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Regional Refining Models for Alternative Fuels Using Shale and Coal Synthetic Crudes

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Annual Report for period 20 March 1979 to 19 March 1980 for the Project
Identification and Evaluation of Optimized Alternative Fuels

Alternative Fuels Utilization Program

November, 1980

Prepared For

U.S. Department of Energy

Assistant Secretary for Conservation and Solar Energy

Office of Transportation Programs

Under Contract No. AC01-79CS-50017

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Prepared For

**U.S. Department of Energy
Assistant Secretary for Conservation and Solar Energy
Office of Transportation Programs
Washington D.C. 20585**

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FOREWORD

The work reported herein was performed under Department of Energy Contract No. DE-AC01-79CS-50017. Southwest Research Institute, San Antonio, Texas, was the prime contractor. Subcontractors were Bonner & Moore Associates, Inc., Houston, Texas and The Standard Oil Company of Ohio, Technology and Planning Department, Cleveland, Ohio. The contract was administered by the Office of Procurement Operations, Washington, D.C. Technical Project Manager was Dr. Ralph D. Fleming, Alternative Fuels Utilization Branch at DOE Headquarters.

ABSTRACT

The initial phase has been completed in the project to evaluate alternative fuels for highway transportation from synthetic crudes. Three refinery models were developed for Rocky Mountain, Mid-Continent and Great Lakes regions to make future product volumes and qualities forecast for 1995.

Projected quantities of shale oil and coal oil syncrudes were introduced into the raw materials slate. Product slate was then varied from conventional products to evaluate maximum diesel fuel and broadcut fuel in all regions. Gasoline supplement options were evaluated in one region for 10 percent each of methanol, ethanol, MTBE or synthetic naphtha in the blends along with syncrude components.

Compositions and qualities of the fuels were determined for the variation in constraints and conditions established for the study. Effects on raw materials, energy consumption and investment costs were reported. Results provide the basis to formulate fuels for laboratory and engine evaluation in future phases of the project.

ACKNOWLEDGMENTS

Meeting the objectives in the first year of the project required the efforts of many participants. The co-authors, Allen Mesch, Joe Dickson and Frank Frederick of Bonner & Moore contributed to the planning and design of the case studies as well as the execution and documentation of computer runs. Robert Rightmire and Warren Wotring of SOHIO helped get the project off to a good start and contributed advice and data as needed throughout.

Thanks are extended to many SwRI staff members: To John Russell who originated the project, provided guidance to keep it on track, and authored sections of the report. To Brent Bailey for data handling and computer graphics. To Jim Pryor for editorial advice. To Myrtie Santee, Gladys Tate and Judy Brandle who persevered through typing multiple drafts to produce an eminently readable report.

The use of facilities and technical support from the U.S. Army Fuels and Lubricants Research Laboratory at Southwest Research Institute is appreciated. Analytical work was done with the concurrence of the U.S. Army Mobility Equipment Research and Development Command (MERADCOM).

Norman R. Sefer
Principal Investigator
Southwest Research Institute

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SUMMARY

Southwest Research Institute has completed the initial phase of the project to identify and evaluate alternative fuels for future highway transportation. Bonner & Moore Associates provided a substantial portion of the synfuels optimization phase in using their Refinery and Petrochemical Modeling System (RPMS) to construct regional refinery models for a series of computer case study evaluations.

Description

The studies show how shale oil and coal oil may be used in a given processing scheme along with petroleum crudes to make specification products. Volumes of 300,000 B/D shale oil and 200,000 B/D coal oil were forecast to be available in 1995. Refineries in the Rocky Mountain, Mid-Continent or Great Lakes regions are expected to receive these syncrudes because of their location near production or transportation systems.

Forecasts of 1995 crude supply and product demand reflect regional differences in raw materials, product slate and product specifications. Composite refinery models were constructed using known 1979 configurations; facilities additions needed to make 1995 products were defined by the model in the base case for each region.

Because crude processing capacity is different in the three regions, inclusion of the projected volume of syncrudes in the crude slate resulted in different proportions in each region (conventional product cases shown):

	% of Total Raw Materials	
	Shale Oil 300,000 B/D	Coal Oil 200,000 B/D
Rocky Mountains	34.1	23.4
Mid-Continent	17.3	11.5
Great Lakes	9.4	6.2

Shale oil and coal were processed separately in Rocky Mountain cases; they were charged simultaneously in the other regions but fractions were segregated for independent identity through processing and blending. The processing scheme applied hydrogenation pretreatment to both shale oils and one of three coal oils before distillation. Fractions from distillation were then further hydrotreated except for light naphtha and the residual streams.

Computer runs optimized many factors within the refinery, including a balance of cost effects. For example, the prescribed products were made with minimum raw materials, thereby controlling the major refinery cost. New facilities were provided only as needed since their investment cost (annualized) and operating costs are included in the total costs. Catalytic reforming octane level was balanced against yield loss. Certain feedstocks could bypass some operations if not needed for quality improvements. Finally, all components were blended in the best combinations to meet product specifications.

Product options were evaluated in all three regions to study the effect of varying product types, including:

- Conventional products, 1995 forecast demand.
- Maximum diesel fuel, replacing 30 percent of gasoline.
- Broadcut fuel, replacing 40 percent of gasoline.

Broadcut fuel is a wide boiling range product, blended with components of both gasoline and diesel fuel, for use in advanced or modified engines which could be available in 1995. It is an example of fuels which require less processing than current motor fuels.

Gasoline supplements were evaluated in conjunction with shale and coal oils in the Rocky Mountain cases. Concentration of 10 volume percent of the following was used:

- Methanol
- Ethanol
- MTBE
- Synthetic naphtha from methanol

Conclusions

The refinery models demonstrated the changes in operation and products when shale and coal oil are included in the crude slate. Compositions determined for highway transportation fuels will be used to prepare test fuels for evaluation in the next phase of the project.

Each barrel of shale or coal oil replaced 0.95 or 1.03 barrels of petroleum new material, respectively. Investment cost and energy consumption increased for both syncrudes, but more so for shale oil because it received more processing. Heavy fractions of coal oil went directly to No. 6 fuel oil because of properties less desirable in downstream processing.

Increasing diesel fuel production to the near-maximum level saved raw materials, partly by reducing product quantity because of better fuel economy for diesel. Other savings resulted from lower processing energy, except in one case where it increased because total distillate production was excessive.

Broadcut fuel production also saved raw materials. Product quantity savings were less than diesel fuel because fuel economy is between gasoline and diesel fuel. However, processing savings are larger than diesel fuel so the net effect on raw materials is similar for either product option.

Broadcut fuel supply could be expanded while diesel fuel was near its limit in the maximum diesel cases. Broadcut fuel offers substantial savings in investment costs with syncrudes or with petroleum. Early development of engines to use broadcut fuel (or any fuel requiring less processing) is desirable to avoid building facilities to make conventional fuels.

Methanol, ethanol, MTBE and synthetic naphtha all saved varying amounts of raw materials and energy consumption, although raw materials and energy used to make these supplements were not included.

I. INTRODUCTION

A. Background

Early in 1976, Southwest Research Institute completed a survey study (1)* which provided an assessment of the impact of coal and oil shale derived crudes upon the composition of gasoline. The interplay between petroleum, coal, and shale resources involved in optimum utilization of U.S. fossil resources was recognized and emphasized by all Federal and private organizations contacted. In that same year, a much more comprehensive study (2) was initiated to:

- a. serve as a reference text for candidate conversion processes to derive liquid hydrocarbon and methanol fuels from coal or oil shale, and,
- b. develop a methodology for projecting the compositions of these fuels in order to provide a means for estimation of energy consumption, environmental effects, and economic factors.

In April 1978, The Department of Energy (DOE) published the Alternative Fuels Utilization Program (AFUP) Planning Document (3) wherein the basic AFUP goal was identified, "to foster the use of alternative fuels by lowering the uncertainty costs associated with their use in highway vehicle systems." Uncertainty costs were taken to include direct dollar costs, social costs, and information costs. Consequently, a lowering of these items would most certainly require identification of optimum resource utilization, minimum pretreatment and refinery energy expenditure, and maximum fuel economy. With these criteria, together with identified linear programming methodology (2) and an increasing knowledge of the compositional aspects of coal- and shale-derived liquids, this present study was formulated to establish a viable systems engineering approach which can be continuously updated as new laboratory and refining data are acquired.

In October 1978 (immediately prior to the initiation of this contract), a conference (4) on "Composition of Transportation Synfuels: R&D Needs, Strategies and Actions" served to define further the areas where data could be applied to an optimization study. In parallel with this activity, DOE-AFUP had been devising a detailed Project Planning Document (5) and an Alcohol Fuels Program Plan (6) which identified AFUP focus and scope together with a project activity policy emphasizing a broad-to-narrow approach. This present study was devised and timed to be compatible with these AFUP policies and goals.

B. Objectives.

This report describes work accomplished in the first year of a 3-year, 4-task program intended to:

- Define chemical compositions and physical properties of alternative fuels derived from petroleum, coal, and shale oils.

* Underlined numbers in parentheses designate references at the end of each section.

- Formulate, blend, and produce R&D-scale quantities of prototype synthetic fuels.
- Identify problems associated with the use of these alternative fuels in conventional and advanced engine.
- Characterize promising fuel/engine combinations for minimum energy consumption in highway vehicles systems.

C. Organization and Approach

The four principal project activities (Tasks) into which work has been categorized are:

- Task 1: Synfuels Optimization-application of linear programming techniques in a variety of scenarios to define chemical and physical characteristics of alternative transportation fuel optimized for minimum costs to satisfy product demands.
- Task 2: Synfuels Formulation for Experimental Evaluation-formulation and preparation of experimental batches of prototype synthetic fuels for use in bench test and internal combustion engine evaluations. These fuel formulations will have been based upon but not limited to results developed in Task 1.
- Task 3: Synfuels Formulation for Other Researchers-formulation, blending, and distribution of R&D-scale quantities of prototype synfuels as defined in Task 2 for use in laboratories other than SwRI who have programs and/or facilities in which testing of these synfuels will provide data relevant to the DOE Alternative Fuels Utilization Program.
- Task 4: Synfuels Performance Evaluation-bench test and engine evaluations using SwRI facilities to screen and evaluate prototype synfuels to provide feedback information to the database established in Task 1 for further modification and refinement of linear programming modeling criteria.

D. Status

This first year's activities reported herein have entailed work solely on Task 1: Synfuels Optimization. Central to this effort has been the application of the Refinery and Petrochemical Modeling Systems (RPMS) developed by Bonner & Moore Associates, Houston, Texas, who have served as principal subcontractor. Proper utilization of RPMS for this projective study required the expansion of an existing database on syncrude compositions and properties to include those from the most current known candidate processes for both coal- and shale-derived crudes. After this expansion, it was necessary to install quantitative data for syncrude hydrotreating pretreatment for sulfur and nitrogen removal as needed for these crudes to be processes by conventional refineries.

Changes were made from the preceding study (2), where quantity of coal- or shale-derived crude to a single refinery configuration was modeled

as a timewise step function with increasing ratio of syncrude-to-petroleum crude in 5-year increments from 1985-2000. Modeling for this present study differs from the earlier one in that three separate regions (Rocky Mountain, Mid-Continent, and Great Lakes) have been established with a composite refinery configuration for each region extrapolated to the year 1995. Product slates have been forecast starting with gasoline-dominant. Then diesel-penetration and wide boiling range fuel-penetration variations are presumed. The concept of a wide boiling range fuel has been defined more precisely. As a corollary activity, RPMS modeling included an alcohol/ether fuel blending option so that selected blending components could be incorporated as octane improvers and finished gasoline supplements.

The main intent is to generate a comprehensive collection of formulations of such fuels which would then provide the basis for blending and laboratory and engine tests. The 4-task organization of this present program, together with the modular activities just described, is shown schematically in Figure 1.1.

Future work will emphasize the physical aspects of this program including actual formulation and blending (Tasks 2 and 3), experimental evaluation (Task 4), plus the initial stages of a repository function in which SwRI will be a technical clearing house for AFUP-related synfuels data exchange and storage. In this last activity (emphasizing Task 3), R&D-scale quantities of available prototype synfuels will commence to be furnished to other laboratories as described above with the understanding that data derived from these materials will be furnished to DOE, or to SwRI as their designated representative, for summarization and correlation.

E. Report Structure

The summary of the report is found in the section just preceding this Introduction. Following the Introduction are seven other sections which proceed from the general outline to more specific descriptions of the project work. The sections also approximate the chronological sequence of project activities from planning through execution to evaluation of results and future plans as indicated in the following paragraphs:

- Section II, Development of Scenarios, establishes the general plan for case studies considering major factors of time, location and syncrude quantities. The variations in product demand and gasoline supplement options provide the basis for a schedule of twenty-six cases to run.
- Section III, Fuels Production Model, describes the modeling system and development of three regional models and product forecasts for 1995. Details of modeling are discussed along with computer results for three regional base cases.
- Section IV, Syncrude Processing, defines the selection of shale oils and coal oils along with their processing scheme and key data for use in the models.
- Section V, Gasoline Supplements, discusses the four components to be used in gasoline and their incorporation into the models.

FIGURE 1.1 IDENTIFICATION, FORMULATION AND EVALUATION OF ALTERNATIVE HIGHWAY TRANSPORTATION FUELS

- Section VI, Results and Discussion, presents summaries of results and then examines specific area in more detail on products, raw materials, energy consumption and investment costs. The numerous tables and figures are arranged by category in groups for all three regions.
- Section VII, Conclusions, analyzes results in several areas to compare impacts of the major variables on the fuel, inputs and processing.
- Section VIII, Future Work, outlines the application of results to succeeding project phases of fuels formulation and testing.
- The Appendix contains a list of acronyms and abbreviations, with a brief definition where needed.

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2. Southwest Research Institute, "Identification of Probable Automotive Fuels Composition: 1985-2000," U.S. Department of Energy Report No. HCP/W3684-01/1, UC-96, May 1978.
3. "Program Planning Document, Highway Vehicle Alternative Fuels Utilization Program (AFUP)," U.S. Department of Energy Report No. DOE/CS-0029, UC-96, April 1978.
4. "Composition of Transportation Synfuels: R&D Needs, Strategies and Actions (Conference Proceedings)," DOE Report No. CONF-7810176, June 1979.
5. "Project Planning Document, Highway vehicle Alternative Fuels Utilization Program (AFUP)," U.S. Department of Energy Report No. DOE/CS-0093, UC-96, July 1979.
6. "Alcohol Fuels Program Plan," U.S. Department of Energy Report No. DOE/US-0001/2, March 1978.

II. DEVELOPMENT OF SCENARIOS

This section describes the planning to make the study a realistic representation of probable future developments. It also establishes the framework for the optimization cases.

A. Time

Predictions were developed for the year 1995. Substantial shale oil and coal oil production is expected by that date. In the 15 years between now and then, there will be time for assumed changes in engine types to have significant effects on the vehicle population.

B. Location

Syncrudes are expected to have major impact in the inland states. The East, West, and Gulf Coasts regions are reasonably well supplied with crude oils from other sources and are not accessible by existing pipelines from the source of western shale oils in Colorado, Utah and Wyoming. Gulf Coast refining capacity is about 40% of the U.S. total and the projected syncrude volume would have minor impact on products in that region. Source of coal syncrudes is more difficult to predict but coal resources are available in all three regions defined for the study as well as the Gulf and East Coasts.

Regional definitions were developed considering the following factors:

- Processing plants near source of production or served by available pipelines or other bulk transportation.
- Areas of common product quality and similar production objectives.
- Availability of data on crude supply, product demand, and transfers of crude and products across regional boundaries.

The regions selected for the study are shown on the map on Figure 2.1 and include the following states:

<u>Rocky Mountains</u>	<u>Mid-Continent</u>	<u>Great Lakes</u>
Colorado	Arkansas	Illinois
Montana	Kansas	Indiana
New Mexico	Missouri	Kentucky
Utah	Oklahoma	Michigan
Wyoming	Texas (North of Dallas-Ft. Worth)	Minnesota
		Ohio
		Wisconsin

C. Syncrude Availability

A forecast of 300,000 B/D shale oil production in 1995 was derived from a study by J.S. Hutchins, "Oil Shale 1979 and the \$3 Tax Credit",

FIGURE 2.1 REGIONS FOR COMPOSITE FUELS PRODUCTION MODELS

presented at the Twelfth Oil Shale Symposium, Golden, Colorado in April, 1979. This forecast considered economic, environmental and technological factors and concluded that some modest economic incentive was necessary to have any shale oil production. An article in the Wall Street Journal of August 16, 1979 reported that 200,000 B/D by the early 1990's was considered both feasible and probable.

Similar forecasts were not available for coal liquids. However, coal has the same obstacles to overcome in economics, environment, and technology. Since coal oil development was behind shale oil and costs were somewhat higher, a forecast of 200,000 B/D coal liquids appeared to be a reasonable basis. (Coal oil is used in this report for liquids derived from coal. The term was adopted by API in 1966 and no longer applies to kerosene from petroleum.)

Since the time these forecasts were made, some national objectives have been revised as a result of changes in international relations and imported crude supply patterns. Federal incentives have been provided to encourage process development and syncrude production from shale and coal. Total volumes as high as 2,500,000 B/D of syncrudes have been proposed, although that level may not be possible to attain in the next 10 to 15 years.

The subject project considered 500,000 B/D synthetic crudes in each of three regions. This may be interpreted as a total 1,500,000 B/D in all three regions to make results more consistent with future possible developments.

D. Product Options

Baseline projections were planned for each region to set 1995 product demand assuming conventional crudes and products. Syncrudes then would be added to replace a portion of the raw material supply. Product variations which were to be evaluated in each region include:

- Conventional products
- Maximum diesel fuel (limit set by refinery parameters)
- Maximum broadcast fuel (limit related to engine availability)

E. Gasoline Supplement Options

Four blending components were selected for use in the study. These are:

- Methanol
- Ethanol
- Methyl-tertiary-butyl ether (MTBE)
- Synthetic naphtha from methanol

These are materials with potential for usage in all regions and with adequate literature data for evaluation. Other similar components may be limited in supply or distribution or were lacking in data availability.

F. Case Study Schedule

Table 2.1 presents the final schedule of cases included in the study for all regions.

The plan allows the evaluation of varying from conventional product demand to maximum diesel and broadcut fuels with shale and coal oils in all three regions. The four gasoline supplements are used in the Rocky Mountain Region where synthetic crudes are at the highest concentration in plant charge. Broadcut fuels are evaluated with petroleum as well as synthetic crudes in all regions.

A brief description of the cases is given near the beginning of Section VI, to supplement the Table 2.1 Schedule.

G. Projection of New Engine Penetration

A projection of potential market penetration by new engine types was needed to establish a maximum level of product demand for diesel and broadcut fuels that could be forecast for 1995.

A convenient relationship between vehicle age and vehicle miles traveled (VMT) has been published by DOE (1):

<u>Vehicle Age, Years</u>	<u>% of Total VMT</u>
1	17.1
2	14.3
3	12.6
4	11.1
5	10.0
6	8.8
7	7.4
8	5.8
9	4.4
10	3.0
11+	5.5

Assumptions of rate of introduction of new vehicles or engines then can be used to generate a curve of VMT which is directly related to market penetration. For example, if a new vehicle accounts for 10% of sales in the first year, 20% of sales in the second year and on to 100% of sales in the tenth year, a curve as in Figure 2.2 is obtained.

TABLE 2.1 PROJECT CASE STUDY SCHEDULE

	ROCKY MOUNTAIN REGION																MID-CONTINENT & GREAT LAKES (Separate)				
Case No.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	1	2	3	4	5
Crudes																					
Petroleum	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
Shale Oil		X	X	X				X	X	X	X							X	X	X	
Coal Oil					X	X	X					X	X	X	X			X	X	X	
Fuel Types																					
Conventional	X	X			X			X	X	X	X	X	X	X	X		X	X			
Max Diesel			X			X													X		
Broadcut				X			X								X				X	X	
Blend Components																					
Methanol								X				X									
Ethanol									X				X								
MTBE										X				X							
Synthetic Naphtha											X				X						

FIG. 2.2 PER CENT VEHICLE MILES -NEW CARS

Using a new vehicle factor of 6% in the above relationship produces a more conservative projection also plotted on Figure 2.2. The percentage of total VMT for two factors at 5-year intervals is:

<u>Year</u>	<u>Percentage of Total VMT</u>	
	<u>10% Factor</u>	<u>6% Factor</u>
5	21.3	12.8
10	64.1	38.5
15	92.8	55.7
20	100.0	60.0

Market penetration of vehicles with engines capable of using broadcast fuels was projected on the following schedule. Engine development would proceed on Stirling, turbine or a suitable internal combustion engine which would be introduced in the 1985 model year. If used in 6% of new vehicles that year and an additional 6% each following year, the new engine would account for 38.5% of total VMT in ten years. Although somewhat hypothetical, this derivation provides a reasonable basis for the potential 40% of the vehicle population with the new type engine in the 1995 broadcast fuel cases.

Predictions have been made of diesel engine sales as part of fuel forecasts. DuPont estimated 5% of all cars and light trucks sold in 1985 would be diesel-powered.(2) A sensitivity analysis allowed this value to go as high as 25%. A forecast from Ethyl Corporation (3) estimated diesel sales to 1993. A moderate extrapolation of their schedule to 1995 and use of the VMT relationship described above gives a projection of diesel automobiles and light trucks in the total vehicle population, as follows:

<u>Year</u>	<u>Diesel as Share of Car Market, % (3)</u>	<u>Diesel Vehicles on Road,% (est.)</u>
1980	1.0	0.2
1985	6.0	2.9
1990	11.3	7.5
1993	14.7	10.7
1995	17.1(Est.)	12.9

This estimate of 12.9% diesels in the 1995 light vehicle population would apply to the baseline prediction for that year. The percentage of diesels could increase more rapidly than these projections because of enthusiastic acceptance by the public and the desire to improve fuel economy for resource conservation. Maximizing diesel fuel in this study was desirable to facilitate measuring the effects with synthetic crudes. Other studies have shown that the diesel fuel population will probably be limited by capability of refineries to increase diesel fuel production. Therefore, a definition was needed for a reasonable maximum level of diesel fuel production.

A study by Bonner & Moore concluded that a maximum of about 60% of total motor fuel could be supplied as diesel fuel.(4) About half of this

amount was "new" diesel fuel produced as an increment over the baseline projection. The limiting quantity was the amount of diesel components present in the crude plus diesel components produced by conversion processes with present technology while meeting other products demands. At that point the ratio of gasoline to total distillate was 0.54.

Amoco investigated the economics of increasing diesel fuel while decreasing gasoline production.(5) They found that about 30% of total motor fuel could be supplied as diesel fuel with existing technology without unusual problems. An additional increment of diesel fuel was provided for off-highway use, amounting to about 8% of total motor fuel. A more recent study was made to update and expand the previous work.(6) Product slates were forecast for 1995 and proportions of gasoline and diesel fuel were varied. Maximum diesel fuel production was at 0.7 ratio of gasoline to total distillate. The conclusion was that additional diesel fuel amounting to about 30% of total motor fuel could be produced and, in fact, was the optimum production level to maximize transportation miles per barrel of crude (along with an optimum gasoline octane level).

A similar study was made by Exxon in the 1990-2000 time frame. (9) Maximum savings in refining cost and energy usage occurred when diesel fuel was increased from the 10% level to 46-55% of total automotive fuel, equivalent to about 0.66 to 0.49 gasoline to total distillate ratio. Higher levels of diesel fuel were made at increasing cost to a maximum feasible 73% of transportation fuel or 0.30 gasoline to distillate ratio.

Based on the above four studies, it was concluded for the 1995 maximum diesel cases that the equivalent of 30% of the vehicle population could be shifted from gasoline to diesel fuel. Stated another way, this assumes that an additional 30% of the vehicles on the road in 1995 were produced with diesel engines instead of gasoline engines.

An additional correction was applied on product volumes to adjust for the difference in average fuel economy of the vehicles with different engine types. Data were available on an equivalent ratio of engine power to vehicle weight which stated a 35-39% increase in miles per gallon for diesel over gasoline.(7) Another source reported that a diesel engine gives 36% better MPG at the same horsepower and inertia weight.(8) A factor of 35% was selected for use in the maximum diesel cases, although a diesel engine at this economy level may not assure the same acceleration performance. More precisely, the volume of gasoline replaced was multiplied by 1.00/1.35 or 0.7407 to arrive at the equivalent volume of diesel fuel. In effect, this method assumes a constant number of miles driven with motor fuel production in each regional series of cases.

A similar adjustment was made for broadcast fuel. Efficiency of a future turbine, Stirling or spark-assisted diesel engine should approach that of a diesel engine. However, average fuel economy would be about 92% of the diesel because of lower BTU content of the broadcast fuel. Therefore, the broadcast fuel would obtain 24% more miles per gallon than gasoline. Gasoline volume displaced was multiplied by 1.00/1.24 or 0.8065 to determine the equivalent volume of broadcast fuel.

A summary of the product volumes for maximum diesel and broadcast fuel cases is given on Table 3.13 in the following section.

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III. FUELS PRODUCTION MODELS

With the scenario framework and the case study outline from the preceding section completed, the next task was development of fuels production models. The principal methodology for this effort was the Refinery and Petrochemical Modeling System (RPMS) developed by Bonner & Moore Associates of Houston, Texas. This system has an extensive data base which facilitates building refinery models. This section describes the basis for construction of the models to represent the refining industry in each region which will be likely to process syncrudes in the future. The development is outlined through the running of three regional base cases for 1995 operation.

A. The Refinery and Petrochemical Modeling System

The RPMS is a computer-based management tool. Consisting of both processors and extensive data libraries, the system permits the rapid construction and solution of linear programming models to address complex economic analysis and planning problems within the refining and petrochemical industries.

It is necessary to understand that RPMS is not a model. It is a system for the creation, validation, documentation and use of models. It accepts technology-oriented statements, logical requests and data tabulations and converts these into a Linear Programming (LP) matrix and reports. The user may supply data explicitly, or the system may retrieve data from any of several data bases or libraries.

RPMS is not an optimization program. Rather its function is the generation of models for optimization and associated reports. It requires the support of a mathematical programming system in order to perform the actual model optimization.

Finally, RPMS is not a matrix generation and reporting language. Most of the RPMS programs are written in the Bonner & Moore GAMMA language for matrix generation and reporting. The library files are also in GAMMA format. RPMS is a higher-level system using GAMMA to collect the data and to program the modeling and data-handling techniques appropriate to the refining and petrochemical industries.

The DATA Component. The heart of the basic system is the DATA processor. This program receives the user input data (in the form of GAMMA tables and lists) specifying the characteristics of the model to be constructed. After analyzing the content of this input, the program selectively retrieves from user and system libraries the additional data needed to support the user's modeling requests. All of the data analyses and calculations required for generation of the matrix are then performed by the DATA program itself.

The CHEK Component. The CHEK (check) program performs a large number of numerical and logical checks on the completed data structure produced by the DATA program. For example, each potential process unit operating variable is checked for exact material balance closure, and every refinery stock is tested to verify that the completed model will include both producing

and consuming activities. This program produces a condensed "logical flow sheet" of the configuration to be represented by the finished model, indicating all raw materials, products, inventories, blends, process units, and stream origins and dispositions.

The DISP Component. The DISP (display) program, like the CHEK program, does not contribute directly to the generation of the model. Its function is to prepare a formatted, documentation-quality set of reports of the final technological data entering the model. In addition to all user-supplied data describing such things as raw material availabilities and costs, product demand structures and prices, etc., it includes a complete display of all process and blending data retrieved from the library files or developed by the DATA program.

The MATX Component. The MATX program has two functions: the conversion of the DATA program output into the proper input format for the LP, and the generation of the report controls. It has been separated from the DATA program so that its functions will not be executed needlessly when the CHEK or DISP reports show errors of sufficient magnitude to require data revision and reexecution of the DATA program.

The MMOD Component. Finally, the MMOD program is used to generate model revisions from user input in a format similar to the DATA program input. In a sense, it may be thought of as combining the functions of both the DATA and MATX programs with respect to model changes, since it is responsible for input and analysis of the user revision requests, validation of these requests against the problem structure created by the DATA program, and their output in a form suitable as input to the LP program itself. The MMOD input and output provides documentation of model changes in a format consistent with the original problem statement.

RPMS Solution Reports. Solution analysis reports produced by RPMS fall into eight groups:

- 1) New Facility Investment Summary
- 2) Overall Material and Economic Balances
- 3) Blending Summaries (Recipe and Specification)
- 4) Stream Production/consumption Reports
- 5) Utility and Chemical Reports
- 6) Final Economic Summary
- 7) Unit Detail Reports
- 8) Miscellaneous Status Reports

B. Refinery Model

The RPMS was used to develop a linear programming model of a refinery. The model is a complete representation of crude conversion into final products by processing in the various refinery operating units. A linear programming model is a set of mathematical equations in which the variables are related to each other in linear combination. The model represents, in mathematical terms, the operation of a variety of refinery process units and the flow of petroleum fractions among these units. The representations describe how the units respond to changes in feedstock qualities and operating conditions. The equations for each unit allow for consumption of utilities

such as fuel, steam, and electricity and the investment costs associated with building new units or expanding capacity of existing units. The model provides for changes in stream flows and unit operating conditions to make a desired set of products. The properties of the individual components of a product blend are blended linearly to meet product inspections. The model is driven either to minimize costs to meet a specific product slate or to maximize refinery cash flow.

When individual refiners use linear programming to plan their operations and strategies, the models are tailored to their specific refinery and to the nature of the planning questions to be answered. When the objective of a study is to provide estimates of how the refining industry will respond to several alternative situations, as in this present study, a model tailored to a specific refinery is not appropriate. Instead, a "composite" model of the refineries in a given region is used.

In a composite model, the ratios between the various process unit capacities represented in the model are the same as the ratios between the total of the process unit capacities existing in the section of the refining industry under study. For example, if the sum of the catalytic cracking unit capacities in a region being studied is 40% of the sum of the crude distillation capacities, then the catalytic cracking capacity represented in the model will be 40% of the crude distillation capacity represented in the same model. The selection of absolute size for one of the processes (usually the crude distillation unit) then determines the size of all the other process units.

So far as process yields and variable operating costs are concerned there are no economy of scale effects. The absolute size selection can be made at the discretion of the analyst. A 100,000 B/D size for the existing crude distillation capacity was chosen for the composite refinery model for the Rocky Mountain region.

The representation of each individual process in the composite model is designed to simulate typical yields, operating costs, operating flexibilities, etc. for the process type. The simulation of a specific process is the same for existing plants as for new plants. When capacity above the existing level is utilized, the fixed costs associated with the new capacity are included in the determination of an economic optimum solution.

Economies of scale are important when sizing new units, so the selection of new unit sizes must not be arbitrary, as was the selection the existing refinery size. The most acceptable results for industry studies are produced when the costs associated with new process capacities are based on the "typical" sizes for such units as may have been recently constructed or for which planned construction has been announced.

If the results of the study show 43,000 B/D of new capacity will be needed by 1995 and the typical size of a new unit is 10,000 B/D, then 4.3 new units would be expected to be added to the industry.

C. Refinery Configurations-1979 Basis

Refinery Configuration for the 1979 basis is shown pictorially in Figure 3.1; 1979 configurations as a percent of atmospheric crude unit capacity are shown in Table 3.1. Unit capacities were obtained from the "Annual Refining Report" published by The Oil and Gas Journal.(1) The refinery capacities reported are as of January 1, 1979. The configurations were calculated by summing the unit capacities excluding topping refineries which are very simple operations usually containing only an atmospheric distillation unit but no conversion processing such as a catalytic reformer or catalytic cracker.

There are 28 to 32 refineries in each region. Comparison of the three regions in Table 3.1 shows principal similarities and differences. The Great Lakes Region has the greatest refinery capacity, nearly twice as much as the Mid-Continent and five times as much as the Rocky Mountains. The most notable differences in configuration are the larger percentages of catalytic cracking, alkylation and coking in the Mid-Continent and Great Lakes regions relative to the Rocky Mountains. These are due to historical feedstock availabilities and product demands which determine individual refinery configurations.

Refinery Size. Initial refinery configurations were based on the 1979 figures reported in Table 3.1. In the Rocky Mountains Region crude capacity was normalized to 100,000 B/D before beginning the computer runs. In the Mid-Continent and Great Lakes Regions the average capacities reported in Table 3.1 were used as a basis. The differing choices reflect the personal preference of the analysts in developing each of the regional models.

D. Crude Supply Forecasts

Crude Oil Production. Crude oil production was forecast from 1975 state-by-state production data obtained from U. S. Bureau of Mines reports. Statistics are reported for Petroleum Administration for Defense (PAD) Districts of the U.S. as shown on the map on Figure 3.2.

The sweet/sour crude breakdown was determined from a review of a Bureau of Mines report entitled "Sulfur Content of Crude Oil" which analyzed 1971 production. The basic data in this report were adjusted for significant sweet/sour additions from 1971 through 1975. Production was decreased in future years based on the historical rate of production decline from 1971 to 1976. These are as follows:

<u>PAD District</u>	<u>Decline Rate %</u>
I	0
II	3.9
III	3.5
IV	1.1
V	2.7

These decline rates imply that U.S. production based on 1975 capacity will decline from 8360 MBPD to 4430 MBPD in 1995 as shown in Table 3.2.

In addition to this volume, new production is expected from those sources shown on Table 3.2. These additions indicate that total production

FIGURE 3.1 REFINERY CONFIGURATION 1979 BASIS

TABLE 3.1 REFINERY CONFIGURATION 1979 BASIS

	<u>Rocky Mountains</u>	<u>Mid-Continent</u>	<u>Great Lakes</u>
No. of Refineries	28	32	31
Crude Capacity, BPSD	630,700	1,539,200	3,067,800
Average Capacity, BPSD	22,530	48,100	98,960

UNIT CAPACITIES, % OF CRUDE

Vacuum Distillation	31.5	28.5	37.8
Catalytic Reforming	20.5	23.2	22.4
Catalytic Cracking	30.3	36.0	34.5
Hydrocracking	1.0	0.5	4.8
Alkylation	5.4	9.2	6.3
Coking	2.5	6.8	6.2

FIGURE 3.2 PETROLEUM ADMINISTRATION FOR
DEFENSE (P.A.D.) DISTRICTS

TABLE 3.2 U.S. CRUDE PRODUCTION
MBPD

	1975			1995		
	<u>Sweet</u>	<u>Sour</u>	<u>Total</u>	<u>Sweet</u>	<u>Sour</u>	<u>Total</u>
PADD I						
Florida	-	114.7	114.7	-	114.7	114.7
New York	2.4	-	2.4	2.4	-	2.4
Pennsylvania	10.7	-	10.7	10.7	-	10.7
Virginia	-	-	0.0	-	-	0.0
W. Virginia	6.8	-	6.8	6.8	-	6.8
Sub-Total	<u>19.9</u>	<u>114.7</u>	<u>134.6</u>	<u>19.9</u>	<u>114.7</u>	<u>134.6</u>
PADD II						
Illinois	71.5	-	71.5	32.2	-	32.2
Indiana	12.5	.2	12.7	5.6	0.1	5.7
Kansas	109.1	52.8	161.9	49.2	23.8	73.0
Kentucky	20.7	-	20.7	9.3	-	9.3
Michigan	55.2	11.7	66.9	24.9	5.3	30.2
Missouri	0.1	0.1	0.2	-	-	0.1
Nebraska	7.4	9.4	16.8	3.3	4.2	7.5
N. Dakota	35.2	20.8	56.0	15.9	9.4	25.3
Ohio	26.5	5.6	32.1	12.0	2.5	14.5
Oklahoma	370.0	76.9	446.9	166.9	34.7	201.6
S. Dakota	-	1.3	1.3	-	0.6	0.6
Tennessee	2.1	-	2.1	0.9	-	0.9
Sub-Total	<u>710.3</u>	<u>178.8</u>	<u>889.1</u>	<u>330.2</u>	<u>80.6</u>	<u>400.9</u>
PADD III						
Alabama	33.5	3.4	36.9	16.4	1.7	18.1
Arkansas	10.3	34.6	44.9	5.0	17.0	22.0
Louisiana	1719.4	76.2	1795.6	842.5	37.3	879.8
Mississippi	34.6	93.0	127.6	17.0	45.6	62.6
New Mexico	135.0	124.3	259.3	66.2	60.9	127.1
Texas	2153.4	1193.2	3346.6	1055.2	584.7	1639.9
Sub-Total	<u>4086.5</u>	<u>1524.7</u>	<u>5611.2</u>	<u>2002.3</u>	<u>747.2</u>	<u>2749.5</u>
PADD IV						
Colorado	13.1	90.8	103.9	10.5	72.8	83.3
Montana	42.0	48.0	100.0	33.7	38.5	72.2
Utah	98.0	10.4	108.4	78.6	8.3	86.9
Wyoming	130.7	217.9	348.6	104.8	174.8	279.6
Sub-Total	<u>283.8</u>	<u>367.1</u>	<u>650.9</u>	<u>227.6</u>	<u>294.4</u>	<u>522.0</u>

TABLE 3.2 U.S. CRUDE PRODUCTION(CONT'D)
MBPD

	1975			1995		
	Sweet	Sour	Total	Sweet	Sour	Total
PADD V						
Alaska	165.0	26.2	191.2	95.4	15.1	110.5
Arizona	1.7	-	1.7	1.0	-	1.0
California	102.3	780.5	882.8	59.1	451.1	510.2
Nevada	-	0.3	0.3	-	0.2	0.2
Sub-Total	269.0	807.0	1076.0	155.5	466.4	621.9
TOTAL	5369.0	2993.0	8362.0	2725.5	1703.3	4428.8
NEW PRODUCTION						
Expanded Yates Production (Texas)	-	50	60			
Enhanced Recovery California 100						
Oklahoma & Texas 600	200	600	800			
Other 100						
New Discoveries in Overthrust Belt (Wyoming/Idaho)	400	-	400			
Elk Hills	55	75	130			
North Slope	-	1600	1600			
Offshore California	-	400	400			
South Alaska	600	-	600			
East Coast Offshore	-	100	100			
	1255	2805	4080			
GRAND TOTAL	3980.5	4528.3	8508.8			

will decrease to 8500 MBPD in 1995 from the 1978 average value of 8684 MBPD (U.S. DOE Monthly Energy Review, April 1979). These new production figures are based on a review of a number of sources including: The Energy Information Administration's Annual Report to Congress, April 1978 and miscellaneous energy studies prepared by PIRINC, Shell Oil, Exxon, Phillips, Mobil, Gulf Oil, Purvin and Gertz, and Pace Company.

Regional forecasts were then developed using this total crude oil forecast as a basis.

Refinery capacity for each region was obtained by using Annual Refining Survey from the Oil and Gas Journal. The capacities are those of January 1, 1979. These capacities have been further subdivided by reference to the NPRA study: "Capabilities of U.S. Refineries to Process Sweet/Sour Crude Oil" done in March 1978.

Regional capacities were extrapolated to 1995 by increasing the values by 1.5 percent/year which is the forecasted annual growth in petroleum demand from 1979 to 1995. The break-down between sweet and sour capacity was determined by assuming all new capacity would be capable of handling sour crudes. No conversion of sweet crude capacity to sour crude feedstocks was assumed. This information is summarized in Table 3.3 and has been used to determine crude quality requirements for each region.

Regional feedstocks are summarized in Table 3.4, which shows four cases spanning the range of syncrude input. In the base case, no synthetics are processed in the refinery. When synthetics are introduced, either domestic or imported sweet crude will be backed out. Three cases could be considered for synthetics: running just shale oil, running just coal oil, or running both in combination.

Swing Crude Definition. For each region, petroleum "swing crudes" were defined whose volume would be variable when the given volume of synthetics was charged to the refinery. In the Rocky Mountain Region cases two crude types were defined: a low sulfur crude which was a mix of 23% of Wyoming Average (Elk Basin) and 77% Wyoming Light (Grass Creek) and a high sulfur crude which was represented by Wyoming Heavy (Steamboat Butte). Distillation curves for high sulfur and low sulfur crude are shown in Figure 3.3. Total quantity of these crudes was allowed to vary, but in a constant ratio to each other. Therefore, the swing crude was the mix of low and high sulfur crudes shown in Table 3.5.

In the Mid-Continent Region, three crude types were defined: a local crude, an inter PADD sour, and an inter-PADD sweet. The inter-PADD sweet crude was the swing crude; the local crude was represented by a mix of 34% Mid-Continent Average Pipeline, 27% Kansas "A", and 39% Oklahoma Sweet. The inter-PADD sour imports represent movements from PADD III and PADD IV. The crudes chosen to represent this mix were 15% Wyoming Heavy, 12% Wyoming Average, and 73% West Texas Heavy. The inter-PADD sweet imports represent movements from PADD III and IV. The crudes chosen to represent this mix were 11% Gulf Coast Average, 23% West Texas Light, 38% South Louisiana Average, and 28% Wyoming Light. The swing crude in this region was inter-PADD sweet. The volumes of the others were fixed.

In the Great Lakes Region, four crude types were defined: a local crude, North Slope, an imported sweet crude, and an imported sour. The imported sweet crude was used as the swing crude. The local crude was

TABLE 3.3 REFINERY CAPACITY
MBPSD

REGION	1979			1995		
	Sweet	Sour	Total	Sweet	Sour	Total
ROCKY MOUNTAIN	498.6	200	698.6	498.6	350.9	849.5
GREAT LAKES	1799.4	1330	3129.4	1799.4	2005.9	3805.3
MID-CONTINENT	1519.5	100	1619.5	1519.5	449.8	1969.3

(1) 1970 capacity based on the NPRA study "Capability of U.S. Refineries to Process Sweet/Sour Crude Oil," March 15, 1978.

(2) All expansions after 1979 are sour crude based expansions.

(3) 1979 capacity is based on Oil and Gas Journal Annual Refining Survey as reported in the March 26, 1979 issue.

TABLE 3.4 FEEDSTOCKS SLATES FOR AUTOMOTIVE FUELS STUDY
MBPD

<u>%</u> <u>Syn</u>		<u>Domestic</u> <u>Sweet</u>	<u>Domestic</u> <u>Sour</u>	<u>Imported</u> <u>Sweet</u>	<u>Imported</u> <u>Sour</u>	<u>Syn</u>	<u>Total</u>
ROCKY MTN REGION							
0	No Synthetics	500	350	0	0	0	850
35	Shale Oil	200	350	0	0	300	850
24	Coal Oil	300	350	0	0	200	850
59	Both	0	350	0	0	500	850
CREAT LAKES REGION							
0	No Synthetics	280	10	1520	2000	0	3810
8	Shale Oil	280	10	1220	2000	300	3810
5	Coal Oil	280	10	1320	2000	200	3810
13	Both	280	10	1020	2000	500	3810
MID-CONTINENT REGION							
0	No Synthetics	1380	450	140	0	0	1970
15	Shale Oil	1220	450	0	0	300	1970
10	Coal Oil	1320	450	0	0	200	1970
25	Both	1020	450	0	0	500	1970

FIG. 3.3 ROCKY MOUNTAIN CRUDE DISTILLATION

PETROLEUM CRUDES

represented by a mix of 34% Mid-Continent Average Pipeline crude, 27% Kansas "A", and 39% Oklahoma sweet. The imported sweet crude was represented by a mix of 16% Forcados, 19.3% Bonny, 34.4% Libyan Mix, 16.8% Ohanet (Algerian), and 13.5% Ekofisk. The imported sour mix was represented by a mix of 71.6% Arabian Light, 13.6% Tia Juana Medium, 9.1% Monagas (Venezuelan) and 5.7% Lagomar (Venezuelan). The swing crude in this region was imported sweet crude. The volumes of the others were again fixed.

The volumes of each of these crudes charged in the base cases in each region are shown in Table 3.5. The compositions and volumes reported were developed from forecasts of individual PADD refinery feedstocks. The forecasts were developed based on historic data and total U. S. energy forecasts.

E. Product Demand Forecasts

Method and Basis. The approach used in developing regional product demands was to develop a national energy forecast and then relate the resultant energy forecasts by sector to representative macroeconomic factors. Individual regional demands were then generated by using state projections of these same macroeconomic factors, the historical relationship of the state to national energy use per macroeconomic factor, and then combining the state forecasts into regional projections.

Figure 3.4 is an information flow diagram of this approach. As indicated in the legend, the double-lined boxes are computer models. The national forecast is developed through the application of rates of growth by sector of demand. These rates of growth can be varied over any time horizon. The sources of supply to satisfy each sector demand are also projected by using a rate of growth, which can be varied with time. Conversion of energy to physical units is based on the most recent historical experience and can be varied externally. The efficiency of power generation is also based on most recent historical experience but can be changed to reflect external information.

Demand forecasts by state were generated on the basis that the historical relationship of state energy demands by sector per appropriate economic factor to the equivalent U.S. ratio will hold into the future. Thus, the state energy demand growth rate by sector uses the national rate of growth, adjusted by the historical ratio of state to national use, and the projected state economic factor growth. This is expressed in the following equation:

$$ROC_{seds} = ROC_{sef} + ROC_{nr} * X$$

where

ROG = Rate of growth
 seds = State energy demand of sector
 sef = State economic factor
 neds = National energy demand of sector
 nef = National economic factor
 nr = neds/nef
 sr = seds/sef
 X = $f(1 + ROG_{sr/1} + ROG_{nr})$, for historical period.

TABLE 3.5 REGIONAL CRUDE FEEDSTOCKS
(BASE CASE COMPOSITIONS)

<u>Rocky Mountain Region</u>	<u>%</u>
Low Sulfur Crude	59
High Sulfur Crude	41
	<u>100</u>
<u>Great Lakes Region</u>	
Local Crudes	10
North Slope	25
Imported Sweet	27
Imported Sour	38
	<u>100</u>
<u>Mid-Continent Region</u>	
Local Crudes	40
Inter-PADD Sour	15
Inter-PADD Sweet	45
	<u>100</u>

FIGURE 3.4 FLOWCHART OF ENERGY FORECAST SYSTEM

The following shows the macroeconomic factor used for each net sector demand.

<u>Sector</u>	<u>Macroeconomic Factor</u>
Residential	Households
Commercial	Population
Transportation	Motor Vehicle Registration (MVR)
Industrial	Personal Income (PI)

The power sector is developed by taking the electrical-energy supply to each sector expanded by the efficiency of generation for that state or region. The ROG of sources of supply to the power sector are based on projected capacity increases of the various types of power-generating plants. Available capacity for the various sources of electrical energy can be entered explicitly.

Data for the desired states are then summed, to produce the desired regional energy product demand forecasts.

Regional Product Demand Forecasts. Product demand forecasts, major product classes, are shown in Table 3.6 for three regions.

The Great Lakes Region is the largest consumer with 1995 demand at 4,062,296 barrels per day. The distribution of products indicates that gasoline will continue to be the largest single product consumed. The percent of gasoline in the total product demand is forecast to drop from around 50% to 36-38% of the total. This is due to a low or negative growth in gasoline demand as shown in Table 3.6. Distillate growth in all three regions is above 2.6% per year and is reflected in distillate becoming an increasing percentage of the total product.

The Great Lakes Region contains the highest product consumption, followed by the Mid-Continent Region (which is less than half of the consumption in the Great Lakes) and the Rocky Mountain Region (under 20% of Great Lakes). The relative product distribution shown in Table 3.6 is similar for all three regions, the main exception being the high consumption of LPG in the Mid-Continent Region.

Refinery Product Demands. The refined product demands shown in Table 3.6 have been modified to produce the product demands imposed on the regional refineries. The distribution of products is shown in Table 3.7. Refinery product demands were developed by adjusting regional product demand forecasts for product imports to and exports from the regions. These imports and exports were based on historical product movements to and from the region. The gasoline pool was divided into regular unleaded (70% of pool) and premium unleaded (30% of pool) grades. The distillate pool was split into No. 2 diesel oil and No. 2 fuel oil based on the historic usage in each region. The residual fuel oil pool was apportioned to low sulfur No. 6 fuel oil (65% of pool) and high sulfur No. 6 fuel oil (35% of pool). The feedstock volume was allocated to gasoline and distillate fractions. LPG demand was not fixed, but allowed to vary depending on the refinery capability to produce LPG from the selected crude and synthetic oil feedstocks.

The breakdown between Unleaded Regular and Unleaded Premium was based on data presented by DuPont in a paper on "Gasoline Octane Quality and

TABLE 3.6 PRODUCT DEMAND FORECASTS

	Rocky Mountain		Mid-Continent		Great Lakes	
	1975	1995	1975	1995	1975	1995
TOTAL DEMAND, B/CD						
LPG	30681	37744	161601	206594	187918	255073
Jet Fuel	31709	49850	51020	81387	118153	199761
Feedstocks	24326	35332	65368	86803	200984	350837
Gasoline	225365	239526	636639	633329	1516442	1545547
Distillate	115154	193426	208582	421299	662870	1153279
Residuals	38704	58984	55698	154429	213745	310023
Lubes, Wax, Asph.	22414	34881	69125	81383	154431	199831
Pet Coke	3987	4974	20634	25119	37486	47945
TOTAL	492339	654718	1268666	1690340	3092027	4062296
DISTRIBUTION, %						
LPG	6.2	5.8	12.8	12.3	6.2	6.4
Jet Fuel	6.4	7.6	4.0	4.8	3.8	4.9
Feedstocks	4.9	5.4	5.2	5.1	6.5	8.6
Gasoline	45.8	36.6	50.2	37.5	49.0	38.0
Distillate	23.4	29.5	16.4	24.9	21.4	28.4
Residuals	7.9	9.0	4.4	9.1	6.9	7.6
Lubes, Wax, Asph.	4.6	5.3	5.4	4.8	5.0	4.9
Pet Coke	0.8	0.8	1.6	1.5	1.2	1.2
TOTAL	100.0	100.0	100.0	100.0	100.0	100.0
GROWTH RATE, 1975-1995, %/YEAR						
LPG		1.04		1.24		1.54
Jet Fuel		2.29		2.36		2.66
Feedstocks		1.88		1.43		2.82
Gasoline		0.31		-0.03		0.10
Distillate		2.63		3.58		2.81
Residuals		2.13		5.23		1.88
Lubes, Wax, Asph.		2.24		0.82		1.30
Pet Coke		1.11		0.99		1.24
TOTAL		1.44		1.45		1.37

TABLE 3.7 PRODUCT DEMAND ON REGIONAL REFINERIES
(% OF TOTAL PRODUCT IN BASE CASE)

<u>Product</u>	<u>Rocky Mountain</u>	<u>Mid-Continent</u>	<u>Great Lakes</u>
LPG	1.1	1.7	2.0
Regular No-Lead	26.1	32.6	27.7
Premium No-Lead	11.2	14.0	11.9
Kero Jet	8.1	6.1	5.3
No. 2 Diesel	15.1	18.3	14.6
No. 2 Fuel Oil	16.8	10.0	20.0
Low Sulfur No. 6	6.6	6.4	4.9
High Sulfur No. 6	3.6	3.4	2.7
Coke	0.8	0.0	2.0
Lubes & Asphalt	4.7	5.2	6.6
Plant Fuel	5.9	2.3	2.2
	<u>100.0</u>	<u>100.0</u>	<u>100.0</u>

Demand" presented at the 1979 API mid-year meeting which indicated that the current 92 RON unleaded gasoline will satisfy 85% of those vehicles requiring unleaded. Their forecasts for future consumption of two grades of unleaded gasoline show the following results:

1985 UNLEADED GASOLINE FORECASTS

	Percent Total Gasoline	Percent Unleaded
Case A		
Unleaded Regular 92 RON	62	77
Higher Octane Unleaded 98 RON	19	23
	<u>81</u>	<u>100</u>
Case B		
Unleaded Regular 92 RON	54	70
Higher Octane Unleaded 98 RON	23	30
	<u>77</u>	<u>100</u>

Case A assumed no further increase in octane requirements would take place beyond 1978. Case B forecasted that by 1985 the requirements of the 50th percentile vehicle would be increased by 1.5 octane numbers and the requirements of the 90th percentile vehicle would be increased by 2.5 octane numbers above the 1975 values. The 70-30 breakdown in Case B was selected for use in the study.

F. Product Specifications

The product specifications employed in building the regional refinery models are shown in Table 3.8. The specifications reported for regular unleaded, premium unleaded, and No. 2 diesel are based on Bonner & Moore's experience in modeling refinery and product blending operations. Gasoline octane requirements and regional differences in these requirements were based on information reported by DOE.(2,3)

Broadcut fuel production has been included for potential use in a future fuel-tolerant engine such as a stratified charge or spark-assisted diesel. Part of the benefit of this type of engine is reported to be improved fuel economy and refinery energy savings. Qualities were defined after consideration of combustion and fuel system needs along with storage, safety, and emissions aspects.

Specifications for the broadcut fuel are given in Table 3.9. Distillation ranges were set to incorporate distillate fuel fractions and thereby increase BTU content on a volume basis which contributes to improved fuel economy. Vapor pressure was included to permit use of gasoline components and gasoline storage facilities. The vapor pressure range selected should keep storage vapor space in safe condition (above the upper explosive limit) down to temperatures of 35°F for 5 pound RVP and 15°F for 9 pound RVP.(4) Sulfur and nitrogen were selected to achieve reasonable emissions.

Not all of the specifications were used in modeling broadcut fuel blending in the regional models. Those used are shown in Table 3.8, selected

TABLE 3.8 TRANSPORTATION FUEL PRODUCT SPECIFICATIONS

	Rocky Mountain		Mid-Continent		Great Lakes	
	Minimum	Maximum	Minimum	Maximum	Minimum	Maximum
REGULAR UNLEADED						
Research ON Clear	90.5		91.5		92.0	
Motor ON Clear	82.0		83.0		83.5	
Reid Vapor Pressure		10.1		10.1		10.1
Pct off at 160°F	18.0	35.0	18.0	35.0	18.0	35.0
Pct off at 210°F	39.0	57.0	39.0	57.0	39.0	57.0
Pct off at 230°F	49.0		49.0		49.0	
Pct off at 330°F	84.0	96.0	84.0	96.0	84.0	96.0
Pct Aromatics		100.0		100.0		100.0
Pct Olefins		100.0		100.0		100.0
Pct Supplement	10.0	10.0				
PREMIUM UNLEADED						
Research ON Clear	93.5		94.5		95.0	
Motor ON Clear	84.0		85.0		85.5	
Reid Vapor Pressure		10.1		10.1		10.1
Pct off at 160°F	18.0	35.0	18.0	35.0	18.0	35.0
Pct off at 210°F	39.0	57.0	39.0	57.0	39.0	57.0
Pct off at 230°F	49.0		49.0		49.0	
Pct off at 330°F	84.0	96.0	84.0	96.0	84.0	96.0
Pct Aromatics		100.0		100.0		100.0
Pct Olefins		100.0		100.0		100.0
Pct Supplement	10.0	10.0				
NO. 2 DIESEL FUEL						
Flash Index ⁽¹⁾		378.2		378.2		378.2
Flash Point, °F	125.0		125.0		125.0	
Wt% Sulfur		0.500		0.500		0.500
Cetane Blending No.	45.0		45.0		45.0	
Pour Point Index ⁽²⁾		640.5		640.5		640.5
Pour Point, °F		20.0		20.0		20.0
BROADCAST FUEL						
Reid Vapor Pressure	5.0	9.0	5.0	9.0	5.0	9.0
Wt% Sulfur		0.250		0.250		0.250
Pct off at 400°F	45.0	88.0	45.0	88.0	45.0	88.0
Nitrogen ppm		200.0		200.0		200.0

$$(1) \log_{10} (\text{FLASH INDEX}) = 42.1093 - 14.286 \log_{10} (\text{FLASH POINT, } ^\circ\text{F} + 460)$$

$$(2) \ln (\text{POUR POINT INDEX}) = -73.0883 + 12.8852 \ln (\text{POUR POINT, } ^\circ\text{F} + 460)$$

TABLE 3.9 BROADCAST FUEL SPECIFICATIONS

	ASTM Test Method	Minimum	Maximum
Gravity, °API	D 287	30.0	57.0
Specific		0.75	0.875
Distillation, °F	D 86		
IBP		---	---
50%		220	400
90%		440	640
EP		---	---
Residue, vol%			1
Reid Vapor Pressure, lb	D 323, D 2551	5	9
Aromatics, vol%	D 1319		50
Sulfur, wt%	D 1552, Note 2		0.25
Nitrogen, ppm wt	D 3431		200
Viscosity, cSt at 100°F	D 445	0.5	6.0
Cloud Point, °F	D 2500		See Note 1
Ash, wt%	D 482		0.01
Carbon Residue on 10% Bottoms	D 524		0.35
Water and Sediment, vol%	D 1796		0.05
Corrosion at 122°F	D 130		No. 3
Oxidation Stability, mg/100 ml	D 2274		2.0

NOTES:

1. Cloud point should follow guidance in ASTM D 975 for diesel fuels, i.e., maximum shall be 6°C above tenth percentile minimum temperature for season and area where used.
2. Sulfur determination allowed by equivalent methods.

because of availability of data on the component streams. The gravity of the broadcast fuel was simply reported rather than being constrained to the specified ranges; only one broadcast blend produced in the computer cases fell slightly outside the gravity range.

G. Additional Modeling Considerations

Forecasts for the refinery fuel products are naturally based on energy requirements to be supplied by each of the fuels. These requirements are then translated to physical volume requirements (barrels) using a standard conversion factor for each fuel product type. Normally, the conversion factor can be considered to be constant and essentially independent of processing sequence and blending operations since specifications of required physical properties on the product do not permit much variation in the heating value (expressed as BTU per barrel). This constant heating value assumption was considered doubtful for two products: low sulfur residual fuel oil and broadcast motor fuel. Depending on the type of crude oils available, the most economical way to supply the low sulfur residual fuel market involves blending significant amounts of light oils into the residual fuel to "dilute" or "blend off" the sulfur in the heavy residuals from crude distillation. The result is a light residual fuel oil with a significantly lower heating value per barrel of fuel oil than has been traditional. The broadcast fuel heating value could also vary several percentage points (depending upon its composition), since distillation and gravity specifications were broad enough to allow anywhere from twenty-five to Seventy-five percent naphtha to be included in the broadcast blend.

The forecast demands for these fuels were expressed in barrels based on assumed heating values as follows:

<u>Fuel</u>	<u>Net Heating Value (10^6 BTU/BBL)</u>
Broadcast	5.40
Low Sulfur Residual	5.88

To assure that the model produced sufficient volume of the fuels (whatever their energy content) to satisfy the forecast demand the volumes of the blends of low sulfur residual and broadcast fuels were corrected to represent barrels of standard fuels with heating values as shown above. The differences between the actual barrels blended and the barrels sold were accounted for in refining loss or gain.

The actual formulation used in the model is expressed as follows:

$$\text{Volume blended} = \sum_i v_i = V,$$

where v_i = the volume of the i th component in the blend.

$$\text{Heating value of Mixture} = \sum_i v_i B_i = H,$$

where B_i is the heating value expressed as million BTU per barrel for component i .

$$\text{Standard barrels} = V_s = H/B_s$$

where B_s = standard heating value, million BTU per barrel

$$\text{Loss due to conversion} = V - V_s$$

H. Model Generation - Regional Base Cases for 1995

Using the data described above, composite refinery models were generated for each of the three regions. Feedstocks to the refineries were defined based on the crude supply forecasts.

Product demands from refining also forecast for each region were scaled down to the model size used and placed as fixed demands (with one exception) on the refinery model. Since the product demand is fixed, product prices are not needed in the model since they do not influence optimization.

The exception is the demand for liquified petroleum gas (LPG) which is primarily propane. There are no refinery processes that can efficiently convert the other parts of crude oil into propane. It is produced mainly as a by-product of cracking and reforming reactions. The actual availability of LPG from a refinery is also dependent upon several factors that cannot be modeled because the refiner has little control over them. For example, small amounts of propane are found in the crude charge, but the propane content of crude shown in standard assays may not relate to what is actually received. Further, the amount of propane produced from catalytic reforming depends on feed characteristics as well as the type and history of the catalyst. It was preferable to let the LPG production from the model vary and therefore a price must be supplied for LPG production. Since the LPG produced from a refinery is mainly a by-product, the model's response is relatively independent of the price placed on the LPG as long as it bears a reasonable relation to the cost of raw material (crude).

Incremental volumes of crude required above the base level defined by 1979 volumes would be met by swing crudes selected for each region. This swing crude was assigned a price so that the refinery model could choose the volume of this crude which it would process within the constraints of the fixed set of product demands. The swing crudes for the three regions and their prices are:

<u>Region</u>	<u>Crude</u>	<u>Price, \$/BBL</u>
Rocky Mountains	Low Sulfur	\$27.00
	High Sulfur	22.00
Mid-Continent	Inter-PADD Sweet	27.00
Great Lakes	Imported Sweet	27.00

In the Rocky Mountains, the two crudes were held in the ratio of 1.44 bbls of low sulfur to 1.00 bbl of high sulfur. The swing crudes were considered to be discretionary crudes (especially in the Mid-Continent and Great Lakes). The 1979 crude prices should not be regarded as rigorous values but only as a directional indicator of the worth of the crude relative to other crudes or products which have been allowed to vary.

In addition to allowing the volume of certain crudes to vary, some products and other feedstocks were allowed to vary in price relative to LPG. These were:

<u>Component</u>	<u>Price, \$/BBL</u>
LPG (product)	\$20.00
Coke (product)	13.50 FOE BBL
Natural Gasoline (feed)	28.00
N-butane (feed)	21.00
Isobutane (feed)	22.00

The results of the base case simulations are shown in Tables 3.10 through 3.12. Table 3.10 contains the overall summary, Table 3.11 shows the processing summary, and Table 3.12 lists the product compositions.

In all three regions, the refinery model responded to the low growth in gasoline demand by not building any new catalytic cracking units. Visbreaking capacity was added in each region. The refinery model chooses to add visbreaking because it adds to the volume of middle distillate material which, as noted above, is growing at over 2.6% per year. The yield of gasoline blendstock fractions is low (about 11% on feed) which is another reason this process is attractive. The crude tower and vacuum unit increases are a natural consequence of the overall increase in demand.

The product compositions are relatively similar in the Mid-Continent and Great Lakes regions as seen in Table 3.11. The main differences are due to octane specifications on the gasolines. The Great Lakes Region gasolines are higher by 0.5 octane number which caused the octane level of the reformat to be higher on average than in the Mid-Continent.

The Rocky Mountain Region is somewhat different due to several factors. Because of altitude, the octane requirements on the gasolines are lower than in the Great Lakes and Mid-Continent, 2.0 and 1.5 numbers respectively. The cut point on the vacuum tower operation was changed from 1050°F to 930°F based on the determination that the 930°F cut point was representative of average historical vacuum tower operations. The 1050°F operation is typical of conditions achieved only in new vacuum units.

In the Rocky Mountain Region the volume of natural gasoline was set at 4200 B/D. In the other regions the model was allowed to choose the volume of natural gasoline to use based on price relative to the swing crude prices. This difference would primarily affect the gasoline composition.

The demand for petroleum coke in the Rocky Mountain region was fixed; in the other regions, it was allowed to swing based on a reasonable price relative to crude oil. Also in the Rocky Mountain Region the hydrotreated kerosene and distillate fractions from different crudes were commingled into two streams: a combined hydrotreated kerosene and a combined hydrotreated distillate. The effects of this commingling will show up in differences in the No. 2 diesel oil blend compositions.

TABLE 3.10 REGIONAL BASE CASES FOR 1995
OVERALL SUMMARY

	Rocky Mountain Region	Mid-Continent Region	Great Lakes Region
RAW MATERIALS B/D			
Low Sulfur Crude	69925	0	0
High Sulfur Crude	48932	0	0
Local Crudes	0	21000	9430
Inter-PADD Sour	0	8140	0
Inter-PADD Sweet	0	24047	0
North Slope	0	0	26190
Imported Sweet	0	0	28119
Imported Sour	0	0	39810
N-Butane	1646	915	768
IsoButane	1386	869	615
Natural Gasoline	4200	0	0
TOTAL RAW MATERIALS	126090	54971	104932
PRODUCTS, B/D			
LPG	1465	992	2214
Regular No-Lead	33400	18185	29846
Premium No-Lead	14300	7794	12791
Broadcut Fuel	0	0	0
Kero Jet	10400	3387	5691
No. 2 Diesel	19400	10220	15702
No. 2 Fuel Oil	21500	5551	21684
Low Sulfur Resid	8500	3571	5318
High Sulfur Resid	4600	1923	2863
Coke	1000	0	2106
Lubcs & Asphalt	6000	2876	7114
Plant Gas Fuel	7620	1285	2363
Volume Loss	(2096)	(813)	(2760)
TOTAL PRODUCTS	126090	54971	104932
UTILITIES			
Plant Fuel, MMBTU/D	37968	8033	14936
Purchased Fuel, MMBTU/D	760	9980	27742
Total Fuel, MMBTU/D	38728	18013	42678
Cat/Chem \$/D	8221	4480	9271
Sulfur, Tons/D	98	9	55
NEW FACILITIES			
Crude Unit	19312	3187	3549
Vacuum Tower	14759	6210	11012
Naphtha Hydrotreater	3667	0	0
Cat Reformer	3162	1372	0
Kero/Gas Oil Htr	21524	0	5504
Visbreaker	1023	1262	11528
Hydrocracker	0	0	0
Cat Cracker	0	0	0
Alkylation	0	0	0
Hydrogen, MSCF/D	0	0	0
Delayed Coke	0	0	0

TABLE 3.11 REGIONAL BASE CASES FOR 1995
PROCESSING SUMMARY

	<u>Rocky Mountain Region</u>	<u>Mid-Continent Region</u>	<u>Great Lakes Region</u>
85-145 LSR Naphtha	9488	2670	3069
GASOLINE REFORMER			
145-200 HTR SR Naphtha	7377	2670	4250
200-330 HTR SR Naphtha	13650	6960	9960
330-400 HTR SR Naphtha		1720	
Htr 170-375 Hydrocrackate	1883	516	4259
Htr Visbreaker Gasoline	81	210	1440
Htr Natural Gasoline	391		
TOTAL FEED	<u>23382</u>	<u>12076</u>	<u>20009</u>
CATALYTIC CRACKER			
700-1050 Htr VGO	12285		
700-930 Htr VGO		5115	16592
Other Gas Oils	11777	8915	6901
TOTAL FEED	<u>24062</u>	<u>14030</u>	<u>23493</u>
DELAYED COKING			
1050+Residue	1067	0	
930+Residue		0	365
970+Slurry	1573	0	4949
TOTAL FEED	<u>2640</u>	<u>0</u>	<u>5314</u>
KERO/DISTILLATE HDS			
550-650 Sr Distillate	3808		
Light Cycle Oil	3724	282	734
650-700 VGO	5886		
700-1050 VGO	13000		
700-930 VGO		5379	17447
TOTAL	<u>26418</u>	<u>5661</u>	<u>18181</u>

TABLE 3.12 REGIONAL BASE CASES FOR 1995
PRODUCT COMPOSITIONS, VOLUME %

	Rocky Mountain Region	Mid-Continent Region	Great Lakes Region
REGULAR UNLEADED			
Light Straight Run	10.8	14.5	12.7
REFORMATE: 100 RON			
Petroleum	21.1	26.6	22.9
Synthetic	0	0	0
Sub-Total	21.1	26.6	22.9
REFORMATE: 90 RON			
Petroleum	21.1	5.0	9.3
Synthetic	0	0	0
Sub-Total	21.1	5.0	9.3
C3/C4 Alkylate	10.0	11.8	11.4
Butanes	7.0	7.3	7.9
Natural Gasoline	9.9	0	0
Cat. Gasoline C5-250			
Petroleum	6.8	12.7	14.8
Synthetic	0	0	0
Sub-Total	6.8	12.7	14.8
Cat Gasoline: 250-410			
Petroleum	13.3	22.1	21.0
Synthetic	0	0	0
Sub-Total	13.3	22.1	21.0
TOTAL REGULAR	100.0	100.0	100.0
PREMIUM UNLEADED			
Light Straight Run	5.7	1.8	11.1
REFORMATE: 100 RON			
Petroleum	22.3	27.2	49.7
Synthetic	0	0	0
Sub-Total	22.3	27.2	49.7
REFORMATE: 90 RON			
Petroleum	22.3	25.4	0
Synthetic	0	0	0
Sub-Total	22.3	25.4	0
C3/C4 Alkylate	11.0	12.0	12.4
Butanes	7.5	9.3	7.7
Natural Gasoline	0	0	0
Cat. Gasoline C5-250			
Petroleum	23.9	18.5	12.2
Synthetic	0	0	0
Sub-Total	23.9	18.5	12.2
Cat Gasoline: 250-410			
Petroleum	7.3	5.8	6.9
Synthetic	0	0	0
Sub-Total	7.3	5.8	6.9
TOTAL PREMIUM	100.0	100.0	100.0
No. 2 DIESEL FUEL			
Trt'd Kero 400-550			
Petroleum	30.7	39.7	48.3
Synthetic	0	0	0
Sub-Total	30.7	39.7	48.3
Trt'd Dist 550-650			
Petroleum	62.7	44.6	45.9
Synthetic	0	0	0
Sub-Total	62.7	44.6	45.9
Trt'd Lt. Cycle Oil	6.6	20.7	5.8
Hydrocracker Kero	0	0	0
TOTAL NO. 2 DIESEL	100.0	100.0	100.0

I. Volumes of Diesel and Broadcut Fuels

After the forecast production in each region was established as on Table 3.10 product volumes were defined for the maximum diesel fuel and broadcut fuel cases. Table 3.13 shows the highway transportation fuels for product option cases in all three regions.

Base case quantities show diesel fuel as 26.9 to 28.9% of highway fuels in 1995. This level is higher than the 10-15% typical of 1980 production. Gasoline to distillate ratio ranges from 0.93 to 1.36.

Part of the gasoline production was replaced by the alternate type of fuel using the following factors.

	<u>Base</u>	<u>Maximum Diesel</u>	<u>Broadcut</u>
a. Percent Gasoline Replaced	0	30	40
b. Relative Fuel Economy	1.00	1.35	1.24
c. Replacement Volume, % (a÷b)		22.22	32.26

The fact that total highway fuel on Table 3.13 in the maximum diesel and broadcut fuel cases is nearly identical was not planned. The plan was to adjust fuel quantities to provide constant miles of travel for the cases in each region. The factors above coincidentally produce almost the same net product differential from the base case.

Inspection of Table 3.13 shows that maximum diesel fuel volume varies from 45.8 to 47.3% of total highway fuel, and gasoline to total distillate varies from 0.54 to 0.73 ratio in those cases. Broadcut fuel ranges from 24.3 to 25.0% of highway fuels, indicating similar proportions for highway fuels in each region.

One additional comparison is useful to describe the three major fuels, as used in this study:

	<u>Gasoline</u>	<u>Broadcut</u>	<u>Diesel</u>
a. Relative Fuel Economy	1.0	1.24	1.35
b. Energy Content, MMBTU/BBL	4.963	5.40	5.49
c. Relative Energy Content	1.0	1.088	1.106
d. Relative Engine Efficiency (a÷c)	1.0	1.14	1.22

The ratios above imply that diesel engines are assumed to be 22% more efficient than spark ignition engines. The rest of the 35% diesel advantage in fuel economy results from higher energy content per volume of fuel.

Broadcut fuel engines are in between with 14% higher efficiency and 24% better fuel economy. It was planned to use 5.04 MMBTU/BBL as energy content of broadcut fuel and 1.22 relative engine efficiency, the same as diesel. However, the value of 5.40 MMBTU/BBL was entered instead. The net effect should be zero if the difference is applied to engine efficiency which is unknown at present, because broadcut fuel volume was adjusted to meet a given BTU demand as explained in Section III-C, Additional Modeling Considerations. The error will be corrected in future case runs.

TABLE 3.13. PRODUCT VOLUMES FOR MAXIMUM DIESEL
AND BROADCAST FUELS

	Base Cases		Maximum Diesel Cases		Broadcast Fuel Cases	
	Volume, B/D	% of Total	Volume, B/D	% of Total	Volume, B/D	% of Total
<u>Rocky Mountains</u>						
Gasoline	47,700	71.1	33,400	52.7	28,600	45.1
Broadcast Fuel	-	-	-	-	15,400	24.3
Diesel Fuel	19,400	28.9	30,000	47.3	19,400	30.6
Total Highway Fuel	67,100	100.0	63,400	100.0	63,400	100.0
Other Distillate	31,900		31,900		31,900	
Gas/Dist Ratio	0.93		0.54		-	
<u>Mid-Continent</u>						
Gasoline	25,979	71.8	18,185	53.2	15,587	45.6
Broadcast Fuel	-	-	-	-	8,376	24.5
Diesel Fuel	10,220	28.2	15,987	46.8	10,220	29.9
Total Highway Fuel	36,199	100.0	34,172	100.0	34,183	100.0
Other Distillate	8,938		8,938		8,938	
Gas/Dist Ratio	1.36		0.73		-	
<u>Great Lakes</u>						
Gasoline	42,637	73.1	29,844	54.2	25,564	46.5
Broadcast Fuel	-	-	-	-	13,766	25.0
Diesel Fuel	15,702	26.9	25,183	45.8	15,702	28.5
Total Highway Fuel	58,339	100.0	55,027	100.0	55,032	100.0
Other Distillate	27,375		27,375		27,375	
Gas/Dist Ratio	0.99		0.57		-	

SECTION REFERENCES

1. "Annual Refining Report", The Oil and Gas Journal, March 26, 1979, pp. 79-156.
2. Motor Gasolines, Winter 1978-1979, Ella Mae Shelton, July 1979, Bartlesville Energy Technology Center.
3. Motor Gasolines, Summer 1978, Ella Mae Shelton, February 1979, Bartlesville Energy Technology Center.
4. Kant, F.H., Cunningham, A.R., and Farrier, M.H., "Effects of Changing the Proportions of Automotive Distillate and Gasoline Produced by Petroleum Refining," Exxon Research and Engineering Co., PB-236 900. Environmental Protection Agency, EPA-460/3-74-018, July 1974.

IV. SYNCRUDE PROCESSING

A. Syncrude Process Selection Criteria

In defining the refinery feedstocks for the alternative fuels study it was necessary to select candidate syncrudes from a number of processes which convert oil shale and coal to liquid materials. The following criteria were used as the most important factors in the selection:

1. Economic viability of process
2. Current status of process development and published data
3. Availability of refinery feedstocks from the process

The goal in this evaluation was not selection of the "best" process but rather the process which was representative of potentially available future syncrude. Although data from specific processes were employed, the processes were considered as generic types. Syncrude conversion processes and their generic groups are shown in Table 4.1.

Oil Shale Processes

Surface retorting of oil shale has many variations, most of which are likely to be commercialized when the proper circumstances prevail. The Paraho process was used in model construction for the following reasons:

1. There is a considerable amount of publicly available data, not only on the shale oil but on refinery processing to finished products. (1)
2. Pilot scale operations have been conducted and plans for commercial production announced.
3. Raw shale oils produced by other retort designs show similar processing results, and thus Paraho can be used as a representative shale oil in the model.
4. The process is intended to produce a refinery feedstock. The indirect operating mode was chosen because it produces a lower pour point oil which will be easier to transport.

In situ retorting of oil shale without removal from the ground also has variations. Fortunately, the shale oils produced are similar in most quality parameters. The Occidental process was used as the example for this generic type for reasons similar to the surface retort example above, plus adequate information was available on processing (2) for reasonably complete modeling.

Coal Liquefaction

Processes were examined for each of five major generic types of coal liquefaction considering the criteria listed above. Three process types were selected for use in the study; two others were set aside as discussed below.

TABLE 4.1 SYNCRUDE CONVERSION PROCESSES

	<u>Generic Process</u>	<u>Examples</u>
Shale Oils	Surface Retort	Paraho, Superior Tosco, Union
	In situ Retort	Occidental, Geokinetics, Rio Blanco
Coal Oils	Pyrolysis	Coed, Toscoal, Garrett, Clean-Coke
	Hydrogenation, Non-Catalytic	SRC-II
	Hydrogenation Catalytic	H-Coal, Exxon Donor Solvent, Synthoil

Pyrolysis processes have several candidates including four examples in Table 4.1. Only COED (Char Oil Energy Development) has been run with a variety of coals and made enough data available to be used as a representative process.

Solvent extraction has undergone considerable investigation. However, it has recently been combined with direct hydrogen usage and apparently major activity has been directed toward this combined approach. For this reason, pure extraction was eliminated as a candidate process.

Non-Catalytic hydrogenation is represented mainly in the SRC-II process which is covered by published information on properties and processing.(3)

Catalytic Hydrogenation research is proceeding on several variations of the process and equipment. More data were available on the H-Coal process and refinery processing which were used in model construction.

Indirect liquefaction involves coal gasification as the first step followed by conversion to liquid process and subsequent refining. Sasol Limited does this commercially in South Africa and recently constructed and started a second, larger plant. It appeared that this process would carry out conversion and processing to finished products in one integrated operation and not make syncrude available for other refineries.

B. Syncrude Processing

The necessary refinery processing of the syncrude charges and fractions as well as processing options allowed were defined after reviewing the results of several research studies carried out on either bench scale or pilot plant equipment.

1. Both retort and in-situ produced shale oils must be hydrotreated before conventional crude distillation. No distinction was made between these two syncrudes once they passed this initial hydrotreat stage.
2. The high nitrogen content of the shale oils (even after whole oil hydrogen pre-treat) is such that further hydrogen treatment is necessary before large concentrations of the distillates can be blended to distillate fuels or can serve as hydro-cracker or catalytic cracker feed. Furthermore, the naphtha fraction must be deeply hydrotreated for essentially complete nitrogen removal to protect reforming catalysts.
3. Only a wide boiling naphtha was taken from the distillation operation and the downstream processing of the naphtha was restricted to (a) hydrotreating followed by catalytic reforming or (b) blending into the Broadcut Fuel. (The standard RPMS crude distillation model yielded light, medium and heavy naphtha streams. Data regarding reforming the syncrude naphtha was available only for the wide boiling naphtha).
4. The gas oil streams from all syncrudes were not allowed to be blended into residual fuel oils. These were hydrotreated and

either hydrocracked or catalytically cracked to lighter products. (However, the entire atmospheric distillation bottoms stream was permitted to go to residual fuel blending.)

5. The light distillate streams (kerosene and heating oil or diesel) were hydrotreated. These streams could be blended without hydrotreating into the broadcut fuel. The hydrotreated streams could then be blended into the light distillate products or hydrocracked or catalytically cracked. Naphtha from hydrocracking was not allowed to be blended directly into gasoline. It was first processed through a catalytic reformer. (Hydrocrackate from syncrudes was judged to be an exceptionally good reformer feed based on data available.)
6. Coal-derived syncrudes from three classes of processes were represented in the model. Pyrolysis derived liquids or liquids from catalytic hydrogen donor processes were judged to be of about equal in quality relative to hydrogen content and other important attributes. (This assumed the pyrolysis product was hydrotreated at the pyrolysis site.) Liquids from non-catalytic hydrogen donor processes were judged to be deficient in hydrogen content relative to the other two classes and were forced to be hydrogen treated prior to the distillation step.
7. Downstream, the coal derived streams were subjected to the same processing alternatives and restrictions as described for shale derived syncrudes. Quality differences between the shale and coal syncrudes were recognized in the downstream processes.

This processing scheme for the syncrudes should not be taken to imply that these steps will be necessary in all cases or that other processing sequences will not be found to be economical. The processing costs represented by this refining scheme will generally be comparable with other viable schemes and the subsequent processing in the model (hydrocracking and catalytic cracking) provides the necessary alternatives to estimate the ultimate allocation of the components derived from syncrude charge stocks among the refinery product pools: gasoline, kerosene, jet fuel, diesel fuel, heating oil, broadcut motor fuel, and residual fuel.

Restricting the gas oil cuts from residual fuel blending is somewhat arbitrary but justifiable. Residual fuels are usually used in large industrial furnaces or power plants and this type of application could also receive its energy requirements directly from coal. It would seem wasteful, therefore, to use a more valuable product in such applications. The option could have been left up to the model, but removing it simplified the model and reduced computing and analysis costs.

Two particular options that have been investigated elsewhere and not included in our model deserve some attention:

1. Shale oil can be charged directly to a coker and the liquid products from the coker then processed through standard refinery equipment. The limited market for petroleum coke in the areas where shale oil will be available would indicate that this route

will be used only to a limited extent. The highly aromatic nature of syncrudes derived from coal makes this option even less attractive. Additionally, coker products from syncrudes tend to retain the nitrogen present in the charge stock, so the need for subsequent hydrogen treat for nitrogen removal would still exist.

2. The highly aromatic nature of the coal syncrudes can be exploited as suggested by UOP. By hydrocracking in two stages in series with selective catalysts in both stages, a naphtha hydrocrackate that preserves many of the original aromatic rings can be produced. The resulting naphtha has a good octane rating relative to other hydrocrackates and is also an exceptionally good feed for catalytic reforming. It was decided not to represent this particular hydrocracking route since it would complicate the model without having major effect on the overall processing cost or gasoline blend compositions.

C. Stream Segregation

One aspect of using a linear program for refinery modeling that must be given careful attention is called the "pooling problem". The problem arises because a refinery charging crudes or streams from different processes, at points ahead of the final disposition of the mixed stream. A non-linearity is therefore introduced into the model. The analyst who sets up the model must use his judgment based on experience with actual refinery operations to decide where in the processing sequence the detailed identities of the streams are to be lost. Further, in generating the model, he must assume proportions among the streams being mixed together in order for the attributes of the mixed stream to be estimated. As a result, the model cannot fully account for the pooling effect where the assumed proportions are not realized in the problem solution. Forcing the model to match the proportions assumed leads to an overly constrained model. The alternative of assuming no commingling or pooling of streams results in a model with too much flexibility.

The problem associated with stream pooling can be partially overcome by recursively solving and modifying the model; the proportions determined from a "solution" are used to recalculate the mixed stream's attributes, the model is revised accordingly and solved again. This technique was used to adjust the sulfur content of the mixed streams.

For the Rocky Mountain regional model, the most significant points of stream pooling or segregation can be generally defined as follows:

1. Ahead of crude distillation, four feed pools were recognized:
 - Low Sulfur crudes
 - High Sulfur crudes
 - Coal-derived syncrudes
 - Shale-derived syncrudes
2. The naphtha fractions immediately downstream of the crude unit are:
 - Naphtha from crude oils
 - Naphtha from shale syncrudes
 - Naphtha from coal syncrudes

3. Middle distillates, heavy gas oils, vacuum residues and atmospheric residues retained the segregation pattern shown for the crude distillation charge.
4. Products from processes after the crude distillation unit were not assumed to be segregated by feed type except for products from catalytic cracking where the products yielded from hydrotreated feeds were kept separate from those yielded from non-hydrotreated feeds.

This pattern of pooling was selected since it has proved to be adequate in many previous refining industry studies. The primary emphasis is on segregating streams according to sulfur content. Segregation between natural and syncrude fractions immediately downstream of the crude distillation unit is necessary because of the dramatic differences in aromatics and nitrogen contents which affect yields from and costs of the processes immediately downstream of the crude distillation unit.

The processing options for shale oil and coal oil are summarized graphically in Figure 4.1 for shale oil and Figure 4.2 for coal oil. The flow diagrams show the processing options allowed in the model. Syncrude fractions are segregated through the process steps described on the diagram. In any processing units downstream of those shown, syncrude fractions are commingled.

Modifications Following the Rocky Mountain Region Cases

The solutions from the Rocky Mountain Model cases were carefully reviewed to see if some improvements were possible and practical before developing the models for the other regions. This analysis revealed that the wide discrepancy in aromatics levels between coal derived syncrudes and natural crudes is probably sufficient to cause refiners to maintain segregated streams beyond the hydrotreating processes for middle distillate cuts. The clue to this need was an observed difficulty in the model in meeting cetane number on diesel fuels and smoke point on jet fuels. In fact, it was necessary to adjust the smoke point and cetane blending value of hydrotreated products to reflect some "prime component" availability from the pool of hydrotreated stocks in order to achieve solutions to cases where the diesel fuel was being maximized. Subsequent models were generated assuming additional segregation through the hydrotreating of the 400°-550°F and 550°-650°F streams.

The necessary data were lacking to model one other feature that appears to be important to refineries processing syncrudes along with natural crudes. It is not currently possible to model various severities of hydrogen treatment for the removal of nitrogen and the saturation of aromatic compounds and the extent to which these treatment effects can be kept independent. Availability of data at intermediate severities in the future would allow investigation of producing fuels at intermediate quality levels less than current specifications.

D. Syncrude Assay Data

Forecasts of costs for syncrudes relative to crude oils in the literature

FIGURE 4.1 PROCESSING OPTIONS - SHALE OILS

FIGURE 4.2 PROCESSING OPTIONS - COAL OILS

show a wide range that precluded allowing the model to choose between syncrude and crude oil. It was elected to estimate the availability of syncrude to the refining industry and to assume that the cost would allow the industry to use it in combination with natural crude. Since syncrudes tend to be light and low sulfur, it was assumed that the syncrudes would back out the light, low sulfur crude oil from the refinery charge. This swing crude would then be available to other regions.

The attributes of the syncrudes were estimated from recent reports that have investigated the make-up of syncrudes and the effects of subjecting them to conventional and unconventional refining processes. The Syncrude assay data used as input to this refinery model are shown in Table 4.2. Syncrude distillations are plotted on Figures 4.3 through 4.5. These data were developed from a variety of sources which are described below.

Shale Oil Processing

1. The raw Paraho shale oil data were obtained from an assay developed for work done in "Identification of Probable Automotive Fuels Composition: 1985-2000", February 1978, page 109. This information has been modified by changing the sulfur distribution based work done at Gulf Science and Technology Company ("Shale Oil: An Acceptable Refinery Syncrude", H. C. Stauffer and S. J. Yanik)
2. The yields and gravities for the hydrotreated Paraho shale oil are based on information contained in "Converting Green River Shale Oil to Transportation Fuels," R. F. Sullivan and B. E. Stangeland, Chevron Research Co., April 1978. The sulfur distributions are based on the raw shale oil and the degree of desulfurization is based on the whole crude properties of raw and hydrotreated shale oil. The lighter fractions were considered to be essentially 100% desulfurized.
3. The fraction properties for the raw Paraho shale oil are from the assay developed for "Identification of Probable Automotive Fuels Composition: 1985-2000". The properties for the hydrotreated fractions were obtained by using engineering judgment applied to data from the following sources:
 - "Converting Green River Shale Oil to Transportation Fuels," R. F. Sullivan and B. E. Stangeland, Chevron Research Co., Eleventh Oil Shale Symposium Proceedings, April 1978.
 - "Composition of Shale Oil and Shale Oil Derived Fuel," E. T. Robinson, Conference on Composition of Transportation Synfuels, San Antonio, Texas, October 1978.
 - "Refining of Paraho Shale Oil into Military Specification Fuels," E. T. Robinson, AIIME Meeting, February 1979.
 - "Refining Shale Oil," R. F. Sullivan, B. E. Stangeland, and H. A. Frumkin, Chevron Research Company and C. W. Samuel, Chevron, U.S.A., API Midyear Meeting, May 1978.

(Text continued on pg. 60)

TABLE 4.2 SYNCRUDE ASSAY DATA USED IN REFINERY MODELS

	Syncrude					
	Shale(3)	Non-Catalytic Hydrogenation Coal(3)	Pyrolysis(3)		Catalytic Hydrogenation	
			Illinois Coal	Wyoming Coal	Illinois Coal	Wyoming Coal
85-145°F						
Yield, Vol%	3.2	3.5	0.7	0.1	1.5	5.0
°API	82.0	69.0	64.0	62.0	69.0	70.0
RON, clear	70.0	80.0	85.0	85.0	85.0	85.0
MON, clear	65.0	69.0	64.0	75.0	80.0	70.0
145-400°F						
Yield, Vol%	16.0	48.5	14.8	8.2	31.5	43.0
°API	51.2	42.3	46.6	41.6	43.2	41.1
N + 2A(1)	56.0	107.0	96.0	127.0	102.0	92.0
400-550°F						
Yield, Vol%	23.5	36.0	25.0	25.7	25.0	24.0
°API	36.0	21.0	29.0	27.0	19.0	27.0
Sulfur, Wt%	0.01	0.02	0.02	0.02	0.14	0.10
Aromatics, Vol%	8.0	67.0	40.0	53.0	49.0	44.0
Cetane	30.0	0.0	29.0	26.0	13.0	26.0
550-650°F						
Yield, Vol%	20.0	5.5	22.0	23.0	12.0	8.0
°API	32.0	15.0	22.0	20.0	9.0	19.0
Sulfur, Wt%	0.01	0.02	0.02	0.02	0.17	0.10
Cetane	39.0	10.0	34.0	30.0	14.0	30.0
650-700°F						
Yield, Vol%	8.0	6.5	10.0	10.0	6.0	4.0
°API	30.5	14.5	18.0	16.0	3.0	15.0
Sulfur, Wt%	0.01	0.02	0.02	0.02	0.19	0.11
K-Factor(2)	11.9	10.8	11.0	10.9	10.0	10.8
700-930°F						
Yield, Vol%	29.0	0	24.0	20.0	14.0	6.0
°API	29.5	-	11.1	11.0	-4.0	10.8
Sulfur, Wt%	0.01	-	0.01	0.01	0.01	0.21
K-Factor(2)	12.0	-	8.0	7.0	-9.8	10.8
930°F + Residuum						
Yield, Vol%	0.3	0	3.5	13.0	10.0	10.0
°API	12.0	-	8.0	7.0	-9.0	2.0
Sulfur, Wt%	0.05	-	0.05	0.05	0.40	0.15

NOTES:

(1) N+2A = Vol% Naphthenes + 2xVol% Aromatics; used as a measure of reforming quality.

(2) Watson characterization factor.

(3) Properties and yields are after whole syncrude hydrotreated.

FIG. 4.3 SYNTHETIC CRUDE DISTILLATION

HYDROTREATED SHALE AND COAL OILS

FIG. 4.4 SYNTHETIC CRUDE DISTILLATION

COAL OILS FROM ILLINOIS COAL

FIG 4.5 SYNTHETIC CRUDE DISTILLATION

COAL OILS FROM WYOMING COAL

- "Shale Oil: An Acceptable Refinery Syncrude," H. C. Stouffer and S. J. Yanik, Gulf Science and Technology, September 1978, American Chemical Society National Meeting
4. The raw in-situ shale oil data was obtained from an assay developed for work done in "Identification of Probable Automotive Fuels Composition: 1985-2000," February 1978, p. 109.
 5. The properties for the hydrotreated fractions were obtained by applying adjustments to data from the following sources:
 - "Prerrefining True In-Situ Shale Oil," Philip L. Cottingham, U. S. DOE, Laramie Energy Research Center, October 1978, The 13th Intersociety Energy Conversion Engineering Conference, SAE.
 - "Distribution of Nitrogen in Hydrocracked In-Situ Shale Oil," Philip L. Cottingham, Ind. Eng. Chem. Prod. Res. Dev., Vol. 15, No. 3, 1976.
 - "High Severity Hydrotreating of Shale Oil," Philip L. Cottingham, Laramie Energy Technology Center
 - "Production of Synthetic Crude From Crude Shale Oil Produced by In-Situ Combustion Retorting," C. M. Frost, R. E. Poulson, and H. B. Jensen, Laramie Energy Research Center, U. S. Department of the Interior, Bureau of Mines, Laramie, Wyoming
 6. Information on hydrotreating whole shale oil was obtained from the following sources:
 - "Composition of Shale Oil and Shale Oil Derived Fuel," E. T. Robinson, Conference on Composition of Transportation Synfuels, San Antonio, Texas, October 1978
 - "Prerrefining True In-Situ Shale Oil," Philip L. Cottingham, U. S. DOE, Laramie Energy Research Center, October 1978, 13th Intersociety Energy Conversion Engineering Conference
 - "Converting Green River Shale Oil to Transportation Fuels," R. F. Sullivan and B. E. Stangeland, Chevron Research Company, April 12-14, 1978, Eleventh Oil Shale Symposium Proceedings.
 7. Information on naphtha pretreating and reforming was obtained from the following sources:
 - "Composition of Shale Oil and Shale Oil Derived Fuel," S. Kumar Kunchal, SOHIO Natural Resources Company, Presented at the Conference on Composition of Transportation Synfuels in San Antonio, Texas, 11-13 October, 1978.
 - "Shale Oil: An Acceptable Refinery Syncrude," H. C. Stouffer and S. J. Yanik, Gulf Science and Technology Company

8. Information on catalytic cracking was obtained from:
- "Shale Oil: An Acceptable Refinery Syncrude," H. C. Stouffer and S. J. Yanik, Gulf Science and Technology Company
 - "Refining Shale Oil," R. F. Sullivan, B. E. Stangeland, and H. A. Frumkin, Chevron Research Company, Richmond, CA, and C. W. Samuel, Chevron, U.S.A., Salt Lake City, UT.
 - "Converting Green River Shale Oil to Transportation Fuels," R. F. Sullivan and B. E. Stangeland, Chevron Research Company, Presented at the Eleventh Oil Shale Symposium Proceedings.
9. Information on distillate hydrotreating was found in:
- "Production of Synthetic Crude from Crude Shale Oil Produced by In-Situ Combustion Retorting," C. M. Frost, R. E. Poulson, and H. B. Jensen, Laramie Energy Research Center
 - "Shale Oil: An Acceptable Refinery Syncrude," H. C. Stouffer and S. J. Yanik, Gulf Science and Technology Company
10. Hydrocracking data were obtained from:
- "Converting Green River Shale Oil to Transportation Fuels," R. F. Sullivan and B. E. Stangeland, Chevron Research Company, Presented at the Eleventh Oil Shale Symposium Proceedings
 - "Refining Shale Oil," R. F. Sullivan, B. E. Stangeland, and H. A. Frumkin, Chevron Research Company, Richmond, CA and C. W. Samuel, Chevron U.S.A., Salt Lake City, UT, May 10, 1978

Coal Oil Processing

1. The COED and H-Coal data were obtained from assays developed for work done in "Identification of Probable Automotive Fuels Composition 1985-2000," February 1978, pp 112-113.
2. The yields and inspections for hydrotreated SRC-II oil were obtained from "Refining the Products from the SRC Coal Liquefaction Process," R. F. Sullivan, B. E. Stangeland, H. A. Frumkin, Chevron Research, 44th Refining Midyear Meeting, May 1979 and from "Refining and Upgrading of Synfuels from Coal and Oil Shales by Advanced Catalytic Processes," January 1979, R. F. Sullivan, prepared for U. S. DOE.
3. Information on fuel oil hydrotreating for the SRC-II coal oil process was obtained from:
 - "Refining of SRC-I and SRC-II, DOE Contract EF-76-C-01-2315, Richard F. Sullivan, Bruce E. Stangeland, and Harry A. Frumkin

4. Data on reforming of coal oils (specifically H-Coal) was obtained from:
 - "Upgrade Coal Derived Distillates," Armand J. de Rosset, Gim Tan, and Lee Hilfman, UOP Inc., Des Plaines, Ill., May 1977, Hydrocarbon Processing, pp. 151-153.
 - "Upgrading of Coal Liquids-Interim Report, Hydrotreating and Reforming H-Coal Process Derived Naphthas," Gim Tan and Armand J. de Rosset, March 1978.
5. Hydrotreating data on naphtha and middle distillates was obtained from:
 - "Upgrading of Coal Liquids-Interim Report, Hydrotreating and Fluid Catalytic Cracking of H-Coal Derived Gas Oils," Gim Tan and Armand J. de Rosset, August 1978
 - "Refining and Upgrading of Synfuels from Coal and Oil Shales by Advanced Catalytic Processes," R. F. Sullivan, Chevron Research Company, April 1979
6. Fluid catalytic cracking yields were obtained from the following sources:
 - "Upgrade Coal Derived Distillates," Armand J. de Rosset, Gim Tan and Lee Hilfman, UOP Inc., Des Plaines, Ill., May 1977, Hydrocarbon Processing, pp. 131-137
 - "Upgrading of Coal Liquids-Interim Report - Hydrotreating and Fluid Catalytic Cracking of H-Coal Derived Gas Oils," Gim Tan and Armand J. de Rosset, August 1978.
7. Hydrocracking yields were obtained from:
 - "Upgrade Coal Derived Distillates," Armand J. de Rosset, Gim Tan and Lee Hilfman, UOP Inc., Des Plaines, Ill., May 1977, Hydrocarbon Processing, pp. 151-153
 - "Upgrading of Coal Liquids-Interim Report, Hydrocracking of H-Coal Process Derived Gas Oils," Gim Tan and Armand J. de Rosset, November 1978

RPMS correlations were used as a basis in interpreting how coal oils and shale oils would be refined. The above data references were consulted to make adjustments and corrections in the RPMS equations to more accurately reflect conditions surrounding the processing of syncrudes.

V. GASOLINE SUPPLEMENTS

Four components included in the project for evaluation as motor gasoline supplements were:

- Methanol
- Ethanol
- MTBE (methyl-tertiary-butyl ether)
- Synthetic naphtha from methanol

Each of these components was blended into the two grades of unleaded gasoline at a concentration of 10 volume percent. This concentration was selected because it is a reasonable level for all four components in order to compare results on a consistent basis. It is also the current minimum amount of ethanol used in gasohol to qualify for tax incentives now expected to continue through 1992. At present, methanol is not authorized by EPA for use in gasoline at any concentration, except in blend with tertiary butyl alcohol (TBA). MTBE is authorized by EPA to be used up to 7 volume percent. It is assumed that these limits could be extended to 10 percent by 1995. There are no regulatory or arbitrary limits on synthetic naphtha because it is all hydrocarbons and is essentially finished gasoline quality.

The main objective of the study was to evaluate the effect on fuel quality and composition of synthetic crudes. As part of that objective, the gasoline supplement options were added to consider their role with synthetic materials in the crude slate. There was no intention to evaluate a range of concentrations or to use mixtures of components in the blend. Also, there was no plan to consider the economics of each component relative to the others since this would be better evaluated by an individual refinery with its unique location, transportation, and price factors.

Blending values of the gasoline supplements are given in Table 5.1. These properties were used to blend with other gasoline components to produce optimum gasoline blends meeting specifications in each case. This is a significant difference from gasohol where the ethanol is added to a finished gasoline already meeting specifications, thereby changing its octanes and volatility properties.

It should be noted that the alcohol blending values for vapor pressure and percent distilled at 160°F are valid only at the 10 percent level since these properties show nonlinear behavior as alcohol concentration is varied. Also, volatility parameters for methanol assume the absence of butane in blends. Significant volumes of methanol cannot be tolerated in blends containing butane without causing potential vapor lock problems. For example, a Vapor Lock Index (VLI) is often specified for gasoline. The equation for this index is:

$$\text{VLI} = \text{RVP} + 0.13 \text{ (percent distilled at } 158^{\circ}\text{F.)}$$

A typical limit of 14.7 VLI is specified for gasolines. This limit would be met by a gasoline with 10.1 pound RVP and 35 percent distilled at 158°F.

The boiling point of methanol is 149°F but it makes azeotropic mixtures with hydrocarbons which boil at lower temperatures. Thus the percent distilled at 158°F is increased by an amount more than the percentage of methanol added. This effect on distillation is the basis for the high blending value for percent distilled at 160°F on Table 5.1. Also, at over 5 percent concentration, methanol raises RVP about 3 pounds which would increase the first term in the VLI equation.

The blending octane numbers in Table 5.1 are based on a review of numerous studies by other researchers (References 1-17). Considerable variation in alcohol and MTBE blending octane values was reported in the literature. This variation results from a combination of factors including:

1. Non-linear blending resulting from factors such as:
 - a. Variation with alcohol concentration, although calculation techniques can be used to minimize this effect.
 - b. A trend toward higher alcohol blending octanes with lower octane gasoline base stocks.
 - c. Variation with hydrocarbon types in the gasoline base stock, particularly aromatics.
2. Difficulty in measuring the octane due to differences in characteristics and detection of knock with blends containing oxygenated compounds.

The blending octanes selected for use in the model tend toward the conservative or low side of the range of reported data.

The change in volumetric fuel economy by adding alcohols to gasoline depends on the carburetor adjustment. Miles per gallon may increase, decrease, or stay the same with alcohol in the gasoline depending on the air/fuel ratio in the individual vehicle (7). Since this condition cannot be predicted and the effect is small (about 5% of fuel use) no adjustment was made to gasoline demand volumes.

A potential problem may occur with methanol blends in the distribution system. If a gasoline containing butane and one containing methanol are mixed, the resulting blend could exceed the VLI limits even if both blends were within specifications separately. This type of mixing may occur in the distribution system and would be likely to occur in the automobile gasoline tank which is typically not supplied consistently from a single source.

The preceding comments on non-linear blending behavior are directed primarily at the oxygenated compounds and do not apply to the synthetic naphtha blending component. Since this is a hydrocarbon stream, its published properties (18) would be expected to blend linearly within the limits of variation for normal gasoline components.

TABLE 5.1 BLENDING VALUES FOR SPECIAL GASOLINE COMPONENTS

	Component			
	MeOH	EtOH	MTBE	Syn. Naph.
Octane Number, Clear				
Research	130.0	128.0	118.0	95.2
Motor	96.0	105.0	101.0	84.3
RVP, psi	60.0	20.0	8.5	7.0
% Distilled at 160°F	250	200	65	25
% Distilled at 210°F	100	100	110	43
% Distilled at 230°F	100	100	110	49
% Distilled at 330°F	100	100	105	82

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VI. RESULTS AND DISCUSSIONS

Results of the refinery model runs are presented in this section for all three regions. Data summaries are grouped in categories so that discussion of conclusions can include comparisons among regions. The main categories are:

- Overall summaries of raw materials, products, utilities, and additions to process units.
- Compositions of highway transportation fuels.
- Impacts of synthetic crudes and gasoline supplements on raw materials and refinery energy consumption.
- Relative investment costs for future expansion with and without synthetic crudes and gasoline supplements.
- Process flowsheets and tables showing volumes of syncrude components through each process step.
- Product quality data on highway fuel blends.

A. Overall Summaries and Case Descriptions

Tables 6.1 through 6.6 contain overall summaries of the individual case runs. The first three tables show RAW MATERIALS purchased and PRODUCTS sold in three groups of cases:

Table 6.1 - Shale Oil Cases
Rocky Mountain Region

Table 6.2 - Coal Oil Cases
Rocky Mountain Region

Table 6.3 - Shale and Coal Oil Cases
Mid-Continent and Great Lakes Regions

In the second group, Tables 6.4 through 6.6, information is tabulated on UTILITIES consumed and NEW CAPACITY added to major processing units in a parallel grouping of cases. Data selected from these summaries are discussed in more detail later in this section.

Since all data tables have similar structure, a description of cases is given below to facilitate identification by case number and an abbreviated name. The cases are the same as outlined on Table 2.1, Project Case Study Schedule, in Section II. The A or B on some case numbers refers to repeat runs made with those computer cases.

TABLE 6.1

RAW MATERIALS AND PRODUCTS
SHALE OIL CASES
ROCKY MOUNTAIN REGION

CRUDE	PETROLEUM		SHALE OIL			Gasoline Supplements			
			Product Options						
Case No.	1	16	2A	3	4	8	9	10	11
Description	Base	Broadcut Fuel	Conventional	Maximum Diesel	Broadcut Fuel	Methanol	Ethanol	MTBE	Synthetic Naphtha
RAW MATERIALS, B/D									
Low Sulfur Crude	69925	69166	26814	28144	25561	28222	28587	26096	25141
High Sulfur Crude	48933	48402	46960	49289	44756	49425	50064	45703	44031
Normal Butane	1646	0	1579	441	796	0	0	1022	1616
Iso-Butane	1386	634	1477	0	0	1495	0	0	0
Natural Gasoline	4200	692	4200	0	4200	1941	73	4200	4200
Shale Oil	0	0	42000	42000	42000	42000	42000	42000	42000
Coal Oil	0	0	0	0	0	0	0	0	0
Supplement	0	0	0	0	0	4770	4770	4770	11475
TOTAL RAW MATERIALS	126090	118894	123130	119874	117323	127853	125494	123791	128463
PRODUCTS, B/D									
LPG	1455	3350	1652	1839	968	3096	2048	1160	1833
Regular Unleaded	33400	20000	33400	23400	20000	33400	33400	33400	33400
Premium Unleaded	14300	8600	14300	10000	8600	14300	14300	14300	14300
Broadcut Fuel	0	15400	0	0	15400	0	0	0	0
Kerosene Jet Fuel	10400	10400	10400	10400	10400	10400	10400	10400	10400
No. 2 Diesel	19400	19400	19400	30000	19400	19400	19400	19400	19400
No. 2 Fuel Oil	21500	21500	21500	21500	21500	21500	21500	21500	21500
No. 6 Low Sulfur	8500	8500	8500	8500	8500	8500	8500	8500	8500
No. 6 High Sulfur	4600	4600	4600	4600	4600	4600	4600	4600	4600
Coke	1000	1000	1000	1000	1000	1000	1000	1000	1000
Lubes & Asphalt	5000	5000	6000	6000	6000	6000	6000	6000	6000
Plant Fuel	7620	1226	3568	4433	1392	5951	6350	5035	3252
(Gain) or Loss	(2095)	(1082)	(1190)	(1799)	(437)	(1294)	(2004)	(1504)	4278
TOTAL PRODUCTS	126090	118894	123130	119874	117323	127853	125494	123791	128463

TABLE 6.2 RAW MATERIALS AND PRODUCTS
COAL OIL CASES
ROCKY MOUNTAIN REGION

CRUDE	PETROLEUM		COAL OIL							
			Product Options				Gasoline Supplements			
Case No.	1	16	5A	5B	6	7A	12	13	14	15A
Description	Base	Broadcut Fuel	Conven- tional	Conven- tional	Maximum Diesel	Broadcut Fuel	Methanol	Ethanol	MTBE	Synthetic Naphtha
RAW MATERIALS, B/D										
Low Sulfur Crude	69925	69166	40646	38997	44541	38878	40646	40646	40646	40646
High Sulfur Crude	48933	48402	47428	45504	51973	45365	47428	47428	47428	47428
Normal Butane	1646	0	2172	2083	0	619	0	0	0	334
Iso-Butane	1386	634	0	1333	0	0	1294	0	0	0
Natural Gasoline	4200	692	4200	4200	0	2547	4200	4200	4200	4200
Shale Oil	0	0	0	0	0	0	0	0	0	0
Coal Oil	0	0	28800	28800	28800	28800	28800	28800	28800	28800
Supplement	0	0	0	0	0	0	4770	4770	4770	11475
TOTAL RAW MATERIALS	126090	118894	123246	120917	125314	116209	127138	125844	125844	132883
PRCDUCTS, B/D										
LFG	1465	3350	1414	1249	4514	2312	2616	2098	2811	4216
Regular Unleaded	33400	20000	33400	33400	23400	20000	33400	33400	33400	33400
Premium Unleaded	14300	8600	14300	14300	10000	8600	14300	14300	14300	14300
Broadcut Fuel	0	15400	0	0	0	15400	0	0	0	0
Kerosene Jet Fuel	10400	10400	10400	10400	10400	10400	10400	10400	10400	10400
No. 2 Diesel	19400	19400	19400	19400	30000	19400	19400	19400	19400	19400
19400										
No. 2 Fuel Oil	21500	21500	21500	21500	21500	21500	21500	21500	21500	21500
No. 6 Low Sulfur	8500	8500	8500	8500	8500	8500	8500	8500	8500	8500
No. 6 High Sulfur	4600	4600	4600	4600	4600	4600	4600	4600	4600	4600
Coke	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000
Lubes & Asphalt	6000	6000	6000	6000	6000	6000	6000	6000	6000	6000
Plant Fuel	7620	1226	6146	3273	9197	721	8235	8126	7908	7979
(Gain) or Loss	(2096)	(1082)	(3414)	(2705)	(3797)	(2224)	(2813)	(3480)	(3975)	1588
TOTAL PRODUCTS	126090	118894	123246	120917	125314	116209	127138	125844	125844	132883

TABLE 6.3 RAW MATERIALS AND PRODUCTS
SHALE AND COAL OIL CASES
MID-CONTINENT AND GREAT LAKES REGIONS

REGION CRUDE	MID-CONTINENT					GREAT LAKES				
	PETROLEUM		SHALE AND COAL OILS			PETROLEUM		SHALE AND COAL OILS		
Case No.	1	5	2	3	4	1	5	2	3	4
Description	Base	Broadcut Fuel	Conven- tional	Maximum Diesel	Broadcut Fuel	Base	Broadcut Fuel	Conven- tional	Maximum Diesel	Broadcut Fuel
RAW MATERIALS, B/D										
Local	21000	21000	21000	21000	21000	9430	9430	9430	9430	9430
Inter-PADD sour	8140	3140	8140	8140	8140					
Inter-PADD sweet	24047	21787	7361	5959	4931					
North slope						26190	26190	26190	26190	26190
Imported Sweet						28119	23940	9894	10116	6145
Imported Sour						39810	39810	39810	39810	39810
Normal Butane	515	1022	1283	581	1418	768	977	1179	1047	1104
Iso-Butane	869	438	789	530	594	615	744	741	0	755
Shale Oil	0	0	9380	9380	9380	0	0	9680	9680	9680
Coal Oil	0	0	6240	6240	6240	0	0	6450	6450	6450
TOTAL RAW MATERIALS	54971	52437	54193	51830	51703	104932	101091	103373	102723	99564
PRODUCTS, B/D										
LPG	992	758	933	741	559	2214	1581	2004	2997	1487
Regular Unleaded	18185	10911	18185	12730	10911	29846	17895	29846	20892	17895
Premium Unleaded	7794	4676	7794	5455	4676	12791	7669	12791	8954	7669
Broadcut Fuel	0	8376	0	0	8376	0	13766	0	0	13766
Kerosene Jet Fuel	3387	3387	3387	3387	3387	5691	5691	5691	5691	5691
No. 2 Diesel	10220	10220	10220	15987	10220	15702	15702	15702	25183	15702
No. 2 Fuel Oil	5551	5551	5551	5551	5551	21684	21684	21684	21684	21684
No. 6 Low Sulfur	3571	3571	3571	3571	3571	5318	5318	5318	5318	5318
No. 6 High Sulfur	1923	1923	1923	1923	1923	2863	2863	2863	2863	2863
Coke	0	0	0	0	0	2106	2139	1414	1802	1407
Lubes & Asphalt	2876	2876	2876	2876	2876	7114	7114	7114	7114	7114
Plant Fuel	1235	808	629	384	284	2363	1532	1708	2558	1162
(Gain) or Loss	(813)	(620)	(876)	(775)	(631)	(2760)	(1863)	(2762)	(2333)	(2194)
TOTAL PRODUCTS	54971	52437	54193	51830	51703	104932	101091	103373	102723	99564

TABLE 6.4 UTILITIES AND NEW FACILITIES
SHALE OIL CASES
ROCKY MOUNTAIN REGION

CRUDE	PETROLEUM		SHALE OIL						
			Product Options			Gasoline Supplements			
Case No.	1	16	2A	3	4	8	9	10	11
Description	Base	Broadcut Fuel	Conven- tional	Maximum Diesel	Broadcut Fuel	Methanol	Ethanol	MTBE	Synthetic Naphtha
UTILITIES									
Plant Fuel	37968	7673	18617	21922	6909	33966	30776	24599	16954
Purchased Fuel	760	26426	27577	23435	32753	11132	11734	16664	26734
Total Fuel, MMBTU/D	38728	34099	46194	45357	39662	45098	42510	41263	43688
Cat and Chemicals, \$/D	8221	6797	18998	18673	17377	18843	17871	17791	32749
Sulfur Made, Tons/D	98	101	102	108	93	110	112	97	93
NEW FACILITIES CAPACITY, B/D									
Crude Distillation	19312	17568	19973	23632	16962	23846	24851	17999	15372
Vacuum Distillation	14759	14529	3705	6895	1473	5902	6581	2392	726
Naphtha Hydrotreater	3667	0	51	264	0	2473	2657	0	0
Catalytic Reformer	3162	0	2182	0	0	1219	0	0	0
Kero/Gas Oil									
Hydrotreater	21524	20618	98287	104170	97989	99330	100630	100565	99380
Visbreaker	1023	0	0	0	0	0	0	0	0
Hydrocracker	0	0	0	0	0	0	0	0	0
Catalytic Cracker	0	0	0	0	0	0	0	0	0
Alkylation	0	0	0	0	0	0	0	0	0
Hydrogen, MSCF/D	0	0	63616	65611	68274	63199	64609	66857	64929
Delayed Coker	0	99	0	0	0	0	0	0	0

TABLE 6.5 UTILITIES AND NEW FACILITIES
COAL OIL CASES
ROCKY MOUNTAIN REGION

CRUDE	PETROLEUM		COAL OIL				Gasoline Supplements			
			Product Options							
Case No.	1	16	5A	5B	6	7A	12	13	14	15A
Description	Base	Broadcut Fuel	Conven- tional	Conven- tional	Maximum Diesel	Broadcut Fuel	Methanol	Ethanol	MTBE	Synthetic Naphtha
UTILITIES										
Plant Fuel	37968	7673	29049	16360	45239	4593	38877	37603	37806	39658
Purchased Fuel	760	26426	10483	23231	0	30239	465	0	0	0
Total Fuel, MMBTU/D	38728	34099	39532	39591	45239	34832	39342	37603	37806	39658
Cat and Chemicals, \$/D	8221	6797	8031	8398	9440	7402	8599	7950	7471	21901
Sulfur Made, Tons/D	98	101	85	89	99	77	86	88	86	79
NEW FACILITIES CAPACITY 3/D										
Crude Distillation	19312	17568	17834	15019	26273	14003	18863	17834	17834	17834
Vacuum Distillation	14759	14259	5256	3773	9338	3029	5250	5250	5250	3993
Naphtha Hydrotreater	3667	0	8237	7499	9227	257	8989	7802	6302	8847
Catalytic Reformer	3162	0	4184	5117	6827	0	3923	2550	3069	6883
Kero/Gas Oil										
Hydrotreater	21524	20618	37075	37608	34320	30266	38898	38256	37199	35310
Visbreaker	1023	0	0	0	0	0	0	0	0	0
Hydrocracker	0	0	575	0	4906	1485	240	1595	2769	1818
Catalytic Cracker	0	0	0	0	0	0	0	0	0	0
Alkylation	0	0	0	0	0	0	0	0	0	0
Hydrogen, MSCF/D	0	0	391	1067	4428	7322	2034	4687	5351	0
Delayed Coker	0	99	132	0	61	104	0	0	253	595

TABLE 6.6 UTILITIES AND NEW FACILITIES
SHALE AND COAL OIL CASES
MID-CONTINENT AND GREAT LAKES REGIONS

REGION CRUDE	MID-CONTINENT					GREAT LAKES				
	PETROLEUM		SHALE AND COAL OILS			PETROLEUM		SHALE AND COAL OILS		
Case No.	1	5	2	3	4	1	5	2	3	4
Description	Base	Broadcut Fuel	Conven- tional	Maximum Diesel	Broadcut Fuel	Base	Broadcut Fuel	Conven- tional	Maximum Diesel	Broadcut Fuel
UTILITIES										
Plant Fuel	8033	5039	4009	2444	1860	14936	9692	10884	14039	7404
Purchased Fuel	9980	10354	16092	15897	14526	27742	28367	33244	27369	31646
Total Fuel, MMBTU/D	18013	15393	20101	18341	16332	42678	38059	44128	41408	39050
Cat and Chemicals, \$/D	4480	3519	5922	5747	5484	9271	8098	11747	11090	10868
Sulfur Made, Tons/D	9	8	15	15	14	55	54	65	63	63
NEW FACILITIES CAPACITY, B/D										
Crude Distillation	3187	927	3267	1865	837	3549	0	2637	2859	0
Vacuum Distillation	6210	5388	3405	2686	2214	11012	9379	7877	7964	6412
Naphtha Hydrotreater	0	0	2256	0	0	0	0	0	0	0
Catalytic Reformer	1372	0	2473	0	0	0	0	0	0	0
Kero/Gas Oil Hydrotreater	0	0	21493	21582	20293	5504	3966	31031	25337	25692
Visbreaker	1262	1311	0	77	0	11528	11651	10101	6388	9475
Hydrocracker	0	0	0	38	0	0	0	0	0	0
Catalytic Cracker	0	0	0	0	0	0	0	0	0	0
Alkylation	0	0	0	0	0	0	0	0	0	0
Hydrogen, MSCF/D	0	0	8887	11997	13461	0	0	15707	15998	18272
Delayed Coker	0	0	0	0	0	0	0	0	0	0

Rocky Mountain Region

<u>Case No.</u>	<u>Name</u>	<u>Description</u>
Petroleum Crudes.		
1	BASE	Base Case: 1995 Product slate.
16	BCF	Broadcut fuel for part of gasoline.
Shale oil in crude slate. Product options series.		
2A	SHALE	1995 Product slate.
3	MAX D	Maximum diesel for part of gasoline.
4	BCF	Broadcut fuel for part of gasoline.
Coal oil in crude slate. Product options series.		
5A,5B	COAL	1995 Product slate.
6	MAX D	Maximum diesel for part of gasoline.
7A	BCF	Broadcut fuel for part of gasoline.
Shale oil in crude slate. Gasoline supplements.		
1995 Product slate.		
8	MEOH	Methanol supplement.
9	ETOH	Ethanol supplement.
10	MTBE	Methy-tert-butyl ether supplement.
11	SYNNAPH	Synthetic naphtha from methanol.
Coal oil in crude slate. Gasoline supplements.		
1995 product slate.		
12	MEOH	Methanol supplement.
13	ETOH	Ethanol supplement.
14	MTBE	Methy-tert-butyl ether supplement.
15A	SYNAPH	Synthetic naphtha from methanol.

Because of changes made in model structure after initial cases were run and reviewed, Rocky Mountain Coal Case 5A should be compared with gasoline Supplement Cases 12, 13, 14 and 15A. Case 5B is consistent with product option cases 6 and 7A.

Mid-Continent and Great Lakes Regions

<u>Case No.</u>	<u>Name</u>	<u>Description</u>
Petroleum Crudes.		
1	BASE	Base Case: 1995 Product slate.
5	BCF	Broadcut fuel for part of gasoline.
Shale and coal oils in crude slate.		
Product options series.		
2	SYNCRUDE	1995 Product slate.
3	MAX D	Maximum diesel for part of gasoline.
4	BCF	Broadcut fuel for part of gasoline.

B. Fuels Compositions

The major objective of this study was to determine the compositions of highway transportation fuels that would be expected in the future when syncrudes derived from coal and shale become a significant fraction of the refining industry's total raw material. Additionally, the effect on the product compositions of adding nonpetroleum-derived gasoline components to the gasoline production were to be determined.

The linear programming model combines a variety of refinery streams to produce a final blend. Unfortunately, this is often so wide a variety as to become unmanageable in a laboratory program. For example, there were over 28 different streams used in preparing the regular no-lead gasolines. In order to reduce the number of components, a Lab Blend Definition Algorithm was developed. The Lab Blend Definition Algorithm involves translating the RPMS components used in the gasoline pool, diesel fuel, and broadcast fuel into a reasonable number of components which could be obtained for use in laboratory formulation. For the gasoline pool, the following streams will be employed:

TABLE 6.7 GASOLINE POOL COMPONENTS

	<u>Petroleum</u>	<u>Shale</u>	<u>Coal</u>
Light Straight Run	X		
Reformate - 100 RON	X		X
90 RON	X	X	X
C3-C4 Alkylate	X		
Cat Gasoline - C5-250°F	X	X	
250-410°F	X	X	
Butane	X		
Natural Gasoline	X		
Methanol	X		
Ethanol	X		
MTBE	X		
Synthetic Naphtha	X		

Those components being used for diesel fuel blending will include the following:

TABLE 6.8 DIESEL FUEL COMPONENTS

	<u>Petroleum</u>	<u>Shale</u>	<u>Coal</u>
Treated Kerosene 400-550°F	X	X	X
Treated Distillate 550-650°F	X	X	X
Treated Light Cycle Oil	X	X	
Hydrocracker Kerosene	X		

In the broadcut fuel blends, the wide boiling naphtha component (145-400°F) from petroleum, shale, and coal have been added to the gasoline and diesel streams listed above.

Each of these component streams include a number of RPMS streams which are allocated to the above components according to the listing shown in Table 6.9.

Using the component stream identifiers just described, results of computer runs on product compositions have been summarized in Tables 6.10 through 6.19. These ten tables contain the volume percentage of each component used to blend each product in a series of cases. Careful reading of the title is necessary to show how the tables are organized with a single product on a table. The sequence of the first group of three tables is:

Shale oil cases, Rocky Mountain region

Table 6.10 Regular Unleaded Gasoline

Table 6.11 Premium Unleaded Gasoline

Table 6.12 Diesel Fuel

The sequence is repeated for two other groups of three:

Coal oil cases, Rocky Mountain region

Shale and coal oil cases, Mid-Continent and Great Lakes regions

Table 6.19, the last tabulation in the group, contains broadcut fuel compositions from all cases in which this product was made.

One of the goals within this study was to produce a variety of blends which can realistically be produced in typical refineries. Table 6.20 summarizes the ranges in compositions which have been obtained from the refinery cases.

Synthetic components are identified where their properties could be expected to differ from a similar petroleum fraction. In gasolines,

(Text continues on pg. 89)

TABLE 6.9 RPMS STREAM ALLOCATION

Blending Component	RPMS Streams	RPMS Name
Light Straight Run	85-145 SR Gaso	1LL
	Mixed C5's	MC5
	Thermal C5's	TC5
	C5-IC6 Hydrocrackate	LHG
	Normal Pentane	NC5
	Natural Gasoline	N12
Reformate	90 RON Reformate	F90
	95 RON Reformate	F95
	100 RON Reformate	F00
C3-C4 Alkylate	Propylene Alkylate	LA3
	Butylene Alkylate	LA4
	Amylene Alkylate	LA5
Cat Gasoline	C5-430 Cat Gaso (T)	FCG
	250-410 Cat Gaso (S)(T)	HWG
	C5-430 Cat Gaso (S)(T)	FWG
	C5-250 Cat Gaso (S)(T)	LWG
	250-410 Cat Gaso (T)	HCG
	C5-250 Cat Gaso (T)	LCG
	C5-250 Coker Gaso	LKG
	C5-420 Poly Gaso	POL
Butanes	n-Butane	NC4
	Butylene	C4U
	Iso-butane	IC4
	Mixed butanes	MC4
Treated Kerosene 400-550°F	200-330 SR Gaso (T)	1MS
	400-550 SR Kero (T)	1SK
	400-550 SR Kero (T)	2SK
	250-400 Coker Gaso (T)	HKG
	400-550 Htr Kero	SKH
Treated Distillate 550-650°F	550-650 SR Dist (T)	1SR
	550-650 SR Dist (T)	2SR
	375-650 H'Crack Dist.	HCD
	550-650 Htr. Sr Dist.	SRH
Treated Light Cycle Oil	430-660 Htr Cy Oil	LCH
Hydrocracker Kerosene	400-550 Hck Kero	HCK
	170-375 H'crackate	HHG

TABLE 6.10 REGULAR UNLEADED GASOLINE COMPOSITION
SHALE OIL CASES
ROCKY MOUNTAIN REGION

CRUDE	PETROLEUM		SHALE OIL Product Options			Gasoline Supplements			
	1	16	2A	3	4	8	9	10	11
Case No.	Base	Broadcut	Conven- tional	Maximum Diesel	Broadcut Fuel	Methanol	Ethanol	MTBE	Synthetic Naphtha
Description		Fuel							
REGULAR UNLEADED, Light Straight Run Reformate: 100 RON	10.8	5.7	9.2	11.4	0.2	0.1	1.3	0.1	9.9
Petroleum	21.1	28.2	10.8	18.4	19.5	4.2	0	0	14.0
Synthetic	0	0	3.6	10.8	3.5	2.0	0	0	14.0
Sub-Total	21.1	28.2	17.1	29.2	23.0	6.2	0	0	23.0
Reformate: 90 RON									
Petroleum	21.1	28.2	6.1	18.5	19.6	16.1	23.1	24.7	9.1
Synthetic	0	0	3.6	10.8	3.5	7.9	11.4	15.2	5.9
Sub-Total	21.1	28.2	9.7	29.3	23.1	24.0	34.5	39.9	15.0
C3/C4 Alkylate	10.0	2.9	14.8	3.2	3.7	11.1	3.4	0.5	5.3
Butanes	7.0	9.1	6.6	8.4	7.9	0	5.7	8.6	7.2
Natural Gasoline	9.9	1.4	6.7	0	16.7	1.2	0	12.6	11.9
Methanol	0	0	0	0	0	10.0	0	0	0
Ethanol	0	0	0	0	0	0	10.0	0	0
MTBE	0	0	0	0	0	0	0	10.0	0
Synthetic Naphtha	0	0	0	0	0	0	0	0	10.0
Cat Gasoline: C5-250									
Petroleum	6.8	19.4	10.2	9.6	9.1	13.8	12.9	7.7	2.3
Synthetic	0	0	5.2	4.1	5.2	6.2	5.8	4.0	1.4
Sub-Total	6.8	19.4	15.4	13.7	14.3	20.0	18.7	11.7	3.7
Cat. Gasoline: 250-410									
Petroleum	13.3	5.1	13.5	3.4	7.1	18.9	18.2	11.0	8.8
Synthetic	0	0	7.0	1.4	4.0	8.5	8.2	5.6	5.2
Sub-Total	13.3	5.1	20.5	4.8	11.1	27.4	26.4	16.6	14.0
TOTAL VOLUME PERCENT	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0

TABLE 6.11 PREMIUM UNLEADED GASOLINE COMPOSITION
SHALE OIL CASES
ROCKY MOUNTAIN REGION

CRUDE	PETROLEUM		SHALE OIL			Gasoline Supplements			
			Product Options						
Case No.	1	16	2A	3	4	8	9	10	11
Description	Base	Broadcut Fuel	Conven- tional	Maximum Diesel	Broadcut Fuel	Methanol	Ethanol	MTBE	Synthetic Naphtha
PREMIUM UNLEADED									
Light Straight Run	5.7	3.5	5.1	1.0	3.9	0	0.3	9.7	0.7
Reformate: 100 RON									
Petroleum	22.3	23.2	33.8	11.3	12.4	21.5	0	8.7	13.6
Synthetic	0	0	19.9	6.6	2.2	10.6	0	5.4	8.7
Sub-Total	22.3	23.2	53.7	17.9	14.6	32.1	0	14.1	22.3
Reformate: 90 RON									
Petroleum	22.3	23.2	0	11.2	12.5	21.6	40.2	8.8	0
Synthetic	0	0	0	6.6	2.2	10.6	19.8	5.4	0
Sub-Total	22.3	23.2	0	17.8	14.7	32.2	60.0	14.2	0
C3/C4 Alkylate	11.0	11.9	0	17.6	18.5	8.6	4.0	15.5	11.2
Butanes	7.5	8.3	8.1	7.7	6.8	0	11.3	6.7	6.7
Natural Gasoline	0	4.9	13.6	0	0	10.7	0.5	0	1.6
Methanol	0	0	0	0	0	10.0	0	0	0
Ethanol	0	0	0	0	0	0	10.0	0	0
MTBE	0	0	0	0	0	0	0	10.0	0
Synthetic Naphtha	0	0	0	0	0	0	0	0	10.0
Cat Gasoline: C5-250									
Petroleum	23.9	21.9	5.3	21.1	18.3	2.1	4.2	8.2	19.0
Synthetic	0	0	2.8	9.0	10.3	0.6	1.6	4.2	11.2
Sub-Total	23.9	21.9	8.1	30.1	28.6	2.7	5.8	12.4	30.2
Cat. Gasoline: 250-410									
Petroleum	7.3	3.1	7.5	5.5	8.3	2.8	5.8	11.5	10.9
Synthetic	0	0	3.9	2.4	4.6	0.9	2.3	5.9	6.4
Sub-Total	7.3	3.1	11.4	7.9	12.9	3.7	8.1	17.4	17.3
TOTAL VOLUME PERCENT	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0

TABLE 6.12 NO. 2 DIESEL FUEL COMPOSITION
SHALE OIL CASES
ROCKY MOUNTAIN REGION

CRUDE Case No.	PETROLEUM		SHALE OIL Product Options			Gasoline Supplements			
	1 Base	16 Broadcut Fuel	2A Conven- tional	3 Maximum Diesel	4 Broadcut Fuel	8 Methanol	9 Ethanol	10 MTBE	11 Synthetic Naphtha
NO. 2 DIESEL FUEL									
Treated Kero 400-550									
Petroleum	30.7	30.7	1.7	28.2	6.9	1.4	0	1.2	1.1
Synthetic	0	0	22.0	13.8	15.5	21.2	18.8	21.6	22.5
Sub-Total	30.7	30.7	23.7	42.0	22.4	22.6	18.8	22.8	23.6
Treated Dist. 550-650									
Petroleum	62.7	53.9	29.6	27.8	30.9	30.6	34.5	30.5	29.7
Synthetic	0	0	46.7	30.2	46.7	46.8	46.7	46.7	46.7
Sub-Total	62.7	53.9	76.3	58.0	77.6	77.4	81.2	77.2	76.4
Treated Lt. Cycle Oil									
Hydrocracker Kero	6.6	15.4	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0	0
TOTAL VOLUME PERCENT	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0

TABLE 6.13 REGULAR UNLEADED GASOLINE COMPOSITION
COAL OIL CASES
ROCKY MOUNTAIN REGION

CRUDE	PETROLEUM		COAL OIL				Gasoline Supplements			
			Product Options							
Case No.	1	16	5A	5B	6	7A	12	13	14	15A
Description	Base	Broadcut Fuel	Conven- tional	Conven- tional	Maximum Diesel	Broadcut Fuel	Methanol	Ethanol	MTBE	Synthetic Naphtha
REGULAR UNLEADED										
Light Straight Run	10.8	5.7	8.8	13.5	9.9	0	0	1.2	0.9	7.0
Reformate: 100 RON										
Petroleum	21.1	28.2	15.0	12.7	21.8	24.8	0	0	5.2	10.7
Synthetic	0	0	10.0	8.9	12.9	4.0	0	0	3.7	7.7
Sub-Total	21.1	28.2	25.0	21.6	34.7	28.8	0	0	8.9	18.4
Reformate: 90 RON										
Petroleum	21.1	23.2	15.0	12.7	21.9	24.8	23.9	36.4	18.1	16.4
Synthetic	0	0	10.0	8.9	12.9	4.0	15.5	24.6	12.9	11.8
Sub-Total	21.1	28.2	25.0	21.6	34.8	28.8	39.4	61.0	31.0	28.2
C3/C4 Alkylate	10.0	2.9	4.0	10.4	2.3	0	12.1	0	0	4.3
Butanes	7.0	9.1	7.9	7.2	2.8	9.1	0	2.5	7.3	7.3
Natural Gasoline	9.9	1.4	12.6	7.6	0	12.7	5.1	12.6	12.6	12.6
Methanol	0	0	0	0	0	0	10.0	0	0	0
Ethanol	0	0	0	0	0	0	0	10.0	0	0
MTBE	0	0	0	0	0	0	0	0	10.0	0
Synthetic Naphtha	0	0	0	0	0	0	0	0	0	10.0
Cat Gasoline: C5-250										
Petroleum	6.8	19.4	5.2	4.8	13.6	15.3	13.9	5.3	12.2	5.4
Synthetic	0	0	0	0	0	0	0	0	0	0
Sub-Total	6.8	19.4	5.2	4.8	13.6	15.3	13.9	5.3	12.2	5.4
Cat. Gasoline: 250-410										
Petroleum	13.3	5.1	11.5	13.3	1.9	5.3	19.5	7.4	17.1	6.8
Synthetic	0	0	0	0	0	0	0	0	0	0
Sub-Total	13.3	5.1	11.5	13.3	1.9	5.3	19.5	7.4	17.1	6.8
TOTAL VOLUME PERCENT	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0

TABLE 6.14 PREMIUM UNLEADED GASOLINE COMPOSITION
COAL OIL CASES
ROCKY MOUNTAIN REGION

CRUDE	PETROLEUM		COAL OIL				Gasoline Supplements			
			Product Options							
Case No.	1	16	5A	5B	6	7A	12	13	14	15A
Description	Base	Broadcut Fuel	Conver- tional	Conven- tional	Maximum Diesel	Broadcut Fuel	Methanol	Ethanol	MTBE	Synthetic Naphtha
PREMIUM UNLEADED										
Light Straight Run	5.7	3.5	2.4	4.6	7.2	6.2	5.1	0	14.8	5.2
Reformate: 100 RON										
Petroleum	22.3	23.2	13.8	15.1	24.4	19.4	21.6	5.4	17.5	12.2
Synthetic	0	0	9.2	10.5	14.4	3.1	14.0	3.7	12.6	8.8
Sub-Total	22.3	23.2	23.0	25.6	38.8	22.5	35.6	9.1	30.1	21.0
Reformate: 90 RON										
Petroleum	22.3	23.2	9.6	15.1	24.4	19.4	21.6	6.2	17.5	12.2
Synthetic	0	0	6.4	10.5	14.4	3.1	14.0	4.2	12.6	8.8
Sub-Total	22.3	23.2	16.0	25.6	38.8	22.5	35.6	10.4	30.1	21.0
C3/C4 Alkylate	11.0	11.9	11.1	5.8	4.4	17.8	1.7	12.4	0	14.3
Butanes	7.5	8.3	7.6	8.3	10.8	8.7	2.9	4.0	5.3	7.5
Natural Gasoline	0	4.9	0	0.9	0	0	0	0	0	0
Methanol	0	0	0	0	0	0	10.0	0	0	0
Ethanol	0	0	0	0	0	0	0	10.0	0	0
MTBE	0	0	0	0	0	0	0	0	10.0	0
Synthetic Naphtha	0	0	0	0	0	0	0	0	0	10.0
Cat Gasoline: C5-250										
Petroleum	23.9	21.9	29.7	23.0	0	15.8	3.8	23.2	3.8	19.7
Synthetic	0	0	0	0	0	0	0	0	0	0
Sub-Total	23.9	21.9	29.7	23.0	0	15.8	3.8	23.2	3.8	19.7
Cat. Gasoline: 250-410										
Petroleum	7.3	3.1	10.2	6.2	0	6.5	5.3	30.9	5.9	1.3
Synthetic	0	0	0	0	0	0	0	0	0	0
Sub-Total	7.3	3.1	10.2	6.2	0	6.5	5.3	30.9	5.9	1.3
TOTAL VOLUME PERCENT	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0

TABLE 6.15 NO. 2 DIESEL FUEL COMPOSITION
COAL OIL CASES
ROCKY MOUNTAIN REGION

CRUDE	PETROLEUM		COAL OIL				Gasoline Supplements			
			Product Options							
Case No.	1	16	5A	5B	6	7A	12	13	14	15A
Description	Base	Broadcut Fuel	Conven- tional	Conven- tional	Maximum Diesel	Broadcut Fuel	Methanol	Ethanol	MTBE	Synthetic Naphtha
NO. 2 DIESEL FUEL										
Treated Kero 400-550										
Petroleum	30.7	30.7	27.3	34.2	46.4	44.8	52.4	56.2	61.3	36.1
Synthetic	0	0	7.1	5.0	1.4	0	0	0	0	2.1
Sub-Total	30.7	30.7	34.4	39.2	47.8	44.8	52.4	56.2	61.3	38.2
Treated Dist. 550-650										
Petroleum	62.7	53.9	47.6	42.8	40.6	37.0	32.6	31.2	29.4	43.8
Synthetic	0	0	18.0	18.0	11.6	16.8	13.0	11.2	9.3	18.0
Sub-Total	62.7	53.9	65.6	60.8	52.2	53.8	45.6	42.4	38.7	61.8
Trt'd. Lt. Cycle Oil	6.6	15.4	0	0	0	1.4	0	0	0	0
Hydrocracker Kero	0	0	0	0	0	0	2.0	1.4	0	0
TOTAL VOLUME PERCENT	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0

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TABLE 6.16 REGULAR UNLEADED GASOLINE COMPOSITION
SHALE AND COAL OIL CASES
MID-CONTINENT AND GREAT LAKES REGIONS

REGION CRUDE	MID-CONTINENT					GREAT LAKES				
	PETROLEUM		SHALE AND COAL OILS			PETROLEUM		SHALE AND COAL OILS		
Case No.	1	5	2	3	4	1	5	2	3	4
Description	Base	Broadcut Fuel	Conver- tional	Maximum Diesel	Broadcut Fuel	Base	Broadcut Fuel	Conven- tional	Maximum Diesel	Broadcut Fuel
REGULAR UNLEADED										
Light Straight Run	14.5	10.3	11.9	15.5	11.6	12.7	0	16.7	12.5	3.3
Reformate: 100 RON										
Petroleum	26.6	13.5	15.7	16.7	14.7	22.9	8.1	21.5	27.0	7.9
Synthetic	0	0	6.1	9.0	5.3	0	0	5.1	3.1	1.1
Sub-Total	26.6	13.5	21.8	25.7	20.0	22.9	8.1	26.6	30.1	9.0
Reformate: 90 RON										
Petroleum	5.0	13.7	15.0	16.7	14.7	9.3	17.7	9.2	25.2	23.1
Synthetic	0	0	5.9	9.0	5.3	0	0	2.2	3.1	3.3
Sub-Total	5.0	13.7	20.9	25.7	20.0	9.3	17.7	11.4	28.3	26.4
C3/C4 Alkylate	11.8	14.9	10.5	12.9	13.2	11.4	19.5	12.4	9.9	17.6
Butanes	7.3	8.1	8.8	7.5	7.8	7.9	7.6	7.8	8.0	7.3
Natural Gasoline	0	0	0	0	0	0	0	0	0	0
Cat Gasoline: C5-250										
Petroleum	12.7	14.4	0	0	12.6	14.8	30.5	6.1	10.2	23.4
Synthetic	0	0	7.4	6.8	0	0	0	0.6	1.0	5.0
Sub-Total	12.7	14.4	7.4	6.8	12.6	14.8	30.5	6.7	11.2	28.4
Cat. Gasoline: 250-410										
Petroleum	22.1	25.0	9.9	0	14.8	21.0	16.6	15.4	0	8.0
Synthetic	0	0	8.8	5.9	0	0	0	3.0	0	0
Sub-Total	22.1	25.0	18.7	5.9	14.8	21.0	16.6	18.4	0	8.0
TOTAL VOLUME PERCENT	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0

TABLE 6.17 PREMIUM UNLEADED GASOLINE COMPOSITION
SHALE AND CCAL OIL CASES
MID-CONTINENT AND GREAT LAKES REGIONS

REGION CRUDE	MID-CONTINENT					GREAT LAKES				
	PETROLEUM		SHALE AND COAL OILS			PETROLEUM		SHALE AND COAL OILS		
Case No.	1	5	2	3	4	1	5	2	3	4
Description	Base	Broadcut Fuel	Conven- tional	Maximum Diesel	Broadcut Fuel	Base	Broadcut Fuel	Conven- tional	Maximum Diesel	Broadcut Fuel
PREMIUM UNLEADED										
Light Straight Run	1.8	0	0	0.7	0	11.1	13.4	0	0.7	11.8
Reformate: 100 RON										
Petroleum	27.2	26.0	21.5	20.2	18.3	49.7	30.6	32.6	37.7	24.6
Synthetic	0	0	8.3	10.9	6.6	0	0	7.7	4.0	3.5
Sub-Total	27.2	26.0	29.8	31.1	24.9	49.7	30.6	40.3	41.7	28.1
Reformate: 90 RON										
Petroleum	25.4	25.9	14.0	12.3	18.4	0	30.5	0	10.5	24.6
Synthetic	0	0	5.5	6.7	6.6	0	0	0	1.3	3.5
Sub-Total	25.4	25.9	19.5	19.0	25.0	0	30.5	0	11.8	28.1
C3/C4 Alkylate	12.0	12.5	10.6	7.9	12.8	12.4	11.3	8.6	6.3	14.2
Butanes	9.3	9.4	8.9	8.7	9.7	7.7	9.7	8.3	8.4	9.3
Natural Gasoline	0	0	0	0	0	0	0	0	0	0
Cat Gasoline: C5-250										
Petroleum	18.5	20.3	24.8	26.1	0	12.2	0	23.9	21.6	3.5
Synthetic	0	0	0	0	18.6	0	0	6.6	7.6	0
Sub-Total	18.5	20.3	24.8	26.1	18.6	12.2	0	30.5	29.2	3.5
Cat. Gasoline: 250-410										
Petroleum	5.8	5.9	6.4	6.5	0.7	6.9	4.5	9.6	1.9	5.0
Synthetic	0	0	0	0	8.3	0	0	2.7	0	0
Sub-Total	5.8	5.9	6.4	6.5	9.0	6.9	4.5	12.3	1.9	5.0
TOTAL VOLUME PERCENT	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0

TABLE 6.18 NO. 2 DIESEL FUEL COMPOSITION
SHALE AND COAL OIL CASES
MID-CONTINENT AND GREAT LAKES REGIONS

REGION CRUDE	MID-CONTINENT					GREAT LAKES				
	PETROLEUM		SHALE AND COAL OILS			PETROLEUM		SHALE AND COAL OILS		
Case No.	1	5	2	3	4	1	5	2	3	4
Description	Base	Broadcut Fuel	Conven- tional	Maximum Diesel	Broadcut Fuel	Base	Broadcut Fuel	Conven- tional	Maximum Diesel	Broadcut Fuel
NO. 2 DIESEL FUEL										
Treated Kero 400-550										
Petroleum	34.7	40.9	34.2	49.7	60.3	48.3	35.6	32.2	33.3	27.4
Synthetic	0	0	6.8	2.8	0	0	0	6.5	1.2	15.9
Sub-Total	34.7	40.9	41.0	52.5	60.3	48.3	35.6	38.7	34.5	43.3
Treated Dist. 550-650										
Petroleum	44.5	38.0	38.0	24.8	12.4	45.9	61.9	39.7	50.2	42.0
Synthetic	0	0	18.3	17.4	19.8	0	0	18.7	11.7	13.3
Sub-Total	44.5	38.0	56.3	42.2	32.2	45.9	61.9	58.4	61.9	55.3
Trt'd. Lt. Cycle Oil	20.7	21.1	2.7	4.3	7.5	5.8	2.5	1.7	3.6	1.4
Hydrocracker Kero	0	0	0	1.0	0	0	0	1.2	0	0
TOTAL VOLUME PERCENT	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0

TABLE 6.19

BROADCAST FUEL COMPOSITION
SHALE AND COAL OIL CASES
ALL REGIONS

REGION CRUDE	ROCKY MOUNTAIN			MID CONTINENT		GREAT LAKES	
	<u>PETROLEUM</u>	<u>SHALE</u>	<u>COAL</u>	<u>PETROLEUM</u>	<u>SHALE & COAL</u>	<u>PETROLEUM</u>	<u>SHALE & OIL</u>
Case No.	16	4	7A	5	4	5	4
BROADCAST FUEL							
Light Straight Run	48.7	35.0	39.9	17.3	7.4	20.3	19.7
145-400 Naphtha							
Petroleum	39.3	0	0	29.5	3.9	41.1	26.2
Synthetic	0	32.3	46.8	0	20.9	0	15.8
Sub-Total	39.3	32.3	46.8	29.5	24.8	41.1	42.0
400-550 Kero							
Petroleum	0	0	0	0	0	0	0
Synthetic	0	8.8	0	0	22.0	0	13.6
Sub-Total	0	8.8	0	0	22.0	0	13.6
550-650 Dist							
Petroleum	10.0	4.8	10.3	23.2	9.5	21.6	4.5
Synthetic	0	0	1.4	0	8.9	0	6.0
Sub-Total	10.0	4.8	11.7	23.2	18.4	21.6	10.5
Lt. Cycle Oil	2.0	16.0	0.4	19.8	16.6	1.1	0
CS-400 Visb Gaso	0	0	0	2.6	0.9	9.4	7.8
N-Butane	0	3.1	1.2	7.6	9.9	6.5	6.4
TOTAL VOLUME PERCENT	100.0	100.0	100.0	100.0	100.0	100.0	100.0

TABLE 6.20 RANGES IN FUEL COMPOSITIONS
ROCKY MOUNTAIN REGION

	Minimum %	Maximum %		Minimum %	Maximum %
REGULAR UNLEADED			PREMIUM UNLEADED		
Light Straight Run	0	16.7	Light Straight Run	0	14.8
Reformate: 100 RON			Reformate: 100 RON		
Petroleum	0	28.2	Petroleum	0	49.7
Synthetic	0	12.9	Synthetic	0	19.9
Reformate: 90 RON			Reformate: 90 RON		
Petroleum	5.0	36.4	Petroleum	0	40.2
Synthetic	0	24.6	Synthetic	0	19.8
C3/C4 Alkylate	0.5	19.5	C3/C4 Alkylate	0	18.5
Butanes	0	9.1	Butanes	0	11.3
Natural Gasoline	0	16.7	Natural Gasoline	0	13.6
Methanol	0	10.0	Methanol	0	10.0
Ethanol	0	10.0	Ethanol	0	10.0
MTBE	0	10.0	MTBE	0	10.0
Synthetic Naphtha	0	10.0	Synthetic Naphtha	0	10.0
Cat Gasoline: C5-250			Cat Gasoline: C5-250		
Petroleum	0	30.5	Petroleum	0	30.2
Synthetic	0	7.4	Synthetic	0	18.6
Cat Gasoline: 250-410			Cat Gasoline: 250-410		
Petroleum	0	25.0	Petroleum	0	30.9
Synthetic	0	8.8	Synthetic	0	6.4
			BROADCAST FUEL		
NO. 2 DIESEL FUEL			Light Straight Run	7.4	48.7
Trt'd Kero 400-550			550-650 SR Dist		
Petroleum	0	61.3	Petroleum	4.5	23.2
Synthetic	0	22.0	Synthetic	0	46.8
Trt'd Dist 550-650			145-400 Naphtha		
Petroleum	12.4	62.7	Petroleum	0	39.3
Synthetic	0	46.8	Synthetic	0	46.8
Trt'd Lt. Cycle Oil	0	15.4	Butanes	0	9.9
Hydrocracker Kero	0	2.0	Lt. Cycle Oil	0	19.8
			C5-400 Visb Gaso	0	9.4
			400-550 SR Kero		
			Synthetic	0	22.0
			Petroleum	0	0

these components are reformat and catalytic gasoline. Other components would be essentially identical from any source. In diesel fuels straight run kerosene and treated distillate are separated into synthetic and petroleum sources. Products from catalytic cracking or hydrocracking were not segregated and usually appear in low concentration in the syncrude cases.

Reformat is stated as amounts of two grades, 90 and 100 Research Octane Number (RON). In actual practice this component would be supplied at the weighted average octane. For example, equal portions of 90 and 100 RON would produce 95 RON.

The same composition data are shown graphically on Figure 6.1 through 6.10. These ten charts are arranged in the same sequence as the preceding tables.

To simplify the graphical representation and emphasize the synfuel components, reformat of both octanes was combined into a single bar. All catalytically cracked gasoline was also combined into a single component. In broadcut fuels, visbreaker gasoline was combined with heavy naphtha since both are normally charge stocks to reforming. Compositions from these tables and charts will be the basis for a range of blends to be selected for engine and laboratory testing in future phases of the project.

The Rocky Mountain cases were further examined to trace the presence of synthetics in the transportation fuels. The percentage of synthetic (either shale oil or coal oil) in the charge was calculated for a rough comparison with the percentage of total synthetics in the transportation fuel blends. These calculations are summarized in Table 6.21. Shale oil concentration ranges from 32.7 to 35.8% of the feed. The average proportion of shale oil derived materials in the products are:

Regular Unleaded	27.5%
Premium Unleaded	24.5%
Diesel Fuel	63.7%
Broadcut Fuel	53.5%

These results indicate that the shale oil components in the gasoline pool are about 70-80% of what would be expected based on synthetics in the feed. The high proportion of shale fractions in the diesel oil and broadcut fuel suggests that these components are advantageous in these products.

Reviewing Table 6.21 for the coal oil cases, concentration ranges from 22.6 to 24.8% of the feed. The average percentages of coal oil derived materials in the transportation fuels are:

Regular Unleaded	22.5%
Premium Unleaded	23.0%
Diesel Fuel	18.8%
Broadcut Fuel	58.1%

These data suggest that the synthetics appearing in the gasoline pool are about what would be expected based on coal oil in the feed. The proportion of synthetics in diesel fuel is 70% of what would be expected and the synthetics in broadcut fuel is over twice what would be expected.

(Text continues on pg. 101)

FIG 6.1 REGULAR UNLEADED COMPOSITION

SHALE OIL CASES - ROCKY MOUNTAIN REGION

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FIG 6.2 PREMIUM UNLEADED COMPOSITION

SHALE OIL CASES - ROCKY MOUNTAIN REGION

FIG 6.3 NO. 2 DIESEL FUEL COMPOSITION

SHALE OIL CASES - ROCKY MOUNTAIN REGION

FIG 6.4 REGULAR UNLEADED COMPOSITION

COAL OIL CASES - ROCKY MOUNTAIN REGION

FIG 6.5 PREMIUM UNLEADED COMPOSITION

COAL OIL CASES - ROCKY MOUNTAIN REGION

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FIG 6.6 NO. 2 DIESEL FUEL COMPOSITION

COAL OIL CASES - ROCKY MOUNTAIN REGION

FIG 6.7 REGULAR UNLEADED COMPOSITION

SHALE & COAL-MID-CONTINENT & GREAT LAKES

FIG 6.8 PREMIUM UNLEADED COMPOSITION

SHALE & COAL-MID-CONTINENT & GREAT LAKES

FIG 6.9 NO. 2 DIESEL FUEL COMPOSITION

SHALE & COAL-MID-CONTINENT & GREAT LAKES

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FIG 6.10 BROADCAST FUEL COMPOSITIONS

SHALE AND COAL OIL CASES - ALL REGIONS

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TABLE 6.21 OCCURENCE OF SYNTHETIC COMPONENTS IN TRANSPORTATION FUELS
ROCKY MOUNTAIN REGION

Case No.	Description	Synthetic In Crude Charge, %	Synthetics in Transportation Fuels, %			
			Regular No-Lead	Premium No-Lead	No. 2 Diesel	Broadcut Fuel
1	Base Case	0	0	0	0	
16	Broadcut Fuel	0	0	0	0	0
	SHALE OIL CASES					
2	Shale Oil	34.1	45.1	28.3	68.7	
3	Maximum Diesel	35.3	31.1	25.0	44.0	
4	Broadcut Fuel	35.8	16.3	20.7	62.2	53.5
8	Methanol	32.9	24.6	22.7	68.0	
9	Ethanol	33.5	25.8	23.8	65.5	
10	MTBE	33.9	24.8	24.2	68.3	
11	Synthetic Naphtha	32.7	24.7	26.5	69.2	
	COAL OIL CASES					
5A	Coal Oil	23.4	22.1	16.2	25.1	
5B	Coal Oil	23.8	21.0	22.1	23.0	
6	Maximum Diesel	23.0	28.1	30.5	13.0	
7A	Broadcut Fuel	24.8	8.0	7.7	16.8	58.1
12	Methanol	22.7	15.5	29.2	13.0	
13	Ethanol	22.9	24.9	7.9	11.2	
14	MTBE	22.9	16.8	28.6	9.3	
15A	Synthetic Naphtha	22.6	21.1	18.8	20.1	

Coal oil based derivatives are a larger portion of the gasoline pool than the shale oil components, primarily because of more gasoline components in coal liquids. This is not overcome by the fact that the vacuum gas oil from shale oil is charged to the catalytic cracker to make more gasoline while vacuum gas oil from coal liquids goes to residual products rather than to gasoline via cracking.

C. Raw Materials Effects

The regional cases have been examined to determine the relative changes in petroleum raw materials requirements caused by introducing synthetics and gasoline supplements. The results of this analysis are shown in Tables 6.22 and 6.23. The differences in petroleum requirements were obtained by calculating differences in the petroleum consumption as defined by the following equation:

$$\text{Petroleum Required} = \text{Low-Sulfur Crude} + \text{High-Sulfur Crude} + \text{Butanes} + \text{Natural Gasoline} - \text{LPG Product} + \text{Purchased Fuel}$$

The product slate (except for LPG) was fixed in each run; LPG was allowed to vary. Therefore, in order to obtain the net differences in petroleum feedstock, the LPG output volumes had to be included. Purchased fuel in MMBTU/D was converted to Barrels Crude Oil Equivalent (BCOE) by using a factor of 5.3 MMBTU/BCOE.

Petroleum effects were calculated on a per-barrel basis. The comparisons between the base and synthetic cases used the volume of synthetic oil added. In the gasoline supplement cases, effect was calculated on a per barrel of supplement basis. For the synthetic naphtha case, the petroleum and fuel effects were reported on a per barrel of methanol basis, not per barrel of synthetic naphtha basis. Methanol yields about 42 volume percent naphtha (or about 54 volume percent hydrocarbon products, including light ends); results relative to 4,770 B/D synthetic naphtha would appear closer to ethanol and MTBE. For the maximum diesel fuel and broadcut fuel runs, the difference was based on changes in the volume of gasoline required.

Model changes were made between the coal syncrude cases and the shale cases in the Rocky Mountains. Therefore, contrasts between the shale oil and coal oil cases must be limited. The petroleum and fuel efficiency values reported are more accurate for the shale cases than for the coal cases.

The introduction of synthetics into the Rocky Mountain Region caused a decrease in the petroleum-based raw materials on nearly a one-to-one basis (Table 6.22). For each barrel of coal oil substituted, 1.03 barrels of petroleum were saved. Introducing one barrel of shale oil replaced 0.95 barrels of petroleum.

The use of methanol, ethanol, MTBE, and synthetic naphtha additives also decreased petroleum requirements. The use of supplements was set at 10 percent by volume in each grade. Ethanol and MTBE were the most efficient, saving over one barrel of petroleum per barrel of supplement.

TABLE 6.22 RAW MATERIAL EFFECTS
ROCKY MOUNTAIN REGION

CASE COMPARISON	INCREMENTAL BARRELS/DAY	PETROLEUM BARRELS/ INCREMENTAL BARREL
Base (1) Coal (5B)*	28,800 Coal Oil	-1.03
Base (1) Shale (2A)	42,000 Shale Oil	-0.95
Base (1) BCF (16)	19,100 Gasoline	-0.22
COAL CASES		
Coal (5B) Max Diesel (6)	14,300 Gasoline	-0.23
Coal (5B) BCF (7A)	19,100 Gasoline	-0.23
Coal (5A) MECH (12)	4,770 Methanol	-0.83
Coal (5A) ETOH (13)	4,770 Ethanol	-1.01
Coal (5A) MTBE (14)	4,770 MTBE	-1.16
Coal (5A) SYN NAP (15A)	11,475 Methanol	-0.58
Coal (5B) SYN NAP (15A)	11,475 Methanol	-0.56
SHALE CASES		
Shale (2A) Max Diesel (3)	14,300 Gasoline	-0.30
Shale (2A) BCF (4)	19,100 Gasoline	-0.22
Shale (2A) MECH (8)	4,770 Methanol	-0.96
Shale (2A) ETOH (9)	4,770 Ethanol	-1.21
Shale (2A) MTBE (10)	4,770 MTBE	-1.19
Shale (2A) SYN NAP (11)	11,475 Methanol	-0.56

* The terms in parentheses refer to the individual computer run numbers.

TABLE 6.23 RAW MATERIAL EFFECTS
MID-CONTINENT REGION

<u>CASE COMPARISON</u>		<u>INCREMENTAL BARRELS/DAY</u>	<u>PETROLEUM BARRELS/ INCREMENTAL BARREL</u>
Base (1)	Syncrude (2)*	15,620 Coal & Shale Oil	-0.97
Syncrude (2)	Max Diesel (3)	7,794 Gasoline	-0.28
Syncrude (2)	BCF (4)	10,392 Gasoline	-0.23
Base (1)	BCF (5)	10,392 Gasoline	-0.21

GREAT LAKES REGION

<u>CASE COMPARISON</u>		<u>INCREMENTAL BARRELS/DAY</u>	<u>PETROLEUM BARRELS/ INCREMENTAL BARREL</u>
Base (1)	Syncrude (2)*	16,130 Coal & Shale Oil	-1.02
Syncrude (2)	Max Diesel (3)	12,791 Gasoline	-0.21
Syncrude (2)	BCF (4)	17,073 Gasoline	-0.21
Base (1)	BCF (5)	17,073 Gasoline	-0.18

* The terms in parentheses refer to the individual computer run numbers.

Synthetic naphtha was the least effective of the supplements (in savings of petroleum feed), backing out 0.58 barrel of petroleum per barrel of feedstock. Methanol was intermediate, replacing 0.83 barrels of petroleum per barrel of supplement. These raw materials effects, however, do not include raw materials used in making the gasoline supplements.

The broadcast fuel and maximum diesel fuel raw material effectiveness was based on changes obtained per unit of gasoline demand reduction. The petroleum savings in both cases were 0.22, and 0.30 barrels of petroleum per barrel of gasoline replaced. The raw material savings are the combined result of less processing and a reduction in product volumes because of better fuel economy for diesel and broadcast fuels.

The comparable analysis done for the Mid-Continent and Great Lakes Regions shows very similar results (Table 6.23). The introduction of a mixed syncrude containing coal oil and shale oil caused a decrease in the petroleum consumption on nearly a one-to-one basis. The introduction of broadcast fuels caused a decrease in petroleum consumption of 0.18 to 0.23 barrels of petroleum per barrel of gasoline replaced. The decrease in petroleum consumption in the maximum diesel case was from 0.21 to 0.28 barrels of petroleum per barrel of gasoline.

D. Energy Consumption Effects

The regional cases were then examined to determine the changes in fuel requirements accompanying the introduction of syncrude into the typical refineries. The results of this analysis are reported in Tables 6.24 and 6.25. The total fuel requirements are based on differences in the total fuel requirements (as reported in Tables 6.4 through 6.6) in MMBTU per day. The total fuel requirement was defined by the following equation:

$$\text{Total Fuel Required} = \text{Plant Gas Fuel} + \text{Plant Liquid Fuel} + \text{Purchased Fuel}$$

The fuel effects were calculated on a per barrel basis with ratios similar to the raw material effects above. Model changes were made between the coal cases and the shale cases in the Rocky Mountains. Therefore, contrasts between the shale and coal oil cases must be limited. The fuel efficiency values reported are more accurate for the shale cases than for the coal cases.

The shale oil case in the Rocky Mountain Region indicated that fuel consumption increased 0.18 MMBTU per barrel of synthetic crude over the all-petroleum base case (Table 6.24). The coal oil case showed 0.03 MMBtu per barrel increase in fuel consumption. This difference was due to the greater requirement for desulfurization in the shale oil case relative to the coal oil case, as indicated in the comparison below:

	Base (1)	Shale Oil (2A)	Coal Oil (5B)
Synthetic Crude, B/D	0	42,000	28,800
Equivalent Light Distillate Desulfurization, B/D	21,524	98,287	37,608
Hydrogen Production, MSCF/D	0	63,616	1,067

TABLE 6.24 ENERGY CONSUMPTION EFFECTS
ROCKY MOUNTAIN REGION

CASE COMPARISON	INCREMENTAL BARRELS/DAY	ENERGY MMBtu/ INCREMENTAL BARREL
Base (1) Coal (5B)*	28,800 Coal Oil	+0.03
Base (1) Shale (2A)	42,000 Shale Oil	+0.18
Base (1) BCF (16)	19,100 Gasoline	-0.24
COAL CASES		
Coal (5B) Max Diesel (6)	14,300 Gasoline	+0.40
Coal (5B) BCF (7A)	19,100 Gasoline	-0.25
Coal (5A) MEOH (12)	4,770 Methanol	-0.04
Coal (5A) ETOH (13)	4,770 Ethanol	-0.40
Coal (5A) MTBE (14)	4,770 MTBE	-0.36
Coal (5A) SYN NAP (15A)	11,475 Methanol	-0.01
Coal (5B) SYN NAP (15A)	11,475 Methanol	-0.15
SHALE CASES		
Shale (2A) Max Diesel (3)	14,300 Gasoline	-0.06
Shale (2A) BCF (4)	19,100 Gasoline	-0.34
Shale (2A) MEOH (8)	4,770 Methanol	-0.23
Shale (2A) ETOH (9)	4,770 Ethanol	-1.77
Shale (2A) MTBE (10)	4,770 MTBE	-1.03
Shale (2A) SYN NAP (11)	11,475 Methanol	-0.22

* The terms in parentheses refer to the individual computer run numbers.

TABLE 6.25 ENERGY CONSUMPTION EFFECTS
MID-CONTINENT REGION

CASE COMPARISON		INCREMENTAL BARRELS/DAY	ENERGY MMBTU/ INCREMENTAL BARREL
Base (1)	Syncrude (2)*	15,620 Coal & Shale Oil	+0.13
Syncrude (2)	Max Diesel (3)	7,794 Gasoline	-0.23
Syncrude (2)	BCF (4)	10,392 Gasoline	-0.36
Base (1)	BCF (5)	10,392 Gasoline	-0.25

GREAT LAKES REGION

CASE COMPARISON		INCREMENTAL BARRELS/DAY	ENERGY MMBTU/ INCREMENTAL BARREL
Base (1)	Syncrude (2)*	16,130 Coal & Shale Oil	+0.09
Syncrude (2)	Max Diesel (3)	12,791 Gasoline	-0.21
Syncrude (2)	BCF (4)	17,073 Gasoline	-0.30
Base (1)	BCF (5)	17,073 Gasoline	-0.27

* The terms in parentheses refer to the individual computer run numbers.

The increased charge required for hydrodesulfurization was based on the requirement that all shale oils must be hydrotreated before being charged to the crude unit. The only one of the three coal oils which was hydrotreated was the material from non-catalytic hydrogenation. The coal liquid from pyrolysis was assumed to be hydrogenated before shipment to the refinery. Also, a higher percentage of the shale underwent a second treating step. The shale vacuum gas oils were hydrotreated before being sent to the FCC unit, whereas the 650°F+ fractions from coal syncrude went directly to residual fuel oils.

The fuel consumption in the Rocky Mountain shale oil case represented a 19 percent increase in total fuel consumption. Coal liquids in the same region required about 2 percent increase in fuel used, an indication of the smaller amount of processing given coal liquids.

All of the Rocky Mountain gasoline supplement cases showed fuel savings relative to their respective synthetic fuel base cases. The fuel savings for the shale oil cases appeared to be higher than those for the coal oil cases. MTBE and ethanol gave higher fuel savings than did methanol and synthetic naphtha. The synthetic naphtha cases included the utility requirements to produce the additive from a methanol feedstock. Although fuel savings were associated with the use of these products, the fuel requirements were not included in preparing each additive. Therefore, any conclusions relative to the overall energy efficiency of these additives would be inappropriate.

Fuel efficiencies for the broadcast and maximum diesel cases were based on changes in refinery fuel used per unit of gasoline demand reduction. The Rocky Mountain shale oil cases showed fuel savings through use of broadcast and diesel fuels. Savings ranged from 0.06 MMBTU per barrel in the maximum diesel fuel case to 0.34 MMBTU per barrel in the broadcast fuel case. These fuel savings equated to 0.01 to 0.06 barrels of petroleum per barrel of gasoline (based on 5.3 MMBTU per barrel of petroleum). Therefore, the energy savings were far less than the savings of 0.22 to 0.30 barrels of petroleum raw material per barrel of feed achieved through the product type shifts from gasoline to diesel and broadcast fuels.

The Rocky Mountain coal cases showed somewhat different results, especially in the maximum diesel case. In this case fuel consumption actually increased. This increase may be partially offset considering the large volume of LPG produced in this case (4514 barrels per day) relative to the coal oil base case (1239 barrels per day). These cases also supported the conclusion that the refinery fuel savings in moving to substitute automotive fuels are not as significant as the petroleum raw material savings achieved via the shift in the product types.

The comparison between the base case and the broadcast fuel case with natural crudes indicated an energy efficiency identical to that calculated for coal oil case but somewhat lower than the shale oil case.

The Mid-Continent and Great Lakes Region cases showed results similar to the above findings (Table 6.25). The fuel consumptions increase when changing to a syncrude slate from the base natural crude slate, +0.13

MMBTU/barrel of syncrude in the Mid-Continent and 0.09 MMBTU/barrel of syncrude in the Great Lakes Region. The maximum diesel cases show decreasing fuel requirements of -0.21 to -0.23 MMBTU/barrel of gasoline. The values for energy savings in these regions with mixed syncrudes are intermediate between the values from the Rocky Mountains where coal oil and shale oil has directionally different effects on fuel consumption in the maximum diesel fuel case.

The broadcast fuel cases are all quite similar in effect. The fuel savings are -0.24 MMBTU/barrel of gasoline in the Rocky Mountains, -0.25 MMBTU/barrel in the Mid-Continent, and -0.27 MMBTU/barrel in the Great Lakes. The syncrude broadcast fuel cases show slightly higher fuel consumptions.

The conclusion is consistent in all regions that petroleum raw material savings are significant in shifting product demand patterns to other fuel types such as maximum diesel or a broadcast fuel. The refinery fuel savings which occur in the same product shift are measurable but minor in magnitude.

E. Investment Effects

The effect on incremental investments required by syncrudes and gasoline supplements is shown in Tables 6.26 and 6.27. The investment ratio represents the investment required in the subject case, for example the coal case (5B) divided by the investment required in the base case (1). The investment required in the base case is chiefly in the crude unit and vacuum tower to allow for the overall demand increase. The coal oil case (5B) includes capability to process syncrude as well. The new facility requirements in barrels per stream day are shown in Tables 6.4, 6.5, and 6.6.

The investment effects indicate that introducing syncrude will require a considerable level of additional investment. In the Rocky Mountain Region, shale oil will require 2.71 times the investment while coal oil will require 1.10 times. In the Mid-Continent this ratio is 3.14 and in the Great Lakes Region the ratio is 2.24 for combined shale oil and coal oil. These additional investments are primarily a reflection of the increased requirement for hydrodesulfurization units and hydrogen production required by the syncrudes.

The broadcast fuel cases show lower investment requirements relative to their base cases. The petroleum crude broadcast fuel cases show lower investment requirements than their respective synthetic broadcast fuel cases. For example in the Mid-Continent Region, the synthetics broadcast fuel case shows an investment ratio of 0.76 compared to a 0.41 ratio for the petroleum broadcast case.

The maximum diesel fuel cases are less consistent at first glance. In the Rocky Mountain Region, the investment ratios for coal oil and shale oil cases are greater than 1.0, while for the Mid-Continent and Great Lakes Regions the investment ratios are 0.80 and 0.92 respectively. The difference may be explained by:

- a. the higher proportion of syncrude in refinery charge in the Rocky Mountains requiring more hydrogenation and hydrogen generation facilities,

TABLE 6.26 INVESTMENT EFFECTS
ROCKY MOUNTAIN REGION

CASE COMPARISON	INCREMENTAL BARRELS/DAY	INVESTMENT RATIO**
Base (1) Coal (5B)*	28,800 Coal Oil	1.10
Base (1) Shale (2A)	42,000 Shale Oil	2.70
Base (1) BCF (16)	19,100 Gasoline	0.76
COAL CASES		
Coal (5B) Max Diesel (6)	14,300 Gasoline	1.72
Coal (5B) BCF (7A)	19,100 Gasoline	0.81
Coal (5A) MEOH (12)	4,770 Methanol	0.99
Coal (5A) ETOH (13)	4,770 Ethanol	1.00
Coal (5A) MTBE (14)	4,770 MTBE	1.04
Coal (5A) SYN NAP (15A)	11,475 Methanol	1.06
Coal (5B) SYN NAP (15A)	11,475 Methanol	1.19
SHALE CASES		
Shale (2A) Max Diesel (3)	14,300 Gasoline	1.05
Shale (2A) BCF (4)	19,100 Gasoline	0.94
Shale (2A) MEOH (8)	4,770 Methanol	1.03
Shale (2A) ETOH (9)	4,770 Ethanol	1.03
Shale (2A) MTBE (10)	4,770 MTBE	0.96
Shale (2A) SYN NAP (11)	11,475 Methanol	1.06

* The terms in parentheses refer to the individual computer run numbers.

** The ratio is the investment for the second case listed divided by the first case on each line.

TABLE 6.27 INVESTMENT EFFECTS
MID-CONTINENT REGION

<u>CASE COMPARISON</u>		<u>INCREMENTAL BARRELS/DAY</u>	<u>INVESTMENT RATIO**</u>
Base (1)	Syncrude (2)*	15,620 Coal & Shale Oil	3.14
Syncrude (2)	Max Diesel (3)	7,794 Gasoline	0.80
Syncrude (2)	Broadcut (4)	10,392 Gasoline	0.76
Base (1)	Broadcut (5)	10,392 Gasoline	0.41

GREAT LAKES REGION

<u>CASE COMPARISON</u>		<u>INCREMENTAL BARRELS/DAY</u>	<u>INVESTMENT RATIO</u>
Base (1)	Syncrude (2)	16,130 Coal & Shale Oil	2.24
Syncrude (2)	Max Diesel (3)	12,791 Gasoline	0.92
Syncrude (2)	Broadcut (4)	17,073 Gasoline	0.85
Base (1)	Broadcut (5)	17,073 Gasoline	0.67

* The terms in parenthesis refer to the individual computer run numbers.

** The ratio is the investment for the second case listed divided by the first case on each line.

- b. higher diesel fuel production relative to gasoline in the Rocky Mountains, and
- c. additional segregation of the hydrotreated kerosene and distillate fractions in the latter two regions which would introduce economic flexibility to the blending operation.

The gasoline supplement cases indicate little impact on investment compared to the amount for syncrude processing. These investments do not include the costs to prepare methanol, ethanol, or MTBE so this factor must be used in interpreting the results.

F. Flowsheets

For the determined reader, four tables provide material balances for synthetic crudes in each of the regional refineries. Each table has an accompanying flowsheet with all streams identified by name and number. Table and figure numbers are:

<u>Table</u>	<u>Figure</u>	
6.28	6.11	Shale Oil - Rocky Mountain
6.29	6.12	Coal Oil - Rocky Mountains
6.30	6.13	Shale Oil - Mid-Continent and Great Lakes
6.31	6.14	Coal Oil - Mid-Continent and Great Lakes

The tables show quantity of each stream in barrels per day (B/D). For instance, Table 6.28 shows 42,000 B/D shale oil to the syncrude hydrotreater. This volume increases to 46,200 B/D charge to the crude unit by addition of hydrogen. The crude unit separation into five streams is shown with their boiling range, e.g., Stream 3, Heavy naphtha, 145-400°F. The 7392 B/D of this stream goes to the naphtha hydrotreater in most cases. Its volume increases to 7466 B/D by hydrotreating to stream 7 which is sent to catalytic reforming. In Case 4, however, 5339 B/D bypassed the hydrotreater as stream 3B and went to broadcut fuel.

Streams to blending with or without hydrotreating show on the flowsheets. Streams to conversion processes such as reforming, cracking and coking are shown but the conversion products do not appear. Those results can be inferred from product compositions on Table 6.10 through 6.19.

One difference between shale oils and coal oils processing is in the process path selected by the model for the 650°F and heavier reduced crude fraction. About half of the shale oil reduced crude is sent to a vacuum unit where it is fractionated into three streams: 650-700°F light vacuum gas oil, 700-930°F heavy vacuum gas oil, and 930°F+ vacuum residual. The vacuum gas oils are desulfurized in a gas oil hydrotreater and then charged to the fluid catalytic cracker. The balance of shale oil 650°F+ reduced crude is sent to No. 6 fuel oil blending.

By contrast, coal oil reduced crude is sent directly to No. 6 fuel oil blending. One reason for this appears to be that the vacuum gas oil from coal liquids is an inferior catalytic cracker feedstock. The other reason is the low residual volume from the coal liquids and the need to make a given volume of No. 6 fuel oil.

TABLE 5.28 SHALE OIL PROCESSING
ROCKY MOUNTAIN REGION

Stream Number	Description	Product Options			Gasoline Supplements			
		Case 2A Conventional	3 Max. Diesel	4 Broadcut	8 Methanol	9 Ethanol	10 MTBE	11 Syn. Naphtha
	Shale Oil A	21000	21000	21000	21000	21000	21000	21000
	Shale Oil E	21000	21000	21000	21000	21000	21000	21000
	TOTAL TO HYDROTREATER	42000	42000	42000	42000	42000	42000	42000
1	Crude Unit Charge	46200	46200	46200	46200	46200	46200	46200
2	Light Naphtha (85-145)	1478	1478	1478	1478	1478	1478	1478
3	Wide Boiling Naphtha (145-400)	7392	7392	7392	7392	7392	7392	7392
3A	To Hydrotreater	7392	7392	2053	7392	7392	7392	7392
3B	To Broadcut Fuel	0	0	5339	0	0	0	0
4	Kerosene (400-550)	10857	10857	10857	10857	10857	10857	10857
4A	To Hydrotreater	10857	10857	9396	10857	10857	10857	10857
4B	To Broadcut Fuel	0	0	1460	0	0	0	0
5	Distillate (550-650)	9240	9240	9240	9240	9240	9240	9240
5A	To Hydrotreater	9240	9240	9240	9240	9240	9240	9240
5B	To Broadcut Fuel	0	0	0	0	0	0	0
6	Reduced Crude (650+)	17233	17233	17233	17233	17233	17233	17233
	TOTAL STREAMS 2-6	46200	46200	46200	46200	46200	46200	46200
7	Hydrotreated Naphtha	7466	7466	2074	7466	7466	7466	7466
8	Hydrotreated Kerosene	10857	10857	9396	10857	10857	10857	10857
9	Hydrotreated Distillate	9060	9060	9060	9060	9060	9060	9060
10	Residual Fuel	8357	8679	8501	8540	8493	8591	8294
11	Vacuum Tower Feed	8876	8554	8732	8692	8740	8642	8939
12	Light Vacuum Gas Oil (650-700)	1904	1835	1873	1864	1875	1853	1917
13	Heavy Vacuum Gas Oil (700-930)	6901	6650	6789	6758	6795	6719	6950
14	Coker Feed	71	59	70	70	70	70	72
15	Hydrotreated LVGO	1833	1833	1804	1795	1805	1785	1846
15A	To Fluid Cat Cracker	1833	1833	1804	1795	1805	1785	1846
15B	To Hydrotreater	0	0	0	0	0	0	0
15C	To Low S No. 6 Fuel Oil	0	0	0	0	0	0	0
16	Hydrotreated HVGO	6562	6562	6457	6427	6462	6389	6610
16A	To Fluid Cat Cracker	6562	6562	6457	6427	6462	6389	6610
16B	To Hydrocracker	0	0	0	0	0	0	0
18	Kerosene to Jet Fuel	4704	6416	5637	4706	5845	5611	5274
19	Kerosene to No. 2 Fuel Oil	1881	298	853	2107	1373	1133	1306
20	Kerosene to Broadcut	0	0	0	0	0	0	0
21	Kerosene to No. 2 Diesel	4272	4142	2906	4044	3640	4113	4277
22	Distillate to No. 2 Fuel Oil	0	0	0	0	0	0	0
23	Distillate to Broadcut	0	0	0	0	0	0	0
24	Distillate to No. 2 Diesel	9060	9060	9060	9060	9060	9060	9060
25	Low S No. 6 Fuel Oil	7078	7224	7076	7066	7019	7078	6921
26	High S No. 6 Fuel Oil	1279	1455	1425	1474	1474	1513	1373

FIGURE 6.11 SHALE OIL PROCESSING
ROCKY MOUNTAIN REGION

TABLE 6.29 COAL OIL PROCESSING
ROCKY MOUNTAIN REGION

Stream Number	Description	Product Options				Gasoline Supplements			
		Case 5A Conventional	5B Conventional	6 Max. Diesel	7A Broadcut	12 Methanol	13 Ethanol	14 MTBE	15A Syn. Naphtha
	Coal Oil A to Hydrotreater	9600	9600	9600	9600	9600	9600	9600	9600
	Coal Oil B to Crude Dist.	9600	9600	9600	9600	9600	9600	9600	9600
	Coal Oil C to Crude Dist.	9600	9600	9600	9600	9600	9600	9600	9600
	TOTAL	28800	28800	28800	28800	28800	28800	28800	28800
1	Crude Unit Charge	29760	29760	29760	29760	29760	29760	29760	29760
2	Light Naphtha (85-145)	854	854	854	854	854	854	854	854
3	Wide Boiling Naphtha (145-400)	10042	10042	10042	10042	10042	10042	10042	10042
3A	To Hydrotreater	10042	10042	10042	10042	10042	10042	10042	10042
3B	To Broadcut Fuel	0	0	0	0	0	0	0	0
4	Kerosene (400-550)	8573	8573	8573	8573	8573	8573	8573	8573
4A	To Hydrotreater	8573	8573	8573	8573	8573	8573	8573	8573
4B	To Broadcut Fuel	0	0	0	0	0	0	0	0
5	Distillate (550-650)	3557	3557	3557	3557	3557	3557	3557	3557
5A	To Hydrotreater	3557	3557	3557	3331	3557	3557	3557	3557
5B	To Broadcut Fuel	0	0	0	226	0	0	0	0
6	Reduced Crude (650+)	6734	6734	6148	6734	6734	6734	6734	6734
	TOTAL STREAMS 2-6	29760	29760	29760	29760	29760	29760	29760	29760
7	Hydrotreated Naphtha	10142	10142	10142	10142	10142	10142	10142	10142
8	Hydrotreated Kerosene	8573	8573	8573	8573	8573	8573	8573	8573
9	Hydrotreated Distillate	3488	3488	3488	3266	3488	3488	3488	3488
10	Residual Fuel	6734	6734	6148	6734	6734	6734	6734	6734
11	Vacuum Tower Feed	6	6	586	6	0	0	0	6
12	Light Vacuum Gas Oil (650-700)	0	0	175	0	0	0	0	0
13	Heavy Vacuum Gas Oil (700-930)	3	3	218	3	0	0	0	3
14	Coker Feed	3	3	193	3	0	0	0	3
15	Hydrotreated LVGO	0	0	175	0	0	0	0	0
15A	To Fluid Cat Cracker	0	0	0	0	0	0	0	0
15B	To Hydrotreater	0	0	169	0	0	0	0	0
15C	To Low S No. 6 Fuel Oil	0	0	0	0	0	0	0	0
16	Hydrotreated HVGO	3	3	207	3	0	0	0	3
16A	To Fluid Cat Cracker	3	3	207	3	0	0	0	3
16B	To Hydrocracker	0	0	0	0	0	0	0	0
18	Kerosene to Jet Fuel	0	0	0	0	0	0	0	0
19	Kerosene to No. 2 Fuel Oil	7186	7600	8157	8573	8573	8573	8573	8160
20	Kerosene to Broadcut	0	0	0	0	0	0	0	0
21	Kerosene to No. 2 Diesel	1387	973	416	0	0	0	0	413
22	Distillate to No. 2 Fuel Oil	0	0	0	0	966	1318	1683	0
23	Distillate to Broadcut	0	0	0	0	0	0	0	0
24	Distillate to No. 2 Diesel	3488	3488	3488	3266	2522	2170	1805	3488
25	Low S No. 6 Fuel Oil	6693	6693	6148	6693	6693	6693	6693	6693
26	High S No. 6 Fuel Oil	35	35	0	35	41	41	41	35

FIGURE 6.12 COAL OIL PROCESSING
ROCKY MOUNTAIN REGION

TABLE 6.30 SHALE OIL PROCESSING
MID-CONTINENT & GREAT LAKES REGION

Stream Number	Description	Mid-Continent, Product Options			Great Lakes, Product Options		
		Case 2 Conventional	3 Max. Diesel	4 Broadcut Fuel	2 Conventional	3 Max. Diesel	4 Broadcut Fuel
	Shale Oil A	4690	4690	4690	4840	4840	4840
	Shale Oil B	4690	4690	4690	4840	4840	4840
	TOTAL TO HYDROTREATER	9380	9380	9380	9680	9680	9680
1	Crude Unit Charge	10318	10318	10318	10648	10648	10648
2	Light Naphtha (85-145)	330	330	330	340	340	340
3	Wide Boiling Naphtha (145-400)	1651	1651	1651	0	0	0
3A	To Hydrotreater	1651	1651	1704	1704	1704	1704
3B	To Broadcut Fuel	0	0	1651	0	0	1704
4	Kerosene (400-550)	2425	2425	2425	2502	2502	2502
4A	To Hydrotreater	2425	2425	2425	2502	2502	2502
4B	To Broadcut Fuel	0	0	0	0	0	0
5	Distillate (550-650)	2064	2064	2064	2130	2130	2130
5A	To Hydrotreater	2064	2064	2064	2130	2130	2130
5B	To Broadcut Fuel	0	0	0	0	0	0
6	Reduced Crude (650+)	3848	3848	3848	3972	3972	3972
	TOTAL STREAMS 2-6	10318	10318	10318	10648	10648	10648
7	Hydrotreated Naphtha	1667	1667	0	1721	1721	0
8	Hydrotreated Kerosene	2425	2425	2425	2502	2502	2502
9	Hydrotreated Distillate	2023*	2023	2023	2088	2088	2088
10	Residual Fuel	0	0	0	0	0	0
11	Vacuum Tower Feed	3848	3848	3848	3972	3972	3972
12	Light Vacuum Gas Oil (650-700)	825	825	825	852	852	853
13	Heavy Vacuum Gas Oil (700-930)	2992	2992	2992	3088	3088	3088
14	Coker Feed	31	31	31	32	32	32
15	Hydrotreated LVGO	795	795	795	820	820	820
15A	To Fluid Cat Cracker	795	795	795	820	820	820
15B	To Hydrotreater	0	0	0	0	0	0
15C	To Low S No. 6 Fuel Oil	0	0	0	0	0	0
16	Hydrotreated HWGO	2846	2846	2846	2937	2937	2937
16A	To Fluid Cat Cracker	2846	2846	2846	2937	2937	2937
16B	To Hydrocracker	0	0	0	0	0	0
18	Kerosene to Jet Fuel	2425	2425	2425	2502	2502	2502
19	Kerosene to No. 2 Fuel Oil	0	0	0	0	0	0
20	Kerosene to Broadcut	0	0	0	0	0	0
21	Kerosene to No. 2 Diesel	0	0	0	0	0	2502
22	Distillate to No. 2 Fuel Oil	0	0	0	0	0	0
23	Distillate to Broadcut	0	0	0	0	0	0
24	Distillate to No. 2 Diesel	1116	2023	2023	2088	2088	2088
25	Low S No. 6 Fuel Oil	0	0	0	0	0	0
26	High S No. 6 Fuel Oil	0	0	0	0	0	0

* 907 bbl to FCC via Stream 9B

FIGURE 6.13 SHALE OIL PROCESSING
MID-CONTINENT & GREAT LAKES REGIONS

TABLE 6.3: COAL OIL PROCESSING
MID-CONTINENT & GREAT LAKES REGION

Stream Number	Description	Mid-Continent, Product Options			Great Lakes, Product Options		
		Case 2 Conventional	3 Max. Diesel	4 Broadcut Fuel	2 Conventional	3 Max. Diesel	4 Broadcut Fuel
	Coal Oil A to Hydrotreater	2080	2080	2080	2150	2150	2150
	Coal Oil B to Crude Dist.	2080	2080	2080	2150	2150	2150
	Coal Oil C to Crude Dist.	2080	2080	2080	2150	2150	2150
	TOTAL	6240	6240	6240	6450	6450	6450
1	Crude Unit Charge	6448	6448	6448	6665	6665	6665
2	Light Naphtha (85-145)	184	184	184	131	131	131
3	Wide Boiling Naphtha (145-400)	2176	2176	2176	2142	2142	2142
3A	To Hydrotreater	2176	2176	2176	2142	2142	2142
3B	To Broadcut Fuel	0	0	0	0	0	0
4	Kerosene (400-550)	1857	1857	1857	1926	1926	1925
4A	To Hydrotreater	1857	1857	568	1926	1926	0
4B	To Broadcut Fuel	0	0	1289	0	0	1925
5	Distillate (550-650)	771	771	771	861	861	861
5A	To Hydrotreater	771	771	771	861	861	177
5B	To Broadcut Fuel	0	0	0	0	0	684
6	Reduced Crude (650+)	1460	1460	1460	1605	1605	1605
	TOTAL STREAMS 2-6	6448	6448	6448	6665	6665	6665
7	Hydrotreated Naphtha	2197	2197	2197	2154	2164	2164
8	Hydrotreated Kerosene	1857	1857	568	1926	1926	0
9	Hydrotreated Distillate	756	756	756	844	844	174
10	Residual Fuel	1446	1446	1446	1591	1591	1591
11	Vacuum Tower Feed	14	14	14	14	14	14
12	Light Vacuum Gas Oil (650-700)	14	14	14	14	14	14
13	Heavy Vacuum Gas Oil (700-950)	0	0	0	0	0	0
14	Coker Feed	0	0	0	0	0	0
15	Hydrotreated LVGO	13	13	13	13	13	13
15A	To Fluid Cat Cracker	0	0	0	0	13	0
15B	To Hydrotreater	13	13	13	7	0	0
15C	To Low S No. 6 Fuel Oil	0	0	0	6	0	13
16	Hydrotreated HVGO	0	0	0	0	0	0
16A	To Fluid Cat Cracker	0	0	0	0	0	0
16B	To Hydrocracker	0	0	0	0	0	0
18	Kerosene to Jet Fuel	150	127	0	0	0	0
19	Kerosene to No. 2 Fuel Oil	1017	1285	0	910	1624	0
20	Kerosene to Broadcut	0	0	568	0	0	0
21	Kerosene to No. 2 Diesel	591	445	0	1016	302	0
22	Distillate to No. 2 Fuel Oil	0	0	0	0	0	0
23	Distillate to Broadcut	0	0	756	0	0	0
24	Distillate to No. 2 Diesel	756	756	0	844	844	0
25	Low S No. 6 Fuel Oil	1446	1446	1446	1591	1591	1591
26	High S No. 6 Fuel Oil	0	0	0	0	0	0

FIGURE 6.14 COAL OIL PROCESSING
MID-CONTINENT & GREAT LAKES REGIONS

G. Product Quality

The product qualities for the four highway transportation fuels are shown in Tables 6.32 through 6.39 for all cases. The limiting gasoline octane specification in the regular and premium unleaded is the motor octane number. The binding distillation specifications are the maximum 35 percent off at 160°F and the maximum 96 percent off at 330°F. The blends are at or near these specifications in nearly all cases.

Gasoline blends using methanol, ethanol or MTBE exceeded the Research octane specification by 0.6 to 4.9 numbers, while just meeting Motor octane because of the relatively high blending Research octanes of these components. A formula octane specification such as $(R+M)/2$ would have reduced this research octane giveaway by about half, but would produce lower Motor octane blends with higher sensitivity.

The controlling qualities on the No. 2 diesel fuel are the maximum sulfur specification of 0.5 wt% and the minimum cetane blending number of 45.0.

In the broadcast fuel blends the controlling specifications are the maximum Reid Vapor Pressure of 9.0 psi, the maximum sulfur of 0.25 wt%, and the maximum nitrogen content of 200 ppm. The maximum nitrogen content specification is only active in the syncrude cases. Distillation curves were calculated for the broadcast fuel blends and are plotted in Figures 6.15 through 6.17.

TABLE 6.32 PRODUCT QUALITIES
SHALE OIL CASES
ROCKY MOUNTAIN REGION

	Specification		1	16	2A	3	4	8	9	10	11
	Minimum	Maximum	Base Case	Broadcut Fuel	Shale Oil	Maximum Diesel	Broadcut Fuel	Methanol	Ethanol	MTBE	Syn Nap
REGULAR UNLEADED											
Specific Gravity			0.756	0.767	0.744	0.769	0.755	0.769	0.765	0.751	0.757
Research ON Clear	90.5		90.5	93.3	90.5	92.5	90.5	95.5	94.7	92.3	90.5
Motor ON Clear	82.0		82.0	82.0	82.0	82.0	82.0	82.0	82.0	82.0	82.0
Reid Vapor Pressure		10.1	10.1	10.1	10.1	10.1	10.1	7.2	8.4	10.1	10.1
Pct off at 160°F	18.0	35.0	35.0	35.0	35.0	35.0	35.0	35.0	35.0	35.0	35.0
Pct off at 210°F	39.0	57.0	49.0	51.7	49.0	50.1	51.5	41.1	43.7	53.1	47.2
Pct off at 230°F	49.0		59.3	61.2	59.5	59.9	60.7	51.4	52.1	60.4	56.7
Pct off at 330°F	84.0	96.0	94.3	96.0	92.8	96.0	94.7	90.6	90.9	93.4	92.5
Pct Aromatics		100.0	29.5	34.2	25.1	34.7	30.6	25.1	24.9	24.0	33.1
Pct Olefins		100.0	7.3	20.6	14.8	14.1	12.5	19.8	22.5	16.2	7.1
Pct Supplement	10.0	10.0	0	0	0	0	0	10.0	10.0	10.0	10.0
PREMIUM UNLEADED											
Specific Gravity			0.753	0.750	0.769	0.743	0.738	0.795	0.774	0.747	0.741
Research ON Clear	93.5		93.5	93.5	93.5	93.8	93.5	97.1	96.4	94.1	93.5
Motor ON Clear	84.0		84.0	84.0	84.0	84.0	84.0	84.0	84.0	84.0	84.0
Reid Vapor Pressure		10.1	10.1	10.1	10.1	10.1	10.1	6.4	10.1	10.1	10.1
Pct off at 160°F	18.0	35.0	35.0	35.0	35.0	35.0	35.0	35.0	35.0	35.0	35.0
Pct off at 210°F	39.0	57.0	52.9	52.6	49.4	54.7	53.4	43.0	45.1	52.9	52.1
Pct off at 230°F	49.0		63.4	63.4	58.5	66.0	64.4	55.4	54.7	62.8	61.5
Pct off at 330°F	84.0	96.0	95.9	96.0	94.5	96.0	94.8	96.0	94.9	93.6	92.1
Pct Aromatics		100.0	28.4	26.9	41.0	23.9	22.1	37.3	29.2	22.4	26.8
Pct Olefins		100.0	18.6	21.4	8.3	26.2	24.6	3.6	13.0	12.7	26.4
Pct Supplement	10.0	10.0	0	0	0	0	0	10.0	10.0	10.0	10.0

TABLE 6.33 PRODUCT QUALITIES
SHALE OIL CASES
ROCKY MOUNTAIN REGION

	Specification		1	15	2A	3	4	8	9	10	11
	Minimum	Maximum	Base Case	Broadcut Fuel	Shale Oil	Maximum Diesel	Broadcut Fuel	Methanol	Ethanol	MTBE	Syn Nap
NO. 2 DIESEL											
Specific Gravity			0.840	0.842	0.843	0.836	0.839	0.843	0.845	0.843	0.843
Flash Index ⁽¹⁾		378.2	378.2	378.2	67.0	378.2	378.2	66.6	32.0	66.0	66.1
Flash Point, °F	125		125	125	200	125	125	201	235	201	201
Wt Pct Sulfur		0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500
Cetane Blending No.	45.0		45.0	45.0	45.0	45.0	45.0	45.0	45.0	45.0	45.0
Pour Point Index ⁽²⁾		640.5	385.7	413.6	235.6	237.3	247.1	231.2	240.8	232.9	236.1
Pour Point, °F		20	2	4	-16	-16	-14	-17	-15	-16	-16
BROADCUT FUEL											
Specific Gravity				0.736			0.762				
Reid Vapor Pressure	5.0	9.0		9.0			9.0				
Wt Pct Sulfur		0.250		0.250			0.250				
Pct off at 400°F	45.0	88.0		88.0			71.6				
Nitrogen PPM		200		0			200				

$$(1) \log_{10} (\text{FLASH INDEX}) = 42.1093 - 14.286 \log_{10} (\text{FLASH POINT, } ^\circ\text{F} + 460)$$

$$(2) \ln (\text{POUR POINT INDEX}) = -73.0883 + 12.5852 \ln (\text{POUR POINT, } ^\circ\text{F} + 460)$$

TABLE 6.34 PRODUCT QUALITIES
COAL OIL CASES
ROCKY MOUNTAIN REGION

	Specification		1	16	5A	5B	6	7A	12	13	14	15A
	Minimum	Maximum	Base Case	Broadcut Fuel	Coal Oil	Coal Oil	Maximum Diesel	Broadcut Fuel	Methanol	Ethanol	MTBE	Syn Nap
REGULAR UNLEADED												
Specific Gravity			0.756	0.767	0.764	0.759	0.787	0.766	0.771	0.780	0.755	0.758
Research ON Clear	90.5		90.5	93.3	90.5	90.5	93.8	92.3	94.6	93.0	93.0	90.5
Motor ON Clear	82.0		82.0	82.0	82.0	82.0	82.0	82.0	82.0	82.0	82.0	82.0
Reid Vapor Pressure		10.1	10.1	10.1	10.1	10.1	6.1	10.1	7.0	6.0	10.1	10.1
Pct off at 160°F	18.0	35.0	35.0	35.0	35.0	35.0	26.9	35.0	35.0	35.0	35.0	35.0
Pct off at 210°F	39.0	57.0	49.0	51.7	48.4	48.1	43.7	52.0	42.1	46.4	52.9	50.4
Pct off at 230°F	49.0		59.3	61.2	58.2	58.6	54.6	61.1	53.0	55.6	60.3	59.5
Pct off at 330°F	84.0	96.0	94.3	96.0	94.6	94.2	96.0	96.0	92.5	95.2	93.3	94.2
Pct Aromatics		100.0	29.5	34.2	34.3	30.6	39.4	34.9	24.7	29.9	26.3	31.7
Pct Olefins		100.0	7.3	20.6	5.5	5.7	14.7	16.8	14.0	7.3	16.9	6.6
Pct Supplement	10.0	10.0	0	0	0	0	0	0	10.0	10.0	10.0	10.0
PREMIUM UNLEADED												
Specific Gravity			0.753	0.750	0.749	0.759	0.788	0.752	0.804	0.757	0.777	0.750
Research ON Clear	93.5		93.5	93.5	93.5	93.5	96.8	93.8	98.4	96.1	95.4	93.5
Motor ON Clear	84.0		84.0	84.0	84.0	84.0	84.0	84.0	84.0	84.0	84.0	84.0
Reid Vapor Pressure		10.1	10.1	10.1	10.1	10.1	10.1	10.1	6.4	8.0	9.3	10.1
Pct off at 160°F	18.0	35.0	35.0	35.0	35.0	35.0	25.0	31.6	35.0	35.0	35.0	35.0
Pct off at 210°F	39.0	57.0	52.9	52.6	53.5	51.9	41.2	50.2	41.5	44.8	52.6	54.0
Pct off at 230°F	49.0		63.4	63.4	63.7	62.1	52.2	62.2	52.8	54.3	61.5	64.9
Pct off at 330°F	84.0	96.0	95.9	96.0	95.2	96.0	96.0	96.0	95.4	90.1	96.0	95.9
Pct Aromatics		100.0	28.4	26.9	27.5	33.2	43.5	28.1	41.9	22.4	35.6	28.6
Pct Olefins		100.0	18.6	21.4	23.0	17.0	7.8	15.8	3.8	22.6	4.0	17.8
Pct Supplement	10.0	10.0	0	0	0	0	0	0	10.0	10.0	10.0	10.0

TABLE 6.35 PRODUCT QUALITIES
COAL OIL CASES
ROCKY MOUNTAIN REGION

	Specification		1	16	5A	5B	6	7A	12	13	14	15A
	Minimum	Maximum	Base Case	Broadcut Fuel	Coal Oil	Coal Oil	Maximum Diesel	Broadcut Fuel	Methanol	Ethanol	MTBE	Syn Nap
NO. 2 DIESEL												
Specific Gravity			0.840	0.842	0.837	0.836	0.836	0.834	0.834	0.833	0.832	0.835
Flash Index ⁽¹⁾		378.2	378.2	378.2	378.2	378.2	378.2	378.2	378.2	378.2	378.2	378.2
Flash Point, °F	125		125	125	125	125	125	125	125	125	125	125
Wt Pct Sulfur		0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500
Cetane Blending No.	45.0		45.0	45.0	45.0	45.0	45.0	45.0	45.0	45.0	45.0	45.0
Pour Point Index ⁽²⁾		640.5	385.7	413.5	341.4	332.0	285.0	328.3	272.7	273.3	277.0	331.9
Pour Point, °F		20	2	4	-3	-4	-9	-4	-11	-11	-10	-4
BROADCUT FUEL												
Specific Gravity				0.736				0.770				
Reid Vapor Pressure	5.0	9.0		9.0				9.0				
Wt Pct Sulfur		0.250		0.250				0.250				
Pct off at 400°F	45.0	88.0		88.0				38.0				
Nitrogen PPM		200		0				200				

$$(1) \log_{10} (\text{FLASH INDEX}) = 42.1093 - 14.286 \log_{10} (\text{FLASH POINT, } ^\circ\text{F} + 460)$$

$$(2) \ln (\text{POUR POINT INDEX}) = -73.0833 + 12.8852 \ln (\text{POUR POINT, } ^\circ\text{F} + 460)$$

TABLE 6.36

PRODUCT QUALITIES
SHALE & COAL OIL CASES
MIDCONTINENT REGION

	Specification		1	5	2	3	4
	Minimum	Maximum	Base Case	Broadcut Fuel	Syncrude	Maximum Diesel	Broadcut Fuel
REGULAR UNLEADED							
Specific Gravity			0.755	0.751	0.764	0.761	0.756
Research ON Clear	91.5		91.7	91.5	92.1	92.5	91.8
Motor ON Clear	83.0		83.0	83.0	83.0	83.0	83.0
Reid Vapor Pressure		10.1	10.1	10.1	10.1	10.1	10.1
Pct off at 160°F	18.0	35.0	35.0	31.6	30.4	34.6	33.4
Pct off at 210°F	39.0	57.0	45.4	43.0	42.0	49.1	46.7
Pct off at 230°F	49.0		56.5	54.7	53.6	60.6	58.2
Pct off at 330°F	84.0	96.0	92.4	91.7	92.8	96.0	94.0
Pct Aromatics		100.0	33.6	30.3	35.2	32.4	31.4
Pct Olefins		100.0	11.5	13.1	7.4	5.5	10.6
PREMIUM UNLEADED							
Specific Gravity			0.763	0.763	0.761	0.762	0.764
Research ON Clear	94.5		94.5	94.5	94.5	94.7	94.5
Motor ON Clear	85.0		85.0	85.0	85.0	85.0	85.0
Reid Vapor Pressure		10.1	10.1	10.1	10.1	10.1	10.1
Pct off at 160°F	18.0	35.0	30.3	29.8	32.3	33.8	28.5
Pct off at 210°F	39.0	57.0	48.4	48.3	50.6	51.6	46.1
Pct off at 230°F	49.0		60.2	60.3	61.9	62.4	58.2
Pct off at 330°F	84.0	96.0	96.0	96.0	96.0	96.0	95.2
Pct Aromatics		100.0	33.7	33.3	33.5	35.4	33.9
Pct Olefins		100.0	13.6	14.9	18.2	19.1	14.1

TABLE 6.37

PRODUCT QUALITIES
SHALE & COAL OIL CASES
MIDCONTINENT REGION

	Specification			5	2	3	4
	Minimum	Maximum	Base Case	Broadcut Fuel	Syncrude	Maximum Diesel	Broadcut Fuel
NO. 2 DIESEL							
Specific Gravity			0.841	0.838	0.851	0.839	0.824
Flash Index ⁽¹⁾		378.2	378.2	378.2	43.8	378.2	378.2
Flash Point, °F	125		125	125	220	125	125
Wt Pct Sulfur		0.500	0.472	0.455	0.261	0.261	0.206
Cetane Blending No.	45.0		45.0	45.5	45.0	45.0	45.0
Pour Point Index ⁽²⁾		640.5	465.6	459.5	407.0	331.7	290.6
Pour Point, °F		20	8	8	3	-4	-9
BROADCUT FUEL							
Specific Gravity				0.797			0.818
Reid Vapor Pressure	5.0	9.0		9.0			9.0
Wt Pct Sulfur		0.250		0.250			0.250
Pct off at 400°F	45.0	88.0		58.0			45.0
Nitrogen PPM		200		0			200

$$(1)\log_{10} (\text{FLASH INDEX}) = 42.1093 - 14.286 \log_{10} (\text{FLASH POINT, } ^\circ\text{F} + 460)$$

$$(2)\ln (\text{POUR POINT INDEX}) = -73.0883 + 12.8852 \ln (\text{POUR POINT, } ^\circ\text{F} + 460)$$

TABLE 6.38

PRODUCT QUALITIES
SHALE & COAL OIL CASES
GREAT LAKES REGION

	Specification		1	5	2	3	4
	Minimum	Maximum	Base Case	Broadcut Fuel	Syncrude	Maximum Diesel	Broadcut Fuel
REGULAR UNLEADED							
Specific Gravity			0.752	0.737	0.756	0.761	0.738
Research ON Clear	92.0		92.2	92.0	92.2	92.5	92.0
Motor ON Clear	83.5		83.5	83.5	83.5	83.5	83.5
Reid Vapor Pressure		10.1	10.1	10.1	10.1	10.1	10.1
Pct off at 160°F	18.0	35.0	34.3	32.6	33.6	35.0	35.0
Pct off at 210°F	39.0	57.0	46.2	50.8	45.0	50.9	54.7
Pct off at 230°F	49.0		57.2	62.3	56.4	61.6	65.7
Pct off at 330°F	84.0	96.0	92.7	94.0	93.1	96.0	96.0
Pct Aromatics		100.0	32.5	22.4	34.0	32.1	21.8
Pct Olefins		100.0	12.9	23.0	7.1	9.9	20.9
PREMIUM UNLEADED							
Specific Gravity			0.763	0.770	0.758	0.758	0.765
Research ON Clear	95.0		95.0	95.0	95.0	95.8	95.0
Motor ON Clear	85.5		85.5	85.5	85.5	85.5	85.5
Reid Vapor Pressure		10.1	10.1	10.1	10.1	10.1	10.1
Pct off at 160°F	18.0	35.0	35.0	29.0	35.0	35.0	29.2
Pct off at 210°F	39.0	57.0	49.9	45.2	51.5	52.5	46.7
Pct off at 230°F	49.0		61.6	57.2	62.2	62.8	58.6
Pct off at 330°F	84.0	96.0	95.9	96.0	94.8	96.0	96.0
Pct Aromatics		100.0	38.4	36.8	35.8	33.5	33.4
Pct Olefins		100.0	9.9	0.5	22.8	26.8	3.6

TABLE 6.39

PRODUCT QUALITIES
SHALE & COAL OIL CASES
GREAT LAKES REGION

	Specification		1	5	2	3	4
	Minimum	Maximum	Base Case	Broadcut Fuel	Syncrude	Maximum Diesel	Broadcut Fuel
NO. 2 DIESEL							
Specific Gravity			0.838	0.830	0.845	0.844	0.836
Flash Index ⁽¹⁾		378.2	378.2	378.2	378.2	378.2	378.2
Flash, °F	125		125	125	125	125	125
Wt Pct Sulfur		0.500	0.500	0.500	0.500	0.500	0.500
Cetane Blending No.	45.0		46.3	47.2	45.0	45.0	45.2
Pour Point Index ⁽²⁾		640.5	445.3	397.6	370.8	339.7	356.3
Pour Point, °F		20	7	3	0	-3	-1
BROADCUT FUEL							
Specific Gravity				0.778			0.791
Reid Vapor Pressure	5.0	9.0		9.0			9.0
Wt Pct Sulfur		0.250		0.247			0.101
Pct off at 400°F	45.0	88.0		77.3			76.5
Nitrogen PPM		200		0			200

$$(1)\log_{10} (\text{FLASH INDEX}) = 42.1093 - 14.286 \log_{10} (\text{FLASH POINT, } ^\circ\text{F} + 460)$$

$$(2)\ln (\text{POUR POINT INDEX}) = -73.0883 - 12.8852 \ln (\text{POUR POINT, } ^\circ\text{F} + 460)$$

FIG 6.15 BROADCAST FUEL DISTILLATIONS

ROCKY MOUNTAIN REGION

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PETROLEUM
CASE 16

SHALE
CASE 4

COAL
CASE 7

FIG 6.16 BROADCAST FUEL DISTILLATIONS

MID-CONTINENT REGION

PETROLEUM
CASE 5

SHALE & COAL
CASE 4

FIG 6.17 BROADCAST FUEL DISTILLATIONS

GREAT LAKES REGION.

PETROLEUM
CASE 5

SHALE & COAL
CASE 4

VII. CONCLUSIONS

Fuels production models were developed to represent composite regional refineries using forecasts of 1995 crude supply and product slates. Within the constraints established and a likely processing scheme, the computer runs optimized the refinery operation and blending to make specification products.

When shale- and coal-derived crudes were included as feedstocks, the models demonstrated how these materials probably would be processed. Identity of the synthetic constituents was maintained as internal feedstocks through processing to finished components for product blends.

The results provide a logical, validated basis for blending test fuels for physical evaluation in following phases of the project. Compositions from the various cases will be used as patterns for blending transportation fuels with petroleum and synthetic components.

Comparisons are made in the following paragraphs of the major effects of processing shale and coal oils in the framework of the study.

A. Raw Materials

The representative synthetic crudes used in this study can replace petroleum raw materials on about one-to-one ratio. In the Rocky Mountain region, a barrel of coal oil replaced 1.03 barrels of petroleum. Shale oil replaced 0.95 barrels. In the other two regions, the syncrudes processed together replaced 0.97 and 1.02 barrels of petroleum.

Production of incremental diesel fuel conserved raw materials when replacing 30% of the gasoline. Part of the benefit was a reduction in product quantity because of better fuel economy for diesel, and part was less processing than needed for gasoline.

Broadcut fuel also achieved savings in raw materials when replacing 40% of the gasoline. Broadcut fuel economy is intermediate between gasoline and diesel fuel, so product savings were smaller. On the other hand, processing requirements for broadcut fuel were substantially reduced by using naphtha without reforming. The net effect on a per barrel basis was comparable to incremental diesel fuel. However, broadcut fuel could supply a greater proportion of the transportation needs while diesel fuel was near its limit in the maximum diesel cases.

Use of gasoline supplements had varying effects on petroleum use. Methanol replaced 0.83 to 0.96 barrel of petroleum and displaced nearly all butane from the gasoline blends. Ethanol replaced 0.96 to 1.21 barrel of raw materials while MTBE replaced a comparable 1.16 to 1.21 barrel. Methanol for synthetic naphtha was less effective, replacing 0.56 barrel of raw material for each barrel of methanol feed; the ratio would increase to 1.35 if based on the volume of synthetic naphtha produced from methanol.

B. Energy Consumption

Using 34% shale oil in raw materials resulted in an increase of about 19% in processing energy, or about 0.7 volume percent of total raw materials. Coal oil at 23% of refinery feedstocks caused a 2% increase in energy used or about 0.1 volume percent on crude. Shale oil was higher because more shale oil was processed and it received more processing.

Processing energy effects were less in the Mid-Continent and Great Lakes regions where combined synthetic crudes were 29% and 16% of feedstocks, respectively. Total energy increased 11.6 and 3.4%, amounting to 0.7 and 0.3 volume percent of raw materials.

Maximum diesel fuel production reduced energy consumption 0.2 and 0.6 volume percent of raw materials except in the Rocky Mountain coal liquids case where it increased by 0.9 volume percent of raw materials because of high total distillate production in the base case.

Broadcut fuel manufacture saved processing energy equivalent to 0.8 to 1.4 volume percent of raw materials when processing synthetic crudes. Similar savings of 0.7 to 1.0 volume percent occurred when making broadcut fuel with petroleum crudes.

Gasoline supplements were used at 10 percent concentration in blends and saved varying amounts of energy expressed as percent of raw materials:

	<u>Energy Savings, Volume %</u>	
	<u>Shale Cases</u>	<u>Coal Cases</u>
Methanol	0.2	0
Ethanol	0.6	0.3
MTBE	0.8	0.3
Synthetic Naphtha	0.4	0

Energy effects in processing for the variables studied are significant and worthy of consideration in planning. They are small compared to the raw materials effects and the quantities are included in the figures for total raw materials discussed above.

C. Investment Cost

Capital costs for additional facilities to process synthetic crudes will be substantial. Shale oil may need more facilities than coal liquids because of the greater amount of processing.

The effect of maximum diesel fuel production apparently depends on the particular refinery situation. Investment costs increased in the Rocky Mountain region but decreased in the other two regions.

Broadcut fuel reduced investment cost in all cases evaluated by reducing amount of downstream processing. This advantage will be available only if a new fuel and engine combination is developed before the facilities are built to produce conventional specification fuels. This same conclusion would apply to other types of fuels with minimal processing or to conventional fuels with revised specifications.

D. Compositions and Product Quality

Gasolines shows Research octane giveaway (octane higher than specified minimum) with methanol, ethanol and MTBE. In this respect the blends are similar to gasohol although the Motor octane, vapor pressure and distillation were controlled. Unlike gasohol, however, use of alcohols as blending components applies their higher octanes to best advantage and allows benefits from adjusting other operations, such as lower catalytic reforming octanes.

Research octane giveaway also occurred in some of the maximum diesel and broadcut fuel cases because gasoline volumes were reduced, leaving a surplus of high octane components.

Wide boiling naphtha from coal oil is a desirable reformer feed and is somewhat better than the average quality naphtha from shale oil. However, when broadcut fuel is made, naphtha from either shale or coal was selectively used in that product to avoid hydrotreating and reforming steps and their costs. Distillate fractions from shale oil were desirable in diesel fuel because of their high cetane number.

VIII. FUTURE WORK

A. Application of Results

Conclusions from the fuels optimization studies in the preceding section provide the foundation for work in subsequent tasks. Blend formulations will be selected from the case studies for three major products--gasoline, diesel fuel, and broadcut fuel. Selections will be based on consideration of:

- o Range of synfuel component volumes
- o Variation in combinations with other components
- o Variation in calculated physical properties
- o Availability of components.

Fuels will be blended with selected formulations in quantities needed for testing at Southwest Research Institute and at other laboratories involved in similar evaluations.

Fuel compositions from other studies, if available and different from those developed in this project, may be included in evaluations.

The testing schedule will be planned in detail for the fuels selected. The main effort will be directed toward performance evaluations in engines available for each type of fuel. If adequate quantities of fuel can be obtained, durability tests will be run. In addition, laboratory evaluations will be made of fuel stability and materials compatibility of selected fuels.

B. Fuels Formulation

Blends will be prepared using components from various processing steps to closely approximate specific product composition and qualities. Petroleum components are generally available and can be obtained as representative streams for use as needed.

Synfuels components, however, have limited availability, particularly those from hydrotreating and processing steps downstream of pre-treatment and distillation. The following tables outline the components and currently known status on availability:

GASOLINE COMPONENTS

	Petroleum	Shale	Coal
Light Naphtha 85-145°F	X		
Reformate 90 RON	X	0	0
100 RON	X		0
CAT Gasoline C ₅ -250°F	X	0	
250-410°F	X	0	
Alkylate	X		
Natural Gasoline 12 lb	X		
Butane	X		
Methanol	X		
Ethanol	X		
MTBE	X		
Synthetic Naphtha			0

DIESEL FUEL COMPONENTS

	Petroleum	Shale	Coal
Kerosene* 400-550°F	X	X	0
Distillate* 550-650°F	X	X	
Light Cycle Oil*	X	0	
Hydrocracker Kerosene	X		

BROADCUT FUEL COMPONENTS

	Petroleum	Shale	Coal
Light Naphtha 85-145°F	X		
Heavy Naphtha 145-400°F	X	X	0
Kerosene* 400-550°F	X	X	0
Distillate* 550-650°F	X	X	0
Light Cycle Oil*	X	0	
Butane	X		

X = available 0 = not available * = Treated

Gasoline blends can be blended to octane and RVP targets by pre-calculation and adjusting the proportions of two octane levels of reformat and of butane.

Synfuel stocks currently on hand include naphtha, kerosene (JP-5) and diesel fuel from Paraho shale oil processed at SOHIO's Toledo Refinery. Also available are middle distillate and full range distillate from SRC-II coal liquefaction at Pittsburg and Midway Coal Mining Company's pilot plant in DuPont, Washington; these latter two fuels are high in aromatics content and should be upgraded by addition of hydrogen for use in conventional engines.

The nonavailability of certain blend stocks indicated above may limit the number of fuels for testing. However, three major coal liquefaction pilot plants are scheduled for startup in 1980; coal liquids from these plants may be converted into products for use in engines. Also, an Air Force project to produce maximum jet fuel from syncrudes may generate by-products of other fuels.

C. Fuels Evaluations

A detailed schedule of engine testing and other laboratory evaluations will be prepared for fuels that can be produced from available components.

Fuels produced in other programs will also be accepted for evaluation. For example, gasoline and diesel fuel produced from coal by Sasol Limited in South Africa would be a welcome addition to the study.

Data from the fuels evaluations will be summarized and interpreted for potential modifications to the original optimization studies.

D. Computer Studies

With refinery models available for all three regions, modifications to incorporate new information will be the basis of revised optimization studies. Modifications may include:

- Feedback from engine and laboratory evaluations of fuels described above.
- Revised product specifications, for example, to meet modified engine requirements or to evaluate a range of gasoline octane levels or diesel fuel cetane specifications.
- New or up-dated syncrude quality data or downstream processing schemes from ongoing process research.
- New technology to upgrade synfuel components by other process techniques.

E. Recommendations for Other Research

Many synfuels studies, including this one, have been directed toward making fuels to meet current specifications. This requirement introduces extensive and expensive processing of syncrudes to upgrade to conventional petroleum quality levels. An alternative would be to provide lower severity processing to intermediate quality levels that would be used in engines modified to accept the lower quality fuels.

An organized approach would outline a range of cetane numbers, hydrogen contents, nitrogen contents, or other parameters for evaluation. Many of the quality parameters are interrelated and cannot be varied independently. However, treating severity changes would result in similar degrees of changes for various measures of quality.

This planning would need to consider specific feedstocks. For instance, a shale oil may be hydrotreated to a nitrogen level that assures stable products. This amount of hydrogen addition causes other changes in sulfur content, boiling range, aromatics content and other qualities related to hydrogen content. The diesel fuel fraction from this degree of treatment is likely to have a cetane number and other properties to make excellent quality diesel fuel although its lubricity may be low from the hydrotreating.

A coal oil syncrude may have less nitrogen and more aromatic molecules than shale oil. Thus hydrogenation to a comparable nitrogen level would change other properties but leave higher levels of aromatics. The diesel fraction would still be aromatic and have a low cetane number. Therefore, coal oil could be treated to additional intermediate levels, producing a diesel fraction of intermediate cetane numbers.

Broadcut fuel variations could follow similar severity studies. Gasoline by nature is a high severity product, mainly because of the need for complete sulfur and nitrogen removal from naphtha to protect reformer catalysts. However, a case could be developed for lower severity pretreatment of syncrude with high severity treating only of naphthas to reforming.

APPENDIX

ACRONYMS AND ABBREVIATIONS

AFUP	Alternative Fuels Utilization Program
API	American Petroleum Institute
ASTM	American Society for Testing and Materials
B or BBL	Barrel (42 U.S. gallons)
BCF	Broadcut Fuel
BCOE	Barrel Crude Oil Equivalent (in this report BCOE = 5.3 MMBTU Net Heating Value)
BFOE	Barrel Fuel Oil Equivalent
BPCD	Barrels per Calendar Day (B/CD)
BPD	Barrels per Day (sometimes B/D)
BPSD	Barrels per Stream Day (B/SD)
BTU	British Thermal Unit
DOE	Department of Energy
EPA	Environmental Protection Agency
ETOH	Ethanol, Ethyl Alcohol
FCC	Fluid Catalytic Cracking
HDS	Hydrodesulfurization
HHV	Higher Heating Value
HTR	Hydrotreated
IBP	Initial Boiling Point
LP	Linear Programming
LPG	Liquefied Petroleum Gas (usually Propane or Butane)
M	Thousand (as in MSCF/D)
MAX D	Maximum Diesel (in this study, 30% of gasoline is converted to diesel fuel)
MEOH	Methanol, Methyl Alcohol

MM	Million (as in MMBTU/D)
MON	Motor Octane Number
MPG	Miles per Gallon
MTBE	Methyl-Tertiary-Butyl Ether
PAD	Petroleum Administration for Defense
PADD	PAD District
R+M/2	Average of Research and Motor Octane Numbers
RON	Research Octane Number
RPMS	Refinery and Petrochemical Modeling System
RVP	Reid Vapor Pressure
SAE	Society of Automotive Engineers
SCF	Standard Cubic Feet
SR	Straight Run
SynNaph	Synthetic Naphtha Made From Methanol
TAME	Tertiary Amyl Methyl Ether
TBA	Tertiary Butyl Alcohol
VGO	Vacuum Gas Oil (LVGO = Light VGO) (HVGGO = Heavy VGO)
VLI	Vapor Lock Index
VT	Vehicle Miles Traveled

DEFINITIONS

Alkylation	Chemical reaction to add an alkyl group to another compound. In petroleum refining, typically reacting an olefin with an iso-paraffin, e.g., butylene with isobutane to make a gasoline component.
Catalytic Cracking	A process to convert high boiling gas oil fractions into lighter materials such as gasoline and distillate by high temperature and catalyst. It is widely used and can make about 40% of the gasoline production from a refinery.
Catalytic Reforming	A process to raise octane ratings of gasoline stocks by converting naphthenes and paraffins to aromatics, with hydrogen as a major byproduct. Severity can be controlled to produce the desired product octane.
Coking	Thermal cracking (pyrolysis) process to convert heavy oils to gasoline and distillate plus gas oil for cat cracking, using high temperature and long residence time. Product coke is a low ash, high BTU solid.
Hydrocracking	Cracking at high hydrogen pressure to suppress coke formation on the catalyst. Converts heavy stocks to lighter products and may saturate aromatic rings as well as olefins.
K Factor	Watson (or UOP) characterization factor used to correlate with many physical and chemical properties. Mathematically, K is the cube root of the average boiling point in degrees Rankine divided by specific gravity at 60°F. High values (12.5 - 13.0) indicate high paraffin content. Low values (10.5 - 11.0) indicate high aromatics.
Sour Crude	Originally indicated presence of dissolved H_2S in crude which smelled "sour". Now generally means high sulfur content, over 0.5 wt%. Local custom may vary and 0.5% - 1.0 wt% be called intermediate and over 1.0 wt% labeled sour.
Sweet Crude	Originally indicated absence of dissolved H_2S and its odor. Now generally means low sulfur content, 0.5% or less.

Swing Crude

A crude type which is allowed to vary or "swing" as opposed to other relatively constant "base" crudes. It is usually marginal in some respect, such as high cost or not required for some special product, so that it could be displaced by a new crude.

Vacuum Distillation

A separation process used on high boiling fractions. Under low pressure, boiling points of these fractions are reduced so distillation can be done without thermal decomposition.

Visbreaking

A thermal cracking (pyrolysis) process to convert heavy oils. Short residence time is used to prevent coke formation. Yield of light products is lower than coking. Unconverted heavy oil is usually lower viscosity than the feed.

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