0
Vacuum Gas Oil (650°F-1050°F)	0.3000	22.3	3.04	0.153	11.8	20.0				
Vacuum Bottoms (1050°F +)	0.2000	5.6	5.55	0.40	9.4	30.8				

Crude Oil Data

°API : 31.4

%S : 2.53

%N : 0.13[A2]

%H : 12.7[B]

Heat of Combustion : 18260.0[G]

Light End Yield (Vol. Fraction)

Refinery Gas	0.0012
LPG	0.0086
Iso-Butane	0.0041
N-Butane	0.0154
Pentanes	0.0302
	0.0595

Crude Oil Name: Paraho Shale

No: 11

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N	%H	Viscosity[C] 210°F (Linear Scale)	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion (Nat) (Btu/lb)[G]
Light Straight Run (IBP-250°F)	0.000	0.00	0.0	0.0	0.0					
Heavy Naphtha (250°F-400°F)	0.015	40.57	0.9023	0.001[A]	12.5					
Light Kerosene (400°F-525°F)	0.075	34.26	0.6587	1.01	12.2	0.0	P 30.0[D] N 53.0 A 17.0	-40.0	14.0	18290.0
Heavy Kerosene (525°F-650°F)	0.160	27.11	0.6910	1.9009	11.5	6.0	P 30.0[D] N 53.0 A 17.0	15.0	12.0	18100.0
Vacuum Gas Oil (650°F-1050°F)	0.660	17.85	0.6008	1.9971	10.9	20.2				
Vacuum Bottoms (1050°F +)	0.090	5.30	0.40	3.06	9.4	31.8				

Crude Oil Data

°API : 19.3

%S : 0.71

%N : 2.00

%H : 11.5

Heat of Combustion : 17760.0[G]

Light End Yield (Vol. Fraction)

Refinery Gas	0.0000
LPG	0.0000
Iso-Butane	0.0000
N-Butane	0.0000
Pentanes	0.0000
	0.0000

Crude Oil Name: Tosco Shale No: 12

Cut \ Property	Yield (Vol. Fraction)	°API	%S	%N	%H	Viscosity[†] 210°F (Linear Scale)	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion (Net) (Btu/lb)[G]
Light Straight Run (IBP-250°F)	0.025	55.88	0.8865	0.0005[A]	13.7					
Heavy Naphtha (250°F-400°F)	0.115	46.78	0.8454	1.0	13.1					
Light Kerosene (400°F-525°F)	0.090	36.11	0.8167	1.45	12.3	0.0	P 30.0[D] N 53.0 A 17.0	-40.0	15.0	18410.0
Heavy Kerosene (525°F-650°F)	0.120	26.61	0.7503	1.8649	11.5	4.0	P 30.0[D] N 53.0 A 17.0	21.0	13.0	18080.0
Vacuum Gas Oil (650°F-1050°F)	0.500	16.54	0.6205	2.1762	10.7	20.8				
Vacuum Bottoms (1050°F +)	0.150	5.4	0.53	2.32	9.5	31.6				

Crude Oil Data

°API : 21.0

%S : 0.67

%N : 1.85

%H : 11.6

Heat of Combustion : 17830.0[G]

Light End Yield (Vol. Fraction)

Refinery Gas	0.0000
LPG	0.0000
Iso-Butane	0.0000
N-Butane	0.0000
Pentanes	0.0000
	0.0000

Crude Oil Name: Garett Shale No: 13

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N	%H	Viscosity[C] 210°F (Linear Scale)	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion[G] (Net) (Btu/lb)
Light Straight Run (IBP-250°F)	0.000	0.0	0.0	0.0	0.0					
Heavy Naphtha (250°F-400°F)	0.033	41.19	0.654	0.001[A]	12.6					
Light Kerosene (400°F-525°F)	0.137	35.30	0.555	0.458	12.5	0.0	P 39.0[D] N 31.0 A 30.0	-30.0	15.0	18380.0
Heavy Kerosene (525°F-650°F)	0.288	28.90	0.598	1.033	12.0	3.5	P 39.0[D] N 31.0 A 30.0	-11.0	13.0	18170.0
Vacuum Gas Oil (650°F-1050°F)	0.497	21.82	0.502	1.586	11.6	17.4				
Vacuum Bottoms (1050°F +)	0.045	2.10	1.32	1.980	9.1	35.0				

Crude Oil Data

°API : 25.0

%S : 0.64

%N : 1.30

%H : 11.8

Heat of Combustion : 18010.0[G]

Light End Yield (Vol. Fraction)

Refinery Gas	0.0000
LPG	0.0000
Iso-Butane	0.0000
N-Butane	0.0000
Pentanes	0.0000
	0.0000

Crude Oil Name: Synthoil (Coal) No: 14

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N	%H	Viscosity[C] 210°F (Linear Scale)	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion[G] (Net) (Btu/lb)
Light Straight Run (IBP-250°F)	0.000	0.0	0.0	0.0	0.0					
Heavy Naphtha (250°F-400°F)	0.017	26.71	0.10	0.30	11.0					
Light Kerosene (400°F-525°F)	0.163	21.60	0.092	0.29	10.8	0.0	P 20.0 N 30.0 A 50.0	-60.0	8.0	17860.0
Heavy Kerosene (525°F-650°F)	0.256	15.90	0.14	0.32	10.4	5.0	P 20.0 N 30.0 A 50.0	-25.0	7.0	17580.0
Vacuum Gas Oil (650°F-1050°F)	0.264	9.40	0.12	0.47	10.1	13.8				
Vacuum Bottoms (1050°F +)	0.300	-4.30	0.31	1.22	8.5	24.2				

Crude Oil Data

°API : 5.9

%S : 0.22

%N : 0.79

%H : 9.2

Heat of Combustion : 17110.0[G]

Light End Yield (Vol. Fraction)

Refinery Gas	0.0000
LPG	0.0000
Iso-Butane	0.0000
N-Butane	0.0000
Pentanes	0.0000
	0.0000

Crude Oil Name: Alaskan - North Slope No: 15

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N [A]	%H [B]	Viscosity [C] 210°F (Linear Scale)	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion [G] (Net) (Btu/lb)
Straight Run (IBP-250°F)	0.074	60.0	0.00	0.0005	14.5					
Heavy Naphtha (250°F-400°F)	0.120	47.6	0.05	0.001	13.8					
Light Kerosene (400°F-525°F)	0.110	36.0	0.23	0.009	13.0	0.0	P 38.0[D] N 38.0 A 24.0	-42.0	17.0	18400.0
Heavy Kerosene (525°F-650°F)	0.130	31.1	0.60	0.028	12.7	8.0	P 38.0[D] N 38.0 A 24.0	15.0[E]	15.0	18250.0
Vacuum Gas Oil (650°F-1050°F)	0.370	21.5	1.15	0.219	11.9	20.0				
Vacuum Bottoms (1050°F +)	0.170	10.7	2.45	0.848	10.4	33.3				

Crude Oil Data

°API : 26.8

%S : 1.04

%N : 0.23

%H : 12.3[B]

Heat of Combustion : 17940.0[G]

Light End Yield (Vol. Fraction)

Refinery Gas	0.001
LPG	0.004
Iso-Butane	0.002
N-Butane	0.007
Pentanes	0.012
	0.026

Crude Oil Name: North Sea - EkoFisk

No: 16

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N [A]	%H [B]	Viscosity [C] 210°F (Linear Scale)	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion [G] (Net) (Btu/lb)
Light Straight Run (IBP-250°F)	0.1385	67.5	0.0003	0.0005	14.9					
Heavy Naphtha (250°F-400°F)	0.1505	50.7	0.0038	0.0010	14.2					
Light Kerosene (400°F-525°F)	0.1220	40.1	0.05	0.003	13.5	0.0	P41.15[D2] N41.15 A17.7	-36.0	21.0	18510.0
Heavy Kerosene (525°F-650°F)	0.1520	34.3	0.10	0.02	13.2	4.0	P40.65[D2] N40.65 A18.7	30.0	18.0	18350.0
Vacuum Gas Oil (650°F-1050°F)	0.2800	24.9	0.19	0.141	12.6	18.2				
Vacuum Bottoms (1050°F +)	0.1410	14.0	0.44	0.500	12.6	29.4				

Crude Oil Data

°API : 35.6

%S : 0.18

%N : 0.112[A2]

%H : 13.7[B]

Heat of Combustion : 18390.0[G]

Light End Yield (Vol. Fraction) [H]

Refinery Gas	0.0025
LPG	0.0025
Iso-Butane	0.0017
N-Butane	0.0033
Pentanes	0.0060
	0.0160

Crude Oil Name: West Texas Sour No: 17

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N [A]	%H [B]	Viscosity [C] 210°F (Linear Scale)	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion [G] (Net) (Btu/lb)
Light Straight Run (IBP-250°F)	0.150	67.0	0.05	0.0005	14.9					
Heavy Naphtha (250°F-400°F)	0.160	50.0	0.25	0.001	14.1					
Light Kerosene (400°F-525°F)	0.130	40.0	0.65	0.004	13.4	0.0	P 40.0[D] N 41.0 A 19.0	-43.0	20.0[F]	18510.0
Heavy Kerosene (525°F-650°F)	0.110	33.0	1.30	0.017	12.7	8.0	P 40.0[D] N 41.0 A 19.0	30.0[E]	18.0[F]	18320.0
Vacuum Gas Oil (650°F-1050°F)	0.253	24.0	1.85	0.167	12.3	17.2				
Vacuum Bottoms (1050°F +)	0.160	10.0	3.30	0.471	10.2	29.8				

Crude Oil Data

°API : 34.0

%S : 1.90

%N : 0.12[A]

%H : 12.7[B]

Heat of Combustion : 18340.0[G]

Light End Yield (Vol. Fraction)

Refinery Gas	0.001
LPG	0.006
Iso-Butane	0.004
N-Butane	0.011
Pentanes	0.015
	0.037

Crude Oil Name: South Louisiana - Ostrica

No: 18

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N [A]	%H [B]	Viscosity 210°F (Linear Scale) [C]	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion (Net) (Btu/lb) [G]
Light Straight Run (IBP-250°F)	0.067	66.2	0.008	0.00026	14.8					
Heavy Naphtha (250°F-400°F)	0.140	48.2	0.04	0.00045	13.9					
Light Kerosene (400°F-525°F)	0.155	38.4	0.05	0.00059	13.5	0.0	P 42.0 [D2] N 41.5 A 16.5	-44.0	18.0	18460.0
Heavy Kerosene (525°F-650°F)	0.170	32.7	0.16	0.004	13.0	3.4	P 42.0 [D1] N 41.5 A 16.5	10.0	16.0	18310.0
Vacuum Gas Oil (650°F-1050°F)	0.355	23.5	0.40	0.035	12.4	19.1				
Vacuum Bottoms (1050°F +)	0.090	9.7	0.96	0.24	10.4	32.8				

Crude Oil Data

°API : 32.3

%S : 0.31

%N : 0.035 [A2]

%H : 12.7 [B]

Heat of Combustion : 18300.0 [G]

Light End Yield (Vol. Fraction)

Refinery Gas	0.0009
LPG	0.0027
Iso-Butane	0.0026
N-Butane	0.0053
Pentanes	0.0110
	0.0225

Crude Oil Name: Louisiana Delta

No: 19.

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N[A]	%H[B]	Viscosity[C] 210°F (Linear Scale)	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion[G] (Net) (Btu/lb)
Light Straight Run (IBP-250°F)	0.073	68.0	0.01	0.0005	15.0					
Heavy Napphtha (250°F-400°F)	0.129	48.2	0.03	0.001	13.8					
Light Kerosene (400°F-525°F)	0.150	38.3	0.11	0.003	13.2	0.0	P 34.4[D] N 52.7 A 12.9	-50.0[E]	20.0[F]	18290.0
Heavy Kerosene (525°F-650°F)	0.175	31.9	0.12	0.011	12.7	8.0	P 34.4[D] N 52.7 A 12.9	2.0[E]	18.0[F]	18230.0
Vacuum Gas Oil (650°F-1050°F)	0.360	22.2	0.40	0.118	12.0	20.0				
Vacuum Bottoms (1050°F +)	0.103	9.6	0.90	0.731	11.6	33.3				

Crude Oil Data

°API : 30.6

%S : 0.30

%N. : 0.12[A1]

%H : 12.8[B]

Heat of Combustion : 18460.0[G]

Light End Yield (Vol. Fraction)

Refinery Gas	0.0020
LPG	0.0020
Iso-Butane	0.0013
N-Butane	0.0027
Pentanes	0.0000
	0.0080

Crude Oil Name: East Texas   No: 20

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N[A]	%H[B]	Viscosity[C] 210°F (Linear Scale)	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion[G] (Net) (Btu/lb)
Light Straight Run (IBP-250°F)	0.158	67.0	0.003	0.0005	14.9					
Heavy Naphtha (250°F-400°F)	0.140	51.0	0.01	0.001	14.3					
Light Kerosene (400°F-525°F)	0.160	40.0	0.05	0.002	13.5	0.0	P 44.0[D] N 39.0 A 17.0	-18.0[E]	20.0[F]	18510.0
Heavy Kerosene (525°F-650°F)	0.070	36.0	0.10	0.016	13.5	8.0	P 44.0[D] N 39.0 A 17.0	30.0[E]	18.0[F]	18400.0
Vacuum Gas Oil (650°F-1050°F)	0.330	27.0	0.38	0.075	12.9	20.0				
Vacuum Bottoms (1050°F +)	0.100	9.0	1.50	0.439	8.9	33.7				

Crude Oil Data

°API : 38.0

%S : 0.30

%N : 0.07

%H : 13.6[B]

Heat of Combustion : 18460.0[G]

Light End Yield (Vol. Fraction)

Refinery Gas	0.0075
LPG	0.0075
Iso-Butane	0.0050
N-Butane	0.0100
Pentanes	0.0120
	0.042

Crude Oil Name: Aneth - Utah　　No:21

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N[A]	%H[B]	Viscosity[C] 210°F (Linear Scale)	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion (Net) (Btu/lb)[G]
Light Straight Run (IBP-250°F)	0.170	71.9	0.013	0.0005	15.6					
Heavy Naphtha (250°F-400°F)	0.180	49.6	0.016	0.001	14.1					
Light Kerosene (400°F-525°F)	0.140	39.0	0.021	0.002	13.5	0.0	P 45.0[D] N 38.0 A 17.0	-38.0	23.0	18500.0
Heavy Kerosene (525°F-650°F)	0.130	36.3	0.02	0.007	13.5	0.0	P 45.0[D] N 38.0 A 17.0	15.0[E]	20.0	18420.0
Vacuum Gas Oil (650°F-1050°F)	0.300	31.7	0.21	0.071	13.9	20.0				
Vacuum Bottoms (1050°F +)	0.040	17.1	0.50	0.941	11.8	33.3				

Crude Oil Data

°API : 40.9

%S : 0.12

%N : 0.06

%H : 13.8[B]

Heat of Combustion : 18520.0[G]

Light End Yield (Vol. Fraction)[H]

Refinery Gas	0.0065
LPG	0.0065
Iso-Butane	0.0043
N-Butane	0.0087
Pentanes	0.0140
	0.0400

Crude Oil Name: Wyoming Sour

No: 22

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N[A]	%H[B]	Viscosity 210°F (Linear Scale)[C]	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion (Net) (Btu/lb)[G]
Light Straight Run (IBP-250°F)	0.055	70.0	0.10	0.0005	15.4					
Heavy Naphtha (250°F-400°F)	0.100	50.0	0.20	0.001	14.2					
Light Kerosene (400°F-525°F)	0.200	35.0	0.60	0.003	12.7	0.0	P 51.0[D] N 35.0 A 14.0	-50.0[E]	16.0[F]	18380.0
Heavy Kerosene (525°F-650°F)	0.190	31.0	1.60	0.010	12.6	8.0	P 51.0[D] N 35.0 A 14.0	25.0[E]	15.0[F]	18240.0
Vacuum Gas Oil (650°F-1050°F)	0.160	20.0	2.60	0.264	11.5	20.0				
Vacuum Bottoms (1050°F +)	0.260	5.0	4.20	0.289	9.4	34.3				

Crude Oil Data

°API : 24.9

%S : 2.40

%N : 0.12[A]

%H : 11.5[B]

Heat of Combustion : 18000.0[G]

Light End Yield (Vol. Fraction)[G]

Refinery Gas	0.005
LPG	0.005
Iso-Butane	0.003
N-Butane	0.007
Pentanes	0.015
	0.035

Crude Oil Name: Oklahoma - Golden Trend

No:23

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N [A]	%H [B]	Viscosity 210°F (Linear Scale) [C]	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion (Net) (Btu/lb) [G]
Light Straight Run (IBP-250°F)	0.183	65.0	0.008	0.0005	14.8					
Heavy Naphtha (250°F-400°F)	0.163	52.0	0.0014	0.001	14.4					
Light Kerosene (400°F-525°F)	0.097	43.0	0.0018	0.005	13.9	0.0	P 50.0[D] N 40.0 A 10.0	-10.0[E]	26.0[F]	18580.0
Heavy Kerosene (525°F-650°F)	0.120	39.0	0.10	0.016	13.9	8.0	P 50.0[D] N 40.0 A 10.0	30.0[E]	23.0[F]	18480.0
Vacuum Gas Oil (650°F-1050°F)	0.275	30.0	0.30	0.154	13.5	20.0				
Vacuum Bottoms (1050°F +)	0.075	15.0	0.55	1.003	11.3	30.2				

Crude Oil Data

°API : 39.9

%S : 0.20

%N : 0.12[A1]

%H : 13.5[B]

Heat of Combustion : 18500.0[G]

Light End Yield (Vol. Fraction)[H]

Refinery Gas	0.015
LPG	0.015
Iso-Butane	0.010
N-Butane	0.020
Pentanes	0.027
	0.087

Crude Oil Name: Elk Hills - California No: 24

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N	%H[B]	Viscosity[C] 210°F (Linear Scale)	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion[G] (Net) (Btu/lb)
Light Straight Run (IBP-250°F)	0.083	55.7			13.9					
Heavy Naphtha (250°F-400°F)	0.157	44.9			13.5					
Light Kerosene (400°F-525°F)	0.192	33.8			12.7		P N A	-60.0[E]	15.0[F]	18340.0
Heavy Kerosene (525°F-650°F)							P N A			
Vacuum Gas Oil (650°F-1050°F)										
Vacuum Bottoms (1050°F +)										

Crude Oil Data

°API : 26.6

%S : 0.61

%N : 0.47

%H : 12.0[B]

Heat of Combustion : 18080.0[G]

Light End Yield (Vol. Fraction)

Refinery Gas

LPG

Iso-Butane

N-Butane

Pentanes

Crude Oil Name: Wilmington - California No: 25

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N[A]	%H[B]	Viscosity[C] 210°F (Linear Scale)	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion[G] (Net) (Btu/lb)
Light Straight Run (IBP-250°F)	0.070	70.3	0.05	0.0005	15.1					
Heavy Naphtha (250°F-400°F)	0.100	51.4	0.10	0.001	14.3					
Light Kerosene (400°F-525°F)	0.120	38.0	0.50	0.023	12.8	0.0	P 25.0[D] N 67.0 A 8.0	-40.0[E]	18.0[F]	18460.0
Heavy Kerosene (525°F-650°F)	0.120	22.0	1.05	0.085	11.7	8.0	P 25.0[D] N 67.0 A 8.0	0.0[E]	16.0[F]	18380.0
Vacuum Gas Oil (650°F-1050°F)	0.226	17.4	1.50	1.015	11.3	20.0				
Vacuum Bottoms (1050°F +)	0.344	7.1	3.40	1.185	9.8	33.3				

Crude Oil Data

°API : 21.7

%S : 1.43

%N : 0.65

%H : 11.5[B]

Heat of Combustion : 17860.0[G]

Light End Yield (Vol. Fraction)[H]

Refinery Gas	0.0025
LPG	0.0025
Iso-Butane	0.0017
N-Butane	0.0033
Pentanes	0.0100
	0.0200

Crude Oil Name: Pembina - Canada

No: 26

Property / Cut	Yield (Vol. Fraction)	°API	%S	%N[A]	%H[B]	Viscosity[C] 210°F (Linear Scale)	PNA	Freeze Point (°F)	Smoke Point (mm)	Heat of Combustion[G] (Net) (Btu/lb)
Light Straight Run (IBP-250°F)	0.1134	70.0	0.01	0.0005	15.4					
Heavy Naphtha (250°F-400°F)	0.1618	52.2	0.01	0.001	14.4					
Light Kerosene (400°F-525°F)	0.1404	41.1	0.016	0.001	13.7	0.0	P 40.5[D2] N 40.5 A 19.0	-32.0	20.0	18540.0
Heavy Kerosene (525°F-650°F)	0.1182	36.0	0.093	0.003	13.5	3.2	P 36.5[D2] N 36.5 A 27.0	13.1	17.0	18400.0
Vacuum Gas Oil (650°F-1050°F)	0.2963	27.6	0.24	0.03	12.2	17.8				
Vacuum Bottoms (1050°F +)	0.1285	14.2	0.57	0.102	11.2	26.2				

Crude Oil Data

°API : 32.7

%S : 0.83

%N : 0.023

%H : 12.8[B]

Heat of Combustion : 18270.0[G]

Light End Yield (Vol. Fraction)[H]

Refinery Gas	0.0075
LPG	0.0075
Iso-Butane	0.0050
N-Butane	0.0100
Pentanes	0.0182
	0.0482

CRUDE ASSAY NOTES

(A) The following distribution of nitrogen between the various cuts was used where data on the nitrogen content of the cuts were not available, but the nitrogen content of the crude oil was known. The distribution is expressed as the per cent of total nitrogen in the crude allocated in each cut.

Cut	Nitrogen
Light Straight Run	0.0005
Heavy Naphtha	0.001
Light Kerosene	0.42
Heavy Kerosene	1.57
Vacuum Gas Oil	35.3
Vacuum Bottoms	62.7

The above was derived from a Pullman Kellogg study on nitrogen and sulfur distribution, primarily for Kuwait crude oils. It is consistent with the general correlation presented in Fig. 4.2 of Petroleum Refining - Technology and Economics, by James Gary and Glen Handwerk, Marcel Dekker, Inc., 1975.

(A_1) The weight per cent of nitrogen in the crude oil was assumed to be 0.12 since better data was not available.

(A_2) The weight per cent of nitrogen in the crude oil was back-calculated applying the distribution presented in A above to the assayed nitrogen contents of the heavy fractions.

(B) The hydrogen content has been estimated from figure 2B2.1 (p 2-11) of the Technical Data Book - Petroleum Refining, Americam Petroleum Institute, Division of Refining, 1966, Port City press, Inc., Baltimore, Md. The above mentioned reference gives the carbon to hydrogen weight ratio as a function of API gravity and mean-average boiling point.

(C) Viscosities are reported as a linear viscosity blending index number at 210°F. Exhibit 6 of Volume I (NASA CR-135333) gives conversion of Saybolt Seconds Universal (SSU) or Saybolt Seconds Furol (SSF) to linear viscosity blending number, provided all viscosities are measured at 210°F.

(D) The PNA values for light and heavy kerosene cuts of this crude oil were estimated from PNA values given for heavy naphtha cuts.

(D_1) The PNA values for the heavy kerosene cut was estimated from the given PNA values for light kerosene cut of this crude oil.

(D_2) Estimated based on given aromatic weight per cent, and PNA values given for heavy naphtha cuts.

(E) Freeze point estimated based on the correlation presented in Petroleum Refinery Engineering, by W.L. Nelson, McGraw-hill Book Co., N.Y., 1969, p. 139, Figure 4-41. Freeze point is correlated as a function of K-factor and mid boiling point, where

$$K = \frac{T_B^{1/3}}{S}$$

T_B = mid boiling point in degrees Rankine
S = specific gravity at 60°F

(F) Smoke point estimated based on correlation presented in Petroleum Refinery Engineering, by W.L. Nelson, McGraw-Hill Book Co., N.Y. 1969, p. 82-83, Table 4-1. Smoke point for light kerosene cut is correlated in terms of mid boiling point and K-factor, where K-factor is a defined in E above.

(G) The net heat of combustion was estimated from Figure 14 A1-1 of the Technical Data Book - Petroleum Refining, American Petroleum Institute, Division of Refining, 1966, Port City Press, Inc., Baltimore, Md. The net heat of combustion presented in the above reference is a function of API gravity.

(H) For this crude oil, light ends composition has been estimated. The total light ends yield was obtained from the assay for this crude. The following light ends composition distribution was assumed:

Refinery Gas	25%
LPG	25%
Iso-Butane	17%
N-Butane	33%
	100%

3.0 PROCESS UNIT YIELD DATA

3.1 Shale and Coal Oil Processing Units

Process unit yield data for the hydrotreating of kerosene fractions and the hydrocracking of gas oil derived from shale and coal oil were obtained from the following reports:

(1) Evaluation of Methods to Produce Aviation Turbine Fuels from Synthetic Crude Oils Phase 2 - Exxon Research and Engineering Co., Government Research Laboratory, Linden, N.J. 07036. Technical Report AFALP-TR-75-10-Volume 2, May 1976.

(2) Synthesis and Analysis of Jet Fuel from Shale Oil and Coal Syncrudes. J.P. Gallagher et. al., Harvey Technical Center, Atlantic Richfield Company. Report designation NASA CR-135112, prepared for National Aeronautics and Space Administration, NASA Lewis Research Center Contract NAS 3-19747. November 17, 1976.

All actual and estimated yield and property data for producing jet fuel components from Paraho, Tosco and Garrett shale oils and from Synthoil (from Kentucky Coal) were obtained from the above reports.

3.2 Petroleum Processing Units

Refinery process unit yields and properties for processing petroleum derived fractions were based on data extracted from the following sources:

(1) U.S. Motor Gasoline Economics, Vol. 1 Manufacture of Unleaded Gasoline, June 1, 1967. Prepared for the American Petroleum Institute by Bonner and Moore Associates, Inc. Houston, Texas.

(2) Gordian Associates in-house data based on extensive collective experience in the petroleum refining industry.

4.0 PROPERTIES AND BLENDING CORRELATIONS

The following correlations were used as the basis for the programmed equations contained in the Gordian Refinery Simulation Model. Sources and the equations derived from the correlations are given where applicable.

A. Hydrogen Content (weight percent)

Where hydrogen content for a given stream is not specified as an input or thru a crude oil assay, the following correlation is used:

Figure 2B2.1 (p.211) of the Technical Data Book - Petroleum Refining American Petroleum Institute, Division of Refining, 1966, Port City Press, Inc., in the form of a nomograph which gives carbon to hydrogen ratio as a function of the API gravity and mean average boiling point.

The method used to represent the nomograph in the program was to reduce it to a table of values and to interpolate linearly betweeen adjacent points. Intervals of 5.0 were taken for the API scale and 25 to 50°F for the mean average boiling point scale. This particular nomograph has been widely used in the petroleum refining industry since the 1950's, however, its accuracy is stated as "unknown". On the other hand, generally acceptable hydrogen balances for petroleum based units observed over many model runs are evidence of a "good" correlation. The same, however, was not observed for cuts derived from shale and coal oil when comparing correlation predictions against actual inspection test data from the sources enumerated in Section 3.0. A plot of predicted vs. actual values indicated that the following correlation adjustments be applied.

Shale oil cuts:	Add 0.25 to the predicted C/H ratio
Coal oil cuts:	Add 0.90 to the predicted C/H ratio

While the above adjustments improve the correlation the need for further work is definitely indicated for adequately correlating shale and coal oil hydrogen contents of cut fractions versus their physical properties. The number of comparison points used to develop the above adjustment factors was too limited the correlation variance too great, and furthermore model run results indicate only a "poor" to "fair" accuracy for overall hydrogen balances for the coal and shale oil hydrotreating units.

The carbon to hydrogen ratios predicted for the petroleum, shale and coal oil cut fractions were adjusted for their sulfur and nitrogen contents in calculating a weight percent hydrogen content. In referencing the nomograph correlation in the model, the following mean boiling points were used for the various fractions:

Light Naphtha	175°F
Heavy Naphtha	325°F
Light Kerosene	462°F
Heavy Kerosene	587°F
Gas Oil	850°F
Fluid Cracker Bottoms	1000°F
Coke	1200°F

Hydrogen content is of course blended by volume.

B. Heat of Combustion (Net)

The following correlation was used:

Figure 14A1-1, p.14-3, Technical Data Book - Petroleum Refining American Petroleum Institute, Division of Refining, 1966, Port City Press, Inc., Baltimore, Md.

The following equation was applied to the correlation as recommended on p.14-5:

$$\Delta H = (8505.4 + 846.81K + 114.92G + 0.12186G^2 - 9.9510KG) \times (1.0 - 0.01S) + 40.5\,S$$

where:

ΔH = net heat of combustion in Btu/#
K = Watson characterization factor
G = API gravity
S = Weight % sulfur

Ash and water content have been omitted from the recommended formula since their effect is nil and their exact quantity is generally unknown. The reliability (see p.14-4) is approximately $\pm$ 180 Btu/# between the predicted values and experimental data for petroleum fractions. The same correlation was applied for shale and coal oil liquids.

Heat of combustion is of course blended by weight.

C. Smoke Point

Nelson gives smoke point vs. Watson characterization factor for kerosene range distillates over a wide range of K factors. The reference is:

Petroleum Refining Engineering, W.L. Nelson, McGraw-Hill Book Co., N.Y., 1969, p.82-83, Table 4-1. A plot of 27 data points over the range 11.0 to 12.3 K factor was reduced to the following correlation equations:

K: 12.0 to 12.3
$$SP = 9969.1 - 1691.536K + 71.91K^2$$

K: 11.6 to 12.0
$$SP = 3955.7 - 687.5K + 30.0K^2$$

K: 11.0 to 11.6
$$SP = -309.23 + 47.5K - 1.6667K^2$$

where SP is the smoke point in millimeters and K is the Watson characterization factor

The general accuracy of the Nelson data was not given. In the absence of data for shale and coal oil kerosene cuts, the above formula were applied to petroleum, shale and coal oil kerosenes. The advisability of separate correlations should be investigated as additional shale and coal oil data become available. It is noted however, that the program logic allows crude oil assay data and input values to override correlation prediction - this was done for shale and coal oil kerosenes (and petroleum derived kerosenes) where test data was available.

Smoke point is blended volumetrically by reciprocal blending. The source for this method is a confidential communication from a major oil company. Their laboratory verification of this method stated that "taking the reciprocal was the least inaccurate (method), with 90% of the results deviating by less than 1.0 mm from the determined value".

D. Freezing Point

The freezing point of individual cuts and of blended fuels is a particularly difficult area. Where assay data was available for crude oil cuts and where freezing points were given in conjunction with process unit yields, these were used in the CBASE and UBASE data bases. Where specific data was altogether lacking, freezing point estimation was based on the correlation presented in Petroleum Refinery Engineering, W.L. Nelson, McGraw-Hill Book Co., N.Y., 1969, p.139, Figure 4-41*. However, the use of Nelson's correlation was limited to non-olefinic petroleum fractions and was therefore not applied to fluid coker, visbreaker, thermal cracker and fluid catalytic cracker products. Shale and coal oil cut fractions were based on data values to the extent possible. Also, UBASE was devised so as to apply changes in freezing point against the freezing point of the feed streams in order to tie the product freezing points as much as possible to the original crude oil assays.

The freezing point of the jet fuel and distillate blends is based on the blending index method of E.B. Reid and H.I. Allen, Estimating Pour Points of Petroleum Distillate Blends, Petroleum Refiner Vol. 30, No. 5, May 1951, p.93. This method is based on thermodynamic considerations and gives a volumetric blending index as a function of pour points and

* Freezing point is correlated as a function of the Watson characterization factor and mid-boiling point.

mid-boiling point of the cut being blended. A regression analysis for light and heavy kerosene fractions (462°F and 588°F mid-boiling point) gave the following equations:

light kerosene: $BI = 10^{(0.01653\ P\ +0.9027)}$

heavy kerosene: $BI = 10^{(0.01941P+0.6987)}$

where BI = volumetric blending index and P = pour point (°F)

It was assumed that freezing point blends in the same manner as pour point. Reid and Allen reported good results for their correlation. Out of a total of 90 blends, the pour point was predicted within ± 5°F for over 90 percent of the cases. Blends included were straight run with straight-run stocks and also mixtures of catalytically and thermally cracked stocks. Shale and coal oil fractions were not included in their experimental work.

E. Other Properties

Sulfur content, nitrogen content, PNA and viscosity are based on crude oil assay value and on inspection tests accompanying process unit yield data. Sulfur, nitrogen and PNA (paraffins, naphthenes and aromatics) are all of course blended by volume. Viscosities are blended by the method shown in Exhibit 6 of Volume I of The Gordian Refinery Simulation Model.

5.0 ECONOMIC DATA

The Gordian Refinery Simulation Model performs an economic calculation for the specific refinery configurations under study. The investment costs of the individual refinery process units are calculated and added to give a total refinery "onsites" investment cost. The "offsites" investment for supporting tankage, steam generation and miscellaneous utilities, off-battery-limits piping, sewers and drains and refinery access facilities are calculated as a function of the Nelson Complexity Factor for specified refinery configuration*. The program also calculates the fixed and variable operating cost components for each process unit and gives an overall economic summary based on crude costs and product revenues.

5.1 Capital Investment Costs

The economic subroutine calculates capital investment cost for each of the specified process units. The onsite investment cost of each unit is calculated from the cost of the unit for a standard reference size and a power law factor to reflect the economies of scale. As stated above, the lump sum offsite investment is calculated based on total onsites investment and the Nelson Complexity Factor.

---

* See Oil and Gas Journal, Sept. 28, 1959, p.73 for the method and examples of the calculation of the Nelson Complexity Factor.

5.1.1 Sources of Data

Data for the capital investment calculation was obtained from published sources of information. These sources included articles in the Oil and Gas Journal, Hydrocarbon Processing, and Chemical Engineering. The essential data extracted was an investment figure in dollars per barrel per stream day, a corresponding capacity figure and the point in time at which the cost was valid.

The data on capital investment costs were all referenced to a common Jan. 1, 1977 basis. This was accomplished by making use of the Nelson Refinery Index as a measure of inflation. The Nelson productivity divisor* is used to correct for productivity advances made in construction of refineries. In order to update a capital investment figure from the year "X" to the year "Y", the figure is multiplied by:

$$\frac{\text{Nelson Refinery Index in year "y"}}{\text{Nelson Refinery Index in year "x"}}$$

and divided by the productivity divisor in year y.

The Nelson productivity divisor varies as a function of the type of refinery unit. Where no data was available, a productivity divisor of 1.06 was assumed.

The unit capital investment costs (Jan. 1, 1977 basis) stored in the program Block Data subroutine for the standard unit reference sizes are given below:

---

* See Oil and Gas Journal, March 1, 1976 p. 120-124.

CAPITAL INVESTMENT COSTS (January 1, 1977 basis)

Refinery Unit	Unit Capital Investment Cost ($/bpsd)	Reference Unit Size (bpsd)	Source
Atmospheric Distillation	190	20,000	OGJ, Feb. 25, 1974, p.71
Vacuum Distillation	198	20,000	OGJ, Mar. 4, 1974, p.100
Catalytic Gas Oil Cracker	699	40,000	OGJ, Apr. 15, 1974, p.66
Thermal Gas Oil Cracker	185	20,000	OGJ, Apr. 8, 1974, p. 74
Kerosene Hydtrotreater	122	30,000	HP, September, 1976
Gas Oil Desulfurizer	614	50,000	OGJ, Mar.1, 1976 p. 120
Distillate Desulfurizer	267	30,000	HP, September, 1976
Fluid Coking	770	20,000	OGJ, May 24, 1976
Vacuum Bottoms Visbreaker	185	20,000	OGJ, Apr. 8, 1974
Distillate Hydrocracker	747	15,000	HP, September, 1974
Gas Oil Hydrocracker	904	20,000	OGJ, Mar. 25, 1974 p. 120
Catalytic Naphtha Reformer	543	20,000	OGJ, Apr. 22, 1974 p. 130
Alkylation	1193	10,000	OGJ, Apr. 8, 1974 p. 74
Polymerization	800	500	"Gordian Estimate"
Isomerization	222	6,650	HP, September, 1974
Hydrogen Manufacture	170/mscfd	50 mmscfd	OGJ, Mar. 25, 1974 p. 120

Note: Alkylation unit investment is in dollars per barrel per day of total alkylate production, polymerization unit investment is in dollars per barrel per day of polymer product and hydrogen plant investment is in dollars per thousand standard cubic feet per day of hydrogen make. All other costs are in dollars per barrels per day of feed stream.

5.1.2 Accounting for Economics of Scale

The following power law formula is used in the model to account for the economics of scale:

$$\text{Capital Investment Cost} = \left(\frac{\text{capacity of process unit}}{\text{Standard reference capacity}}\right)^{N} \times \text{(Investment at Standard reference capacity)}$$

In the above equation, N represents the capacity ratio exponent. For values of N below 1.0 economies of scale exist. The values of N extracted from the literature are listed on the following page along with an average value of the exponent which corresponds to the number used in the program and stored in the Block Data subroutine. The standard reference capacities and the corresponding capital investments used stored in the program are those listed under Section 5.1.1.

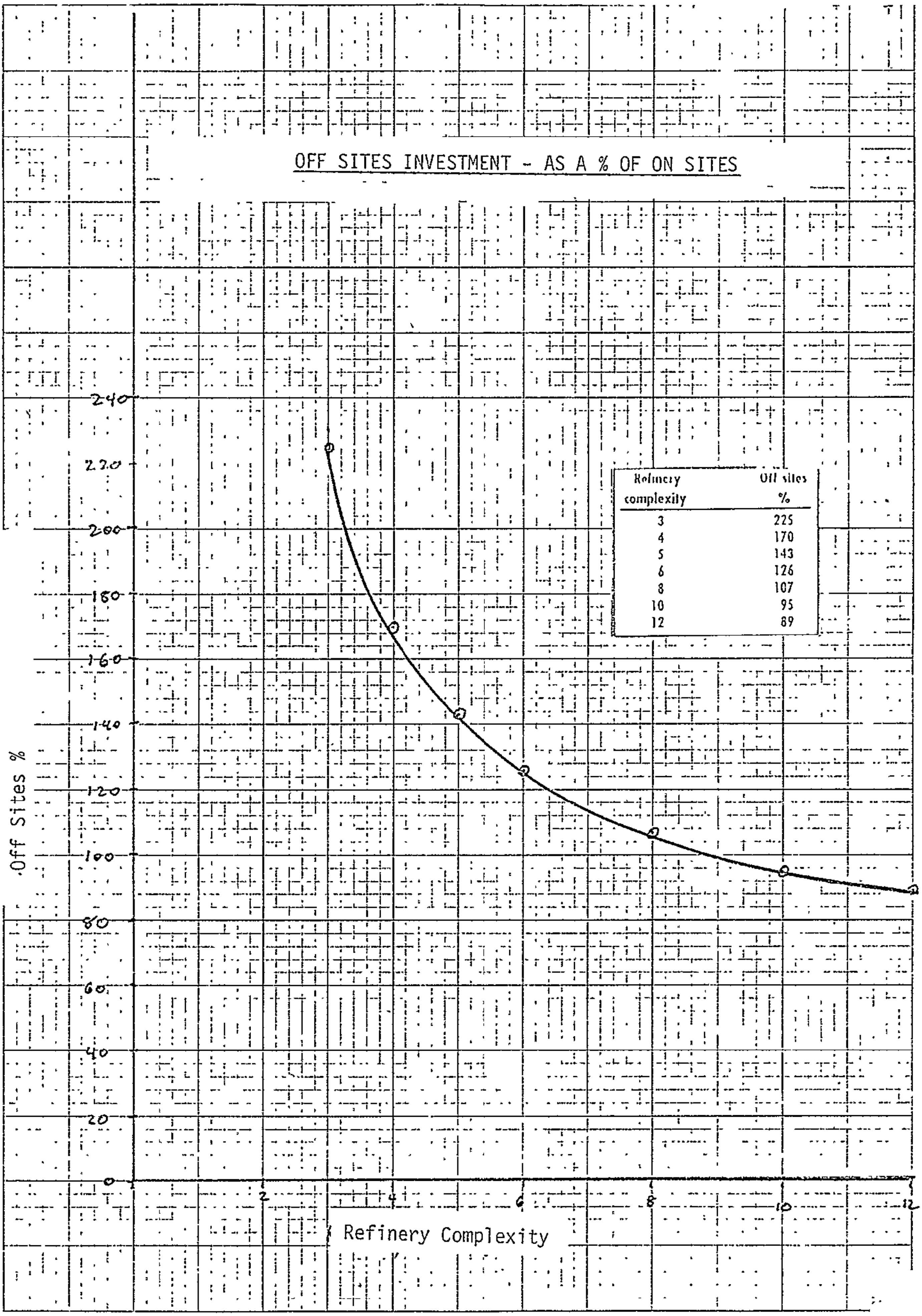
5.1.3 Total Refinery Capital Investment Cost

The total refinery onsite capital investment cost is the sum of the process unit capital costs adjusted for capacity utilization. Since plant capacities are input into the model in units of barrels per calendar day (BPCD), it is necessary to increase the unit capacities to reflect planned maintenance periods and unscheduled unit shutdowns. A 92% operating rate is assumed in the program, but this may be modified by input. The offsites capital investment are then calculated as a percentage of the total shown in Exhibit 1.

Refinery Unit	Capacity Ratio Exponent			
	Hydrocarbon Processing (May, 1975 p.111)	Chemical Engineering (June 15, 1970)	OGJ (see section 5.1.1)	Average*
Atmospheric Distillation	0.70-0.85	0.90	0.77	0.805
Vacuum Distillation	0.70	0.70	0.75	0.717
Catalytic Gas Oil Cracker	0.70	0.55	0.86	0.703
Thermal Gas Oil Cracker		0.70		0.700
Kerosene Hydrotreater		0.65		0.650
Gas Oil Desulfurizer	0.80			0.800
Distillate Desulfurizer	0.65-0.85			0.750
Fluid Coking			0.72	0.720
Vacuum Bottoms Visbreaker		0.65	0.620	0.635
Distillate Hydrocracker	0.75			0.750
Gas Oil Hydrocracker			0.75	0.750
Catalytic Naphtha Reformer	0.70-0.85	0.61	0.80	0.740
Alkylation		0.60	0.60	0.600
Polymerization			0.58	0.580
Isomerization			0.66	0.660
Hydrogen Manufacture	0.65-0.70		0.70	0.680

* The same exponents are assumed for processing shale and coal oil kerosene and gas oil cuts.

EXHIBIT 2



Refinery complexity	Off sites %
3	225
4	170
5	143
6	126
8	107
10	95
12	89

Source: Oil and Gas Journal, July 22, 1974.

5.2 Operating Costs

The economic subroutine calculates the operating costs for the specified refinery configuration. The operating costs are divided into fixed and variable cost components. The cost of electric power is calculated separately. The cost of fuel and steam are not included as a cost item since they are accounted for by the purchase of raw material required to produce the fuel gas and oil consumed by the various refinery processes.

5.2.1 Variable Operating Costs

The variable operating costs include the cost of catalysts, chemicals and water. The process unit consumption data for this section was collected from the following sources:

Chemicals and Catalyst	-	A Guide to Refinery Operating Costs, by W.L. Nelson, Petroleum Publishing Co.,1976
Water	-	The Oil and Gas Journal, June 14, 1976 p.74

The catalyst and chemicals cost figures are in units of cost per barrel of throughput. In order to update the chemicals and catalysts cost, the Nelson-Chemicals Index* was applied to place chemicals and catalysts costs used in the model on a Jan. 1, 1977 basis. Water costs were based on an average reported consumption (gal/barrel), at a unit cost assumed to be $0.05/1000 gals.

The total variable operating costs used in the model (chemicals, catalyst, and water) are shown below:

---

* See Oil and Gas Journal, April 11, 1976 p. 60-61.

Unit	Variable Cost ($/Bbl)
Atmospheric Distillation	0.015
Vacuum Distillation	0.019
Catalytic Gas Oil Cracker	0.074
Thermal Gas Oil Cracker	0.071
Kerosene Hydrotreater	0.200 (assumed for shale and coal oil)
Gas Oil Desulfurizer	0.115
Distillate Desulfurizer	0.115
Fluid Coking	0.029
Vacuum Bottoms Visbreaker	0.022
Distillate Hydrocracker	0.423
Gas Oil Hydrocracker	0.423 (assumed the same for shale and coal oil)
Catalytic Naphtha Reformer	0.183
Alkylation	0.990
Polymerization	0.274
Isomerization	0.043
Hydrogen Manufacture	0.097 ($/mscf)

5.2.2 Fixed Operating Costs

The fixed operating costs include labor and process unit maintenance costs. Labor costs are assumed to be independent of throughput. Units are assumed to operate on a 24 hour per day basis. Labor use (men per shift) estimates were obtained from A Guide to Refinery Operating Costs, by W.L. Nelson, Petroleum Publishing Company, 1976. Labor rates used were: operators - $10.00/hr, supervisors - $12.50/hr. In each case the labor are inclusive of benefits.

Maintenance costs are given as a per cent of the onsite unit capital investment cost. The program utilizes these maintenance factors to calculate the maintenance cost in dollars per day. The maintenance and labor cost numbers used by the program and contained in subroutine Block Data are listed below:

Unit	Labor Cost ($/day)	Maintenance (% Capital Investment Per Annum)
Atmospheric Distillation	806.	4.0
Vacuum Distillation	1002.	3.5
Catalytic Gas Oil Cracker	1545.	4.0
Thermal Gas Oil Cracker	1245.	5.5
Kerosene Hydrotreater	720.*	4.0
Gas Oil Desulfurizer	720.	4.0
Distillate Desulfurizer	720.	4.0
Fluid Coking	1485.	5.5
Vacuum Bottoms Visbreaker	1059.	4.3
Distillate Hydrocracker	1065.*	4.0
Gas Oil Hydrocracker	1065.	4.0
Catalytic Naphtha Reformer	1012.	4.0
Alkylation	1050.	5.5
Polymerization	505.	4.3
Isomerization	1440.	3.5
Hydrogen Manufacture	585.	3.5

5.2.3 Electric Power Costs

Electric power usage for the total refinery is calculated by the model and reported in thousands of kilowatt hours per day. The cost of electric power (in costs per kilowatt hour) is an input data item since it varies between refining situations. In the absence of specific information, a cost of $2.14¢/kWh is recommended. The average cost of power among the "Large Light and Power Class" users is 1.92¢/kWh as obtained from The Statistical Year Book of The Electric Utility Industry, The Edison Electric Institute, NYC, for 1975. Updating this to a January 1, 1977 basis by using the Nelson Industrial Electric Power Index gives a current value of 2.14¢/kWh.

---

* Assumed to be the same for shale and coal oil processing units.

5.3 Summary Economic Calculation

When selecting the option to calculate refinery economics, the user must input values for the delivered cost of crude oils and product realizations - the latter should be refinery netback prices, exclusive of transportation costs from refinery to points of sale. The user must also specify an investment carrying charge to include interest, taxes and a suitable rate of return.

6.0 CONCLUDING REMARKS

This report has presented crude assay data, property and blending data, and economic unit costs and other data for use as bases in The Gordian Refinery Simulation Model. The report is Volume II of three volumes covering the description, application, and documentation of the refinery calculation program. This volume is, however, independent of the other volumes. The information represents a compilation of current data, and correlations can be used for jet fuel production and blending calculations with reference to the Gordian program.

Volume III (NASA CR-135335), covering the program listing and other documentation, is available from the NASA Project Manager. Computer documentation and tapes can be purchased through the Computer Software and Management Information Office (COSMIC), 112 Barrow Hall, University of Georgia, Athens, GA 30602, under the number LEW-13047.