General Disclaimer

One or more of the Following Statements may affect this Document

- This document has been reproduced from the best copy furnished by the organizational source. It is being released in the interest of making available as much information as possible.

- This document may contain data, which exceeds the sheet parameters. It was furnished in this condition by the organizational source and is the best copy available.

- This document may contain tone-on-tone or color graphs, charts and/or pictures, which have been reproduced in black and white.

- This document is paginated as submitted by the original source.

- Portions of this document are not fully legible due to the historical nature of some of the material. However, it is the best reproduction available from the original submission.

COMPUTER MODEL FOR REFINERY OPERATIONS WITH EMPHASIS ON JET FUEL PRODUCTION VOLUME III DETAILED SYSTEMS AND PROGRAMMING DOCUMENTATION

NASA CR-135335

June 27, 1978

Prepared for:

NASA Lewis Research Center
Cleveland, Ohio 44135

Prepared by:

Daniel N. Dunbar
Barry G. Tunnah

Gordian Associates, Inc.
711 Third Avenue
New York, New York 10017

(212) 697-9023

1. Report No.	2. Government Accession No.	3. Recipient's Catalog No.
NASA CR-135335		

4. Title and Subtitle	5. Report Date
Computer Model for Refinery Operations with Emphasis on Jet Fuel Production. Volume III. Detailed Systems and Programming Documentation	May 24, 1978
	6. Performing Organization Code

7. Author(s)	8. Performing Organization Report No.
Daniel N. Dunbar Barry G. Tunnah	1099-I
	10. Work Unit No.

9. Performing Organization Name and Address	11. Contract or Grant No.
Gordian Associates Incorporated 711 Third Avenue New York, New York 10017	NASA3-20620
	13. Type of Report and Period Covered
12. Sponsoring Agency Name and Address National Aeronautics & Space Administration Washington, D.C. 20546	Final
	14. Sponsoring Agency Code

15. Supplementary Notes

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

16. Abstract

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

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

19. Security Classif. (of this report)	20. Security Classif. (of this page)	21. No. of Pages	22. Price*
Unclassified	Unclassified	49	

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

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

TABLE OF CONTENTS

LIST OF EXHIBITS

SUMMARY

This volume of the report on The Gordian Refinery Simulation Model contains the detailed systems and programming documentation for the computer program. The program predicts the flow streams, material, energy and economic balances for a refinery processing shale oil, coal oil, and petroleum crudes with emphasis on the production of jet fuel of varying end point and hydrogen content specifications. This volume includes a detailed description of all program modules, subroutine common blocks and variables, program function statements and data values, files used during program execution and a list of program limitations as determined by the size of dimensioned arrays. The first two volumes of this report and a complete Fortran listing of the program are necessary supplements to this volume.

1.0 INTRODUCTION

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

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

This report deals with the refinery portion of the overall program. In order to have a systematic way of determining the energy efficiency of the production of various product slates involving different crude

sources and different processing schemes, the Lewis Research Center of NASA has supported the development of this computer model for petroleum refinery operation. The primary objectives of this model are:

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

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

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

4. The determination of overall refinery energy efficiency;

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

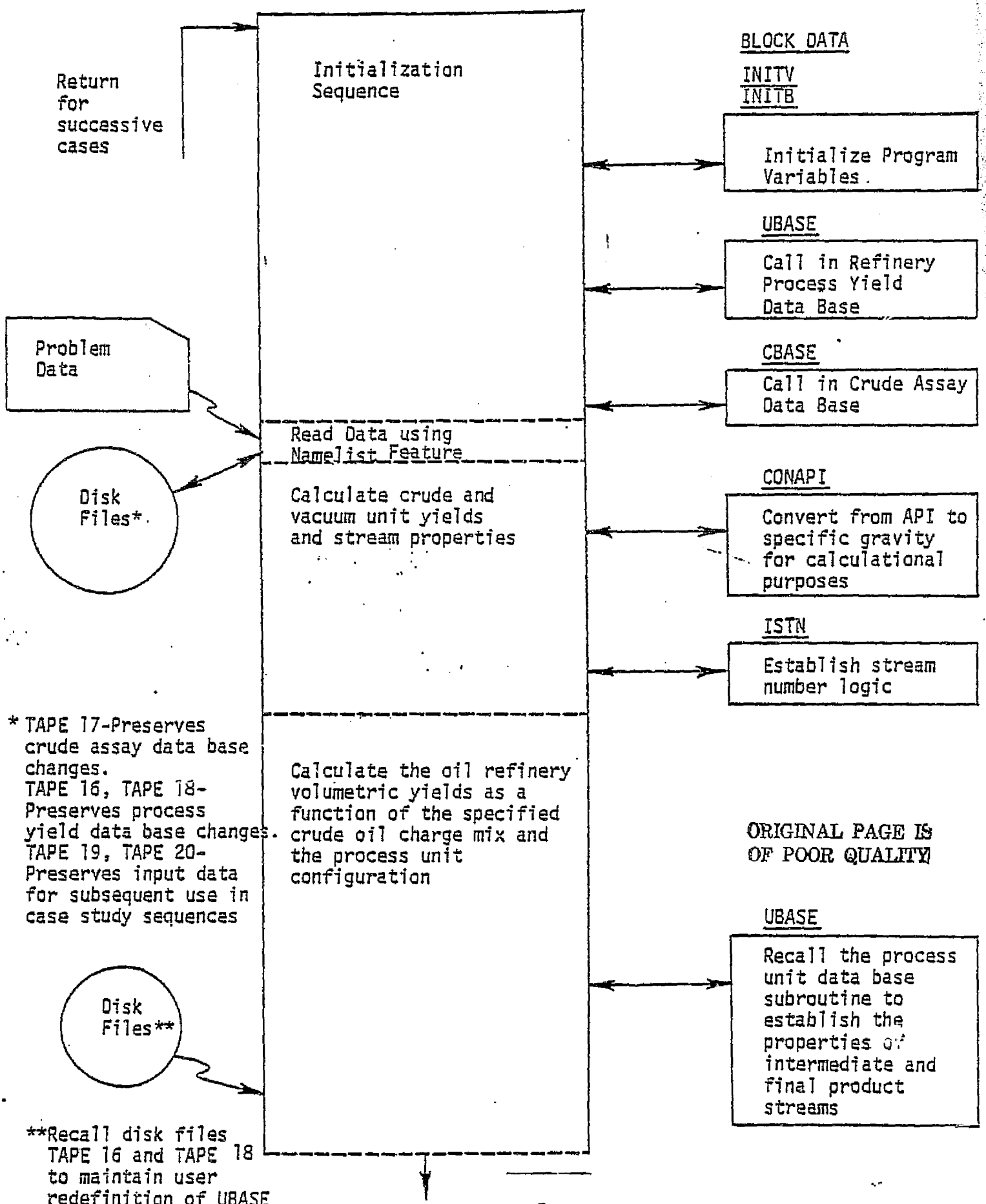
6. The capability of carrying out economic calculations.

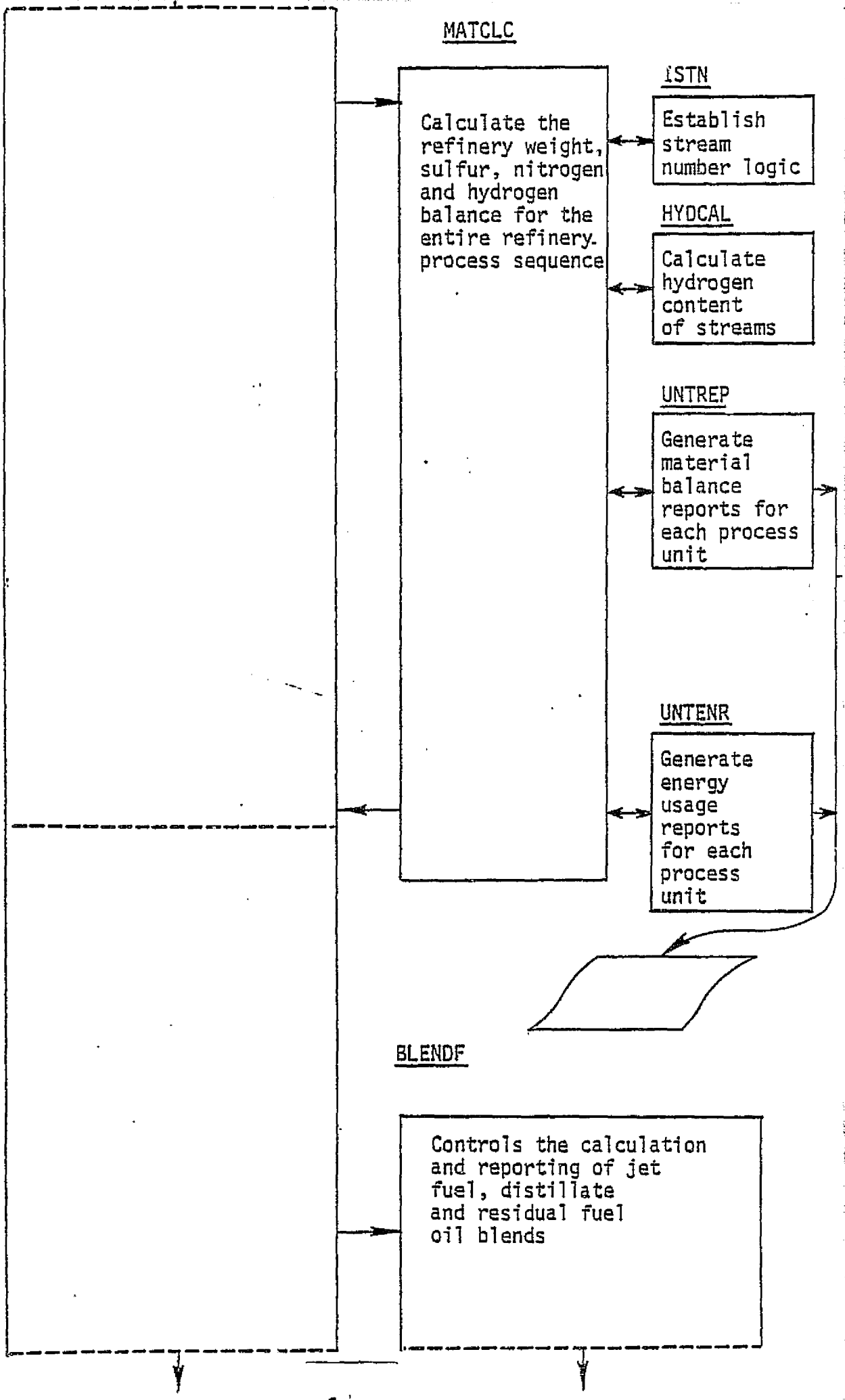
The Gordian Refinery Simulation Model, presented herein, has all the above capabilities. This report is the third of three volumes. Volume I (NASA CR-135333) is a detailed description of the program, input data, and sample output; and Volume II (NASA CR-135334) contains a description of program data bases and correlations. The complete documentation and program tape are available through the Computing Software and Management Information Office (COSMIC) under the number LEW-13047.

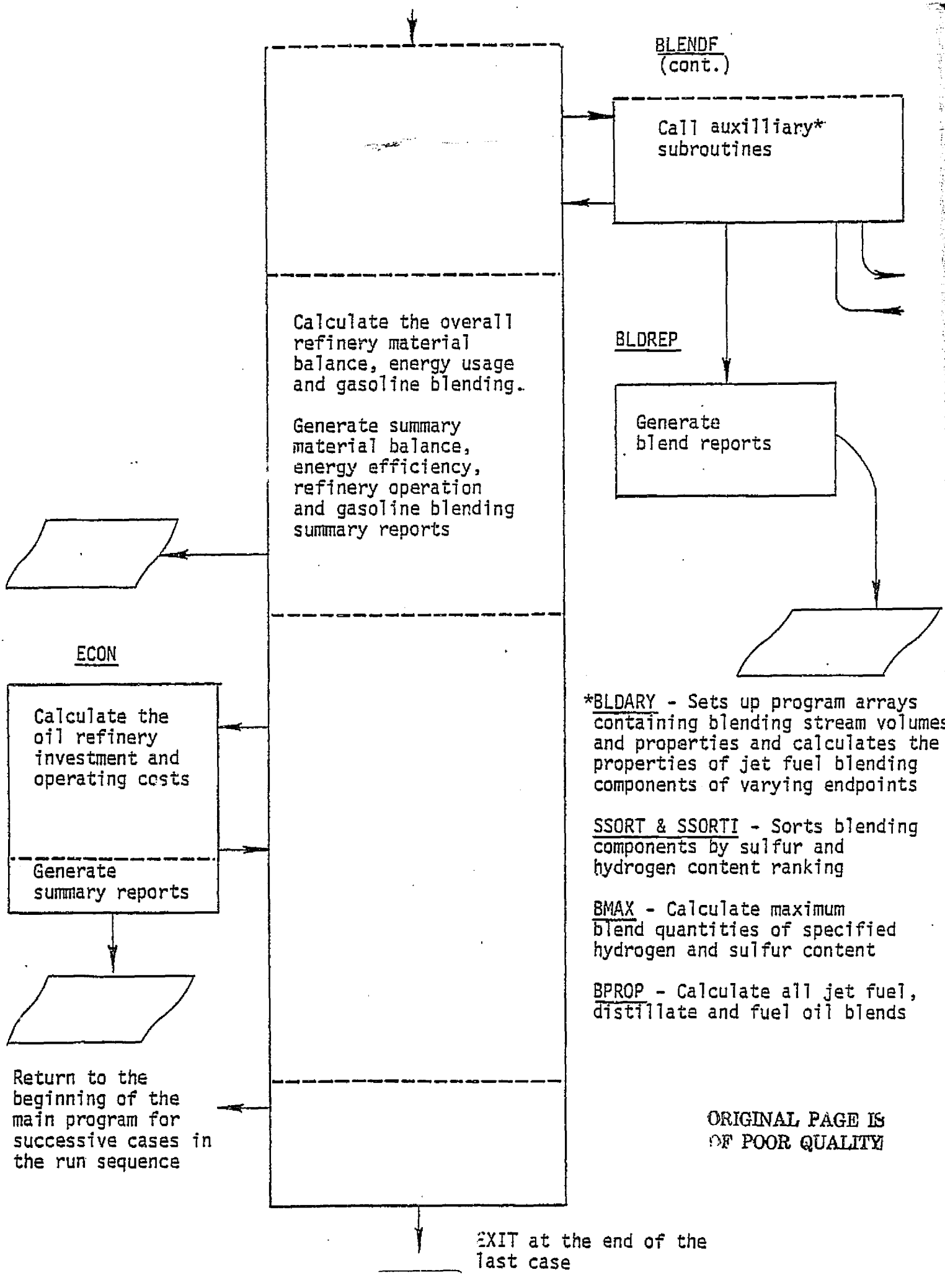
This volume is designed to aid the user in understanding the construction of the program to the point where a programmer could be able to make program changes in order to extend the scope of the calculation, alter data base values, update program correlations and increase the accuracy of the program results.

Exhibit 1 on the following page shows the program logic and the interrelationship between the main program and its subroutines. Reference is made in this volume to the preceding two volumes of this report and to the Fortran program listing. These are therefore required for a complete understanding of the contents.

EXHIBIT 1 - Block Flow Diagram of Program Logic




MATCLC
Calculate the refinery weight, sulfur, nitrogen and hydrogen balance for the entire refinery. process sequence
ISTN
Establish stream number logic
HYDCAL
Calculate hydrogen content of streams
UNTREP
Generate material balance reports for each process unit
UNTENR
Generate energy usage reports for each process unit
BLENDF
Controls the calculation and reporting of jet fuel, distillate and residual fuel oil blends



*BLDARY - Sets up program arrays containing blending stream volumes and properties and calculates the properties of jet fuel blending components of varying endpoints

SSORT & SSORTI - Sorts blending components by sulfur and hydrogen content ranking

BMAX - Calculate maximum blend quantities of specified hydrogen and sulfur content

BPROP - Calculate all jet fuel, distillate and fuel oil blends

2.0 MAIN PROGRAM AND SUBROUTINE DESCRIPTIONS

The following sections contain the detailed descriptions of the main program and the twenty subroutines which comprise the Computer Model for Refinery Operations. Section 2.1 describes the functions of the main program and each of the subroutines and the nature of the calculations performed within each of the program modules. Section 2.2 describes the subroutine calling sequence and the subroutine heirarchy.

2.1 Detailed Description of Program Modules

An overall block flow diagram describing the logic of the Gordian Model for Refinery Operations is shown in Exhibit 1. A description of the sequence of calculations and operations performed within each program module follows:

A. MAIN PROGRAM

The main program performs the following operations and computations in sequence:

(1) Reads changes to the crude oil assay data base and the process unit yield and properties data base. These changes remain in effect for the entire run sequence and are stored on temporary disk files with logical designations of 16, 17 and 18. A detailed description of these files and their contents is given in Section 5.0.

(2) Commencing with main program statement 777, the initializing subroutines INITB and INITV are called to reinitialize variable values for each case.

(3) Calls the process unit yield and properties data base subroutines (UBASE) and the crude oil assay data base (CBASE). This brings all of the model data base values into core.

(4) Reads the problem specific information for each case of the entire run sequence. Base case information is written and stored on disk file 20 while subject case changes to the base case are written on disk file 19.

(5) Commencing with program statement 6, changes to the crude oil assay and process unit yield and property data base are read from disk files 16, 17 and 18 to overlay the CBASE and UBASE subroutines data base values with those supplied by the program user. These changes remain in force throughout the entire job step.

(6) If a base case is being processed the input data is next read from disk file 20. If a subject case is being processed, the file 20 read is followed by a file 19 read, thus overlaying the base case with the subject case changes.

(7) Subroutine CONAPI is called to convert all of the input API gravity values to specific gravities.

(8) Commencing with statement 888 the properties of shale oils, coal oils, and petroleum based oils input to the refinery are blended individually according to volume or weight as appropriate. The main program function statements BFPF and FRFP are called within this calculational sequence to blend freezing point by blending index values. This computational sequence extends to the statement prior to main program statement 9, where the program loops back to statement 888 to do the blending calculation for coal oil and petroleum based refinery feeds (shale oil properties are blended in the first pass thru the loop). Subroutine INITV is called at the beginning of this loop in order to reinitialize various intermediate variables which are used in the blending calculations.

(9) Commencing with main program statement 9, the composite volumes, specific gravity, sulfur, nitrogen and hydrogen contents of the shale oil, coal oil and petroleum based refinery feeds are blended in order that the overall refinery mass, sulfur, nitrogen and hydrogen balances may be calculated at a later stage. The total heat content of the composite refinery feed streams is also computed for later use in the calculation of the overall refinery energy efficiency.

(10) Commencing with the DO LOOP statement 16 individual process unit volumetric balances are calculated. These process unit computations extended for about three hundred and seventy statements until statement 133.

The locations of the calculations for each process unit are specified below:

Statement Number	Process Unit
Seven prior to 16	Kerosene hydrotreater (petroleum)
200	Shale oil kerosene hydrotreater
208	Coal oil kerosene hydrotreater
13	Coker
22	Fluid catalytic cracker
33	Thermal gas oil cracker
34	Gas oil hydrocracker (petroleum)
216	Shale oil gas oil hydrocracker
224	Coal oil gas oil hydrocracker
44	Gas oil desulfurizer (petroleum)
55	Distillate desulfurizer (petroleum)
66	Distillate hydrocracker (petroleum)
77	Catalytic naphtha reformer
88	Butane isomerizer
99	Alkylation unit
111	Polymerization
122	Hydrogen unit

(11) Commencing with statement 133, the effect of hydrotreated kerosene sales, desulfurized diesel sales and raw gas oil sales on the refinery balance and the availability of fuel blending stocks is computed. This calculational sequence extends thru program statement 150.

(12) Subroutine UBASE is recalled to bring into computer storage the specific gravity, freezing point and PNA "deltas". These deltas correspond to the change in properties between the product and feed streams for the specific process units. Files 16 and 18 are reread to overlay these values with those (if any) which are user specified for the run sequence.

(13) Subroutine MATCLC is called to calculate the individual process unit mass balances, along with the sulfur, nitrogen and hydrogen balances. A lengthy sequence of program calculations is thus initiated which take place outside of the main program. During this sequence of calculation, optional reports are generated which give the mass, sulfur, nitrogen and hydrogen balances for each process unit along with the energy efficiency report for each unit within the user specified refinery configuration.

(14) Subroutine BLENDF is next called. Again a lengthy chain of calculations is initiated outside of the main program which calculates the volumes, masses and all properties of the jet fuel, distillate and residual blends produced by the oil refinery. Blend reports are generated during this sequence of calculations.

(15) The final segment of the main program thus has in hand all of the process unit material balance and fuel blend information necessary to calculate the overall refinery balances and to generate the corresponding reports. The sequence of calculation and operations within the final segment of main program is as follows:

(a) Calculate all refinery inputs
(b) Calculate light end products
(c) Calculate excess naphtha product
(d) Calculate the jet fuel product blend
(e) Calculate the distillate fuel product blend
(f) Calculate the residual fuel product blend
(g) Calculate the coke sales
(h) Calculate the kerosene sales (side stream)
(i) Calculate the gas oil sales (side stream)
(j) Calculate the diesel oil sales (side streams)
(k) Summarize the refinery process unit operations as elements of capacity and feed volume arrays
(l) Do the refinery gasoline blend calculations
(m) Generate the overall material balance report (crudes followed by products)
(n) Generate the refinery process unit operations reports
(o) Generate the refinery energy efficiency summary report
(p) Generate the refinery fuel, power and steam summary report
(q) Generate the gasoline pool report

(16) Subroutine ECON is called at the end of the main program to do the optional refinery economic calculations. Following this set of calculations and the generation of the economic summary calculations, a return is made to the main program. The "GO TO 777" statement in the main program loops back to the beginning of the main program in order to begin the calculation for the next case within the job sequence. Note that the read statements which pertain to overlaying the crude oil data base and the process unit yield and properties data base are not repeated since these are performed at the beginning of the entire run sequence and remain in force throughout the entire run. Separate jobs must be submitted if it is desired to make alternative data base changes.

B. BLOCK DATA

The BLOCK DATA subroutine initializes several arrays and variables prior to execution of the program. This initialization of course occurs at the beginning of the execution of the run sequence.

Various subroutines (later described) are used to reinitialize key variables at the beginning of the execution of successive case runs within a run sequence. The following arrays are initialized in BLOCK DATA:

(1) All refinery process unit yield and property arrays
(2) All refinery crude oil volumes and all crude oil array values
(3) The case title is initialized as blanks
(4) All intermediate refinery stream volumes
(5) All refinery fuel blend volumes and properties

In addition all of the refinery stream names are set in array SNAMES, all refinery process unit names in UNAMES and all crude oil names in array CN.

Certain economic subroutine values are also initialized in BLOCK DATA. These include the capital investment costs of the process units (array UNTCPC), the BPD capacities to which these dollar investments correspond (array UNTSTR), the power law coefficients for investment (array UNTEXP), the process unit dollar per barrel investment costs (array UNTVC), the dollar per day labor costs for each process unit (array UNTLC) and the annual process unit maintenance costs expressed as a percentage of the capital investment (array UNTMP). BLOCK DATA also initializes the refinery stream day factor to 0.92 and various mass and energy balance accumulators are initialized to zero.

C. INITB

This subroutine initializes select input variables when a new base case is specified within a run sequence. The classes of variables which are initialized include the process unit capacities, process unit severities, process unit feed volumes (which are calculated during the course of

previous runs) jet and other fuel blend specifications (these are initialized and reinitialized at zero to suppress the blend production unless specified in the input), fuel blend and miscellaneous by product stream productions (initialized at zero), various mass and energy balance accumulators (initialized at zero) and finally the report writer option (IREP) which is initialized at 1 for limited report generation.

D. INITV(IJ)

The purpose of this subroutine is to reinitialize accumulators prior to each run along with refinery stream and blend property arrays. The entire subroutine is invoked by calling INITV(1). A limited number of variables are reinitialized by calling INITV(2) - this is done at various points within a case calculation to reset specific accumulators.

E. CBASE

This subroutine contains the crude oil assay information for the first nineteen crude oils. A complete explanation of the crude array variables is given on pages 27 thru 29 of Volume I.

F. CBASE1

This subroutine contains the crude oil assay information for the twentieth thru the twenty-sixth crude oils. The split into two subroutines is made in order to accomodate the compilation requirements of certain IBM computer operating systems.

G. UBASE(III)

This subroutine contains the following refinery process unit yield and stream quality arrays:

(1) Process unit yields as a function of the feed stream

(2) Sulfur and nitrogen contents of refinery process streams - these are expressed as a function of the feed stream contents.

(3) Octane values at 0 and 3 ml of tetraethyl lead for the gasoline range refinery streams.

(4) Viscosity blending values of distillate and residual fuel.

(5) The specific gravity and heat of combustion of distinct light ends species such as hydrogen.

The above arrays are established within the program at their data base values by calling UBASE(1). The call to UBASE(2) establishes "deltas" for various properties, where the deltas are the differences between the process unit product and feed stream properties. These include changes in specific gravity, freezing point, and paraffin, aromatic and napthene contents. In the case of gas oil feed streams being charged to process units which produce distillate streams, absolute rather than differential freezing point and PNA properties are specified as a function of the process unit severity level.

A complete explanation of all UBASE process unit yield and physical property variables is given on pages 29 thru 45 of Volume I and Exhibits 5 and 6 of that volume.

H. MATCLC

This subroutine converts the volumetric stream balances described in the Main Program to mass balances and computes the sulfur, nitrogen and hydrogen balances. Two function statements are referenced repetitively within MATCLC to convert from specific to API gravity (TAPI) and from API to specific gravity (TSPGG). Both are required since the feed stream specific gravities for each process unit must be converted to API gravity in order to add the data base "delta" API gravity between product and feed streams ..... and this sum must then be reconverted to specific gravity in order to calculate the mass balances.

The initial segment of MATCLC thru statement 141 sets the process unit gravities for the thirteen light end species to the correct values. The logic of the remainder of the subroutine is repetitive in nature, with successive sections calculating the mass, sulfur, nitrogen and hydrogen balances for each process unit specified for the oil refinery configuration.

Four subroutines are called for each process unit calculation:

ISTN - sets the process unit stream numbers according to the stream codes listed in Exhibit 5 of Volume I.

HYDCAL - calculates the hydrogen content of each stream as a function of API gravity, mean boiling point and sulfur and nitrogen content. The sole exceptions are for the petroleum, shale and coal oil crude units since the hydrogen contents for these process unit streams are obtained directly from the crude oil assays (subroutines CBASE and CBASE1) and it is hence not necessary to call HYDCAL. Subroutine HYDCAL returns to MATCLC with a calculated hydrogen content for each stream vs. the value of 0.0 that was originally transmitted from MATCLC. Program initialization sets these values at 0.0 unless overridden by user values. These overides may be provided for selected streams involved in the blending of aviation turbine jet fuel as listed on pages 39 and 40 of Volume I.

UNTREP - generates the process unit material balance report.

UNTENR - generates the process unit energy consumption report.

The specific sections of MATCLC where each process unit calculation is performed are listed below in the order of calculation:

Statement Number	Process Unit
141	Petroleum crude unit
80	Coal oil crude unit
151	Shale oil crude unit
1	Petroleum kerosene hydrotreater
154	Fluid coker
81	Visbreaker
4	Fluid catalytic cracker
5	Thermal cracker
6	Petroleum gas oil hydrocracker
157	Petroleum gas oil desulfurizer
9	Petroleum middle distillate desulfurizer
10	Petroleum middle distillate hydrocracker

Statement Number	Process Unit
6161	Shale oil kerosene hydrotreater
176	Coal oil kerosene hydrotreater
177	Shale oil gas oil hydrocracker
178	Coal oil gas oil hydrocracker
1111	Naphtha reformer
12	Butane isomerizer
13	Alkylation unit
14	Polymerization unit
15	Hydrogen plant

The material balances calculated by subroutine MATCLC are an integral part of the overall program calculations. The UNTREP and UNTENR report subroutines which are called from MATCLC return immediately without issuing reports if the report option indicator IREP is not set at 2 or higher.

I. ISTN (NS, I1, I2...I15)

This subroutine performs an important function in terms of the overall program logic. The calls to this subroutine are made from the main program and subroutine MATCLC in order to identify the coded stream numbers for subsequent strings of volumetric and mass balance calculations (1). The first argument NS is the total number of stream numbers to be coded, and I1 thru I15 are the coded stream numbers themselves. Thus up to fifteen stream numbers may be set, corresponding to (for example) two process unit feed streams and up to thirteen product streams. This is more than sufficient for any of the process units represented in the model. Excess arguments are coded with a dummy variable. For example, the call statement for the alkylation unit mass balance from MATCLC is as follows:

---

(1) A full list of the coded stream numbers is given in Exhibit 5 of Volume I.

Call ISTN (4,8,10,21,22,M,M,M,M,M,M,M,M,M,M,M)

where from Exhibit 5, Volume I,

Stream 8 is isobutane (a feed)
Stream 10 is butylene (a feed)
Stream 21 is light alkylate (a product)
Stream 22 is a heavy alkylate (a product)

The total number of streams involved is four, as indicated by the first call argument. M is a dummy variable which is defined in MATCLC. Feed streams are listed first to accomodate the reporting functions handled by subroutine UNTREP.

Once the series of coded stream numbers is set within subroutine ISTN, the series of stream numbers is transmitted to the other program subroutines through labeled common/ISTNUM/ which contains the array ISTR(66) and NSTOT. In the example of the alkylation process unit, the ISTR array positions will contain the following:

ISTR(1) 8
ISTR(2) 10
ISTR(3) 21
ISTR(4) 22
ISTR(5) spillover
Thru from previous
ISTR(66) calculations

Subsequent calls to calculational and report subroutines will transmit the information that only the first four elements of the ISTR array are to be used. The logic contained within subroutine ISTN has thus informed subroutine MATCLC (and subroutines HYDCAL, UNTREP and UNTENR which also utilize this information) in this example that the mass balance and related calculations are for the alkylation unit. This remains in force until the next call to subroutine ISTN is made.

The calls to subroutine ISTN are made from MATCLC and the main program. The calls from the main program are made to identify the feed and product streams for the petroleum, shale and coal oil crude processing units.

J. HYDCAL (AAA,SSS,NNN,PCTHY,NSTRM)

This subroutine calculates the hydrogen content of process unit streams as a function of API gravity and sulfur and nitrogen content. The calling arguments are listed below:

AAA	specific gravity (converted in HYDCAL to API gravity)
SSS	weight percent sulfur content
NNN	weight percent nitrogen content
PCTHY	the weight percent hydrogen which is returned to the calling subroutine
NSTRM	the number of active streams and thus the number of streams to be accessed within array ISTR.

The calculations within HYDCAL are bypassed for any coded streams with an identification number of 13 or lower since these are distinct light end hydrocarbon compounds (such as propane) whose hydrogen contents are known. The calculations are also bypassed if PCTHY has been prespecified and has a value other than the program initialization value of 0.0. This allows model users the flexibility to make their own estimates of hydrogen content for the key aviation turbine fuel blending streams.

The array STRMBP which is set within HYDCAL contains the mean boiling points for each of the possible sixty-six process streams represented within the model (the first thirteen are set at 0.0 because these light end streams are not referenced). The BPI, APII and CHR arrays contain the correlation values obtained from the Technical Data

Book - Petroleum Refining (1966), Figure 2B2.1, page 2-11, and refer to mean boiling point (°F), API gravity and carbon-to-hydrogen ratio. This correlation forms the basis of the HYDCAL prediction in which a double linear interpolation is performed between the stream API and mean boiling points, with reference to the tabular array values, to arrive at the estimated carbon-to-hydrogen ratio for each stream. Adjustments are then made for the sulfur and nitrogen contents to obtain the weight percent hydrogen content. A bias correction is programmed for shale and coal oil cuts to adjust the petroleum-based correlation which is used for these different hydrocarbon species.

K. UNTREP (YLDARC,SULARC,NITARC,SPGARC,HYDARC,NSTR,NF, UNAME,UNAME1,UNAME2)

This subroutine is called from MATCLC and reports the mass, sulfur, nitrogen and hydrogen balances for each refinery process unit. The report function is bypassed if the report level indicator IREP is set at less than 3. A set of preliminary calculations are always made in UNTREP, however, since they involve the accumulation of mass, sulfur, nitrogen and hydrogen for the overall refinery material balance which is reported from the main program. These are accumulated in the arrays SVWGT, SVSUL, SVNIT, and SVHYD respectively, and are transmitted back to the main program thru the labeled common/OBAL/.

The UNTREP subroutine arguments are listed below:

YLDARC	Stream masses
SULARC	Stream sulfur masses
NITARC	Stream nitrogen masses
SPGARC	Stream specific gravities
HYDARC	Stream hydrogen masses
NSTR	Total number of streams active in the ISTR array
NF	Total number of process unit feed streams
UNAME	The alpha numeric-
UNAME1	process unit-
UNAME2	name

The total mass and component masses are transmitted in units of pounds per day and converted to pounds per hour within UNTREP. Stream specific gravity values are converted to API gravity for reporting purposes. Subroutine UNTREP must distinguish between the process unit feed and product streams in order to report the material balances correctly. Since the CALL ISTN statement always lists feed streams first, the value NF, which provides the number of feed streams in the list, completes the information required by UNTREP. The use of the ISTR array containing the process unit stream code identifiers permits the proper corresponding stream names to be referenced for report purposes.

L. UNTENR (YLDARC,UNAME,UNAME1,UNAME2)

This is a companion subroutine to the above which reports the refinery process unit energy balances if the report level indicator IREP is set at greater than 2. A portion of the subroutine calculation proceeds in all cases and involves the accumulation of energy related arrays for the overall energy consumption report issued by the main program. These arrays are:

SVBTU	Btu's consumed in the form of fuel, power, steam and hydrogen
SVBTUS	The above, converted to SI units
SVFOE	Expressed in barrels FOE
SVPCT	Energy consumption expressed as a percentage of total refinery Btu input

The UNTENR subroutine calling arguments are listed below:

YLDARC	The process unit masses. Only the first four, YLDARC(1) thru YLDARC(4) are referenced
UNAME	The alpha numeric-
UNAME1	process unit-
UNAME2	name

The first four stream identifiers in the YLDARC array always contain the following information for all process units:

YLDARC(1) Strem consumption
YLDARC(2) Fuel consumption
YLDARC(3) Power usage
YLDARC(4) Hydrogen usage

Steam, fuel and hydrogen usage are transmitted in units of barrels of fuel oil equivalent per day and converted to the reporting units within UNTENR. There is a potential for confusion between the hydrogen values for the catalytic reformer and hydrogen plant, which produce hydrogen, and all of the other process units which consume it. Therefore appropriate programming checks are made within subroutine UNTENR.

M. BLENDF

This subroutine provides the logic for calculating the sequence of fuel oil blends ranging from jet fuel aviation turbine blends to residual fuel oil.

The first call from BLENDF is to subroutine BLDARY which sets up the volumetric and properties arrays for the entire forty-seven potential fuel oil blending components. The remaining BLENDF statements are involved with a series of call statements which produce each of the blends. A key to understanding the blending logic is to inspect the element of the VT(I) array to determine the blend being produced, where I is the blend code number. These code numbers are enumerated below:

Blend Code Number	Blend Description
1	The total distillate fuel oil blend.
2	The maximum distillate fuel oil blend that can be produced at SPECMD percent sulfur.

Blend Code Number	Blend Description
3	The remaining middle distillate fuel oil blend after blend 2 is produced from the total distillate fuel oil pool.
4	The middle distillate blend of volu. VM1 and percent sulfur SPM1.
5	The middle distillate blend of volume VM2 and percent sulfur SPM2.
6	The remaining middle distillate fuel oil blend after blends 4 and 5 have been produced.
7	The total residual fuel oil blend.
8	The maximum residual fuel oil blend that can be produced at SPECRF percent sulfur.
9	The remaining residual fuel oil blend after blend 8 is produced from the total residual fuel oil pool.
10	The residual fuel oil blend of volume VR1 and percent sulfur SPR1.
11	The residual fuel oil blend of volume VR2 and percent sulfur SPR2.
12	The remaining residual fuel oil blend after blends 10 and 11 have been produced.
13	The total middle distillate plus residual fuel oil blend after making all fixed volume blends, i.e. blends 4, 5, 10, and 11.
14	The 525°F endpoint aviation turbine jet fuel blend.
15	Blend 14 as limited by the minimum hydrogen content specification HDSPEC.
16	The 650°F endpoint aviation turbine jet fuel blend.
17	Blend 16 as limited by the minimum hydrogen content specification HDSPEC.
18	The aviation turbine jet fuel blend at the specified variable endpoint EPSPEC.
19	Blend 18 as limited by the minimum hydrogen content specification HDSPEC.

The blend specification variables which are underlined above are defined on pages 47 and 48 of Volume I. The general logic reflected in subroutine BLEND is to produce all blends independently of one another wherever possible (this is not possible with blends 4,5, and 6 since 6 is defined as the blend remaining after blends 4 and 5 are produced, and similarly for blends 10, 11, and 12).

A call is made to subroutine BLDREP from BLENDF in order to report the volume, composition and properties of each of the blends produced. These reports cannot be suppressed by user option. The program logic of producing and reporting all of the possible blend combinations yields the maximum information. The overall material balance reported from the main program includes only the following: blend 19; the remaining middle distillate pool after making blend 19 (i.e. blend 1 minus blend 19); and blend 7. These are the aviation turbine jet fuel blends of specified endpoint and hydrogen content, the remaining middle distillate pool and the total residual fuel oil blend. These blends are of prime interest in the overall material and volumetric balances and do not contain overlapping components, as do some of the other blends.

A set sequence of subroutine calls is made from within BLENDF for each of the fuel oil blends produced.

These are:

Subroutine(s)	Function
SSORT or SSORT1	Sorts blending components by maximum sulfur or minimum hydrogen content.
BMAX	Calculates the maximum quantity of a blend of specified sulfur or hydrogen content that can be produced.

Subroutine(s)	Function
BPROP	Calculates the full set of blend properties.
BLDREP	Produces the blend reports.

BMAX is omitted from the calling sequence for a particular blend if the particular blend volume is not limited by a sulfur or hydrogen specification (e.g. blends 1, 7, 14 and 16).

N. BLDARY (IJK)

BLDARY is called a total of three times from subroutine BLENDF. The first call establishes the stream volumes and all related properties for each of the potential forty-seven possible blending components. The second call adjusts these properties and stream volumes for the variable endpoint aviation turbine jet fuel blend (controlled thru the input SPSPEC), and the third call restores the original stream volumes for the middle distillate and residual fuel oil blending sequence contained within the final segments of subroutine BLENDF. The BLDARY argument, IJK, is set at a value of 1 for the first and third call, and at 2 for the second call.

The blend component volume and properties which are set within BLDARY are results of volumetric and mass calculations previously performed in the main program and subroutine MATCLC. The stream properties are established on the basis of internally stored data base property values contained in subroutines CBASE, CBASE1 and UBASE. The following arrays are set up in subroutine BLDARY:

Array	Description
VOL	Stream volume, BPD
API	Stream specific gravity
SUL	Stream sulfur content, weight percent
NIT	Stream nitrogen content, weight percent
HDR	Stream hydrogen content, weight percent
VIS	Stream viscosity blending index @ 210°F
PAR	Stream paraffin content, weight percent
NAP	Stream napthene content, weight percent
ARO	Stream aromatics content, weight percent
FRT	Stream freezing point, °F
SPT	Stream smoke point, millimeters
HTC	Stream heat of combustion, Btu per pound
NUN	Stream unit code (producing unit)
NST	Stream name code

The unit and name codes are established for the purpose of issuing blend reports and they are linked with a set of unit and stream alpha-numeric names which are referenced from subroutine BLDREP. Each element of the above arrays corresponds to a potential blending component, the identity of which is established in subroutine BLDARY. There are a total of forty-seven potential fuel oil blending components as listed below:

Number	Fuel Blending Component Description
1	purchased kerosene
2	hydrotreated light kerosene - petroleum derived
3	hydrotreated light kerosene - shale oil derived
4	hydrotreated light kerosene - coal oil derived
5	hydrocracker light kerosene - petroleum derived
6	hydrocracker light kerosene - shale oil derived
7	hydrocracker light kerosene - coal oil derived
8	raw light kerosene - petroleum derived
9	raw light kerosene - shale oil derived
10	raw light kerosene - coal oil derived
11	reformer endpoint control tower bottoms
12	purchased heavy kerosene
13	hydrotreated heavy kerosene - petroleum derived
14	hydrotreated heavy kerosene - shale oil derived
15	hydrotreated heavy kerosene - coal oil derived
16	hydrocracker heavy kerosene - petroleum derived
17	hydrocracker heavy kerosene - shale oil derived
18	hydrocracker heavy kerosene - coal oil derived
19	raw heavy kerosene - petroleum derived
20	raw heavy kerosene - shale oil derived

Number	Fuel Blending Component Description
21	raw heavy kerosene - coal oil derived (1)
22	desulfurizer distillate from straight run gas oil
23	desulfurizer distillate from coker gas oil
24	desulfurizer light cycle oil(1)
25	desulfurizer light coker gas oil
26	raw light cycle oil
27	raw light coker oil
28	purchased gas oil
29	purchased residual fuel oil
30	desulfurizer petroleum gas oil
31	desulfurizer coker gas oil
32	raw petroleum vacuum gas oil(1)
33	thermal cracker fuel oil cut
34	fluid cracker tower bottoms (1)
35	reduced crude - petroleum derived
36	reduced crude - shale oil derived
37	reduced crude - coal oil derived
38	total coker gas oil
39	heavy coker gas oil
40	vacuum bottoms - petroleum derived
41	vacuum bottoms - shale oil derived
42	vacuum bottoms - coal oil derived
43	visbreaker pitch
44	raw shale gas oil
45	raw coal gas oil
46	hydrotreated shale gas oil
47	hydrotreated coal gas oil

The logic for adjusting the volume and properties of the jet fuel blending components commences following statements 1314 and is contained within the DO LOOP for statement 10. The volume and properties are calculated by linear interpolation between those corresponding to 525 and 650°F, cut points which correspond to yields and properties given in the crude oil assays. The specified jet fuel blend endpoint, EPSPEC, is used to interpolate properties.

0. SSORT (IL, IU)

This subroutine sorts the volume and property arrays in order of increasing sulfur content for middle distillate and residual fuel oil

(1) Petroleum derived.

blends. This sort is required in order to calculate the maximum quantities of fuel oil blends that can be produced with a specified sulfur content. The original component volumes and their corresponding properties are held in permanent arrays (for the duration of the run) which are set up in BLENDF, the subroutine which calls SSORT. These permanent arrays are necessary in order to reestablish the initial blend component values for subsequent blend calculations performed in BLENDF. The permanent blend arrays are identified below:

Working Array	Permanent Array	Property
VOL	VHOLD	Volume
API	AHOLD	Specific gravity
SUL	SHOLD	Sulfur
NIT	NIHOLD	Nitrogen
HDR	HHOLD	Hydrogen
VIS	VIHOLD	Viscosity
PAR	PAHOLD	Paraffins
NAP	NAHOLD	Napthenes
ARO	ARHOLD	Aromatics
SPT	SPHOLD	Smoke Point
FRT	FRHOLD	Freezing Point
HTC	HCHOLD	Heat of Combustion
NST	NSHOLD	Stream Number
NUN	NUHOLD	Producing Unit

The subroutine arguments IL and IU define the range of blending components to be sorted and are selected from the blend component numbers defined in subroutine BLDARY.

P. SSORT1 (IL, IU)

This subroutine is analogous to SSORT and differs only in that the sort is according to hydrogen content ranking as opposed to sulfur content. The working arrays are established in SSORT1 in the order of decreasing hydrogen content.

Q. BMAX (IU, IL, IBL, IBT)

This subroutine calculates the maximum volume of a blend of specified sulfur content, or hydrogen content, which can be produced from the fuel oil and jet fuel blend pools.

The subroutine arguments IL and IU define the range of blending components to be considered and are selected from the blend component numbers defined in subroutine BLDARY. Argument IBL is the blend number being calculated by BMAX (these blend identifiers are listed under the description for subroutine BLENDF). Argument IBT is the blend number from which the blend IBL is being produced. For example, the call statement preceding the DO 302 loop in BLENDF is CALL BMAX (1, 11, 19, 18) and conveys the following:

- Limit the calculation to VOL(1) thru VOL(11) corresponding to the range from purchased kerosene to reformer feed preparation tower bottoms (this is the full range of jet fuel blend components as defined in subroutine BLDARY).
- BMAX will calculate the maximum quantity of aviation turbine fuel blend of hydrogen content HDSPEC - blend 19 as defined in subroutine BLENDF.
- The above blend is to be produced from blend 18 - the maximum jet fuel blend volume of endpoint EPSPEC.

The composition of each blend calculated in subroutine BMAX is contained in array COMP (J, IBL), where J is the component number and IBL is the blend number, as defined in subroutines BLDARY and BLENDF, respectively.

The blend calculation will fail in BMAX if an impossible task is set forth, e.g. if all of the jet fuel blend components have a lower hydrogen content than HDSPEC. This situation triggers an error message and the run is then halted. Appropriate input adjustments must be made to obtain a successful run, such as lowering the blend specification or altering the refinery configuration in order to produce blending components of higher hydrogen contents.

R. BPROP (JL, JU, IT)

BPROP calculates the properties of each blend produced. The subroutine arguments denote the range of blend components considered for a particular blend (JL and JU) as defined in subroutine BLDARY, and the blend number (IT) as defined in subroutine BLENDF. The following arrays appearing in BPROP contain the blended properties of each blend. The method of blending is indicated:

Array	Description	Blending Method
AP (IT)	Specific gravity	volumetrically
SU (IT)	Sulfur content	by weight
NI (IT)	Nitrogen content	by weight
HD (IT)	Hydrogen content	by weight
PA (IT)	paraffin content	by weight
NA (IT)	napthene content	by weight
AR (IT)	aromatic content	by weight
HT (IT)	heat of combustion	by weight
VI (IT)	viscosity blending index	volumetrically
SP (IT)	smoke point	by reciprocal volumetric blending
FR (IT)	freezing point	by blending function BFPF as defined in BPROP

Subroutine BPROP is called from BLENDF.

S. BLDREP (IL, IU, JB)

This subroutine is called from BLENDF in order to report each of the blends produced. The blending component names are referenced thru the array SNAMES as defined in the BLOCK DATA subroutine. The refinery process units which produce these jet fuel, distillate and residual fuel oil blends are also reported using the UNAMES array. Specific gravity is converted to API gravity and both are reported. The blending reports issued by subroutine BLDREP are reported for all values of the report option indicator IREP. The BLDREP subroutine arguments denote the range of blend components considered for a particular blend (IL and IU) and the blend number (JB).

T. CONAPI (JJJ)

This subroutine is called to convert all streams (API) gravities to specific gravities (JJJ=1) for the calculation of the process unit material balances and from specific gravity to API gravity (JJJ=2) in order to restore the initial values for reporting purposes.

U. ECON

This subroutine calculates the overall refinery economics if the report option indicator IREP is set at greater than a value of 1. The order of calculation is as follows:

Description	Subroutine Location
Process unit investments	preceding statement 129
Nelson refinery complexity factor	statement 129 thru 14
Refinery offsites investment	statement 14 thru 148
Investment report	statement 148 thru 48
Refinery fixed operating cost calculation and reporting	statement 48 thru 4
Refinery variable operating cost calculation and reporting	statement 4 thru 8

Description	Subroutine Location
Crude oil cost calculation and reporting	statement 8 thru 12
Refinery product revenue calculation and reporting	statement 12 thru 529
Summary refinery economic calculations and reporting	statement 529 thru 801

The above statement numbers refer to the ECON subroutine labels, which are not numbered sequentially.

2.2. Subroutine Heirarchy

The heirarchy of program subroutines is described below. The underlined subroutine calls those which are listed below it.

MAIN PROGRAM

- BLOCK DATA
- INITB
- INITV
- UBASE
- CBASE
- CONAPI
- ISTN
- MATCLC
- BLENDF
- ECON

MATCLC

- ISTN
- HYDCAL
- UNTREP
- UNTENR

BLENDF

- BLDARY
- SSORT
- SSORT1
- BPROP
- BMAX
- BLDREP

CBASE

- CBASE1

3.0 COMMON BLOCK DESCRIPTIONS

3.1 Common Blocks Crossreferenced by Subroutine

Common Block/ Subroutine	BLEND	CB	HTCOM	ISTNUM	LENDEN	IB
REFMOD (Main)	X	X	X	X	X	X
ECON		X				X
CBASE		X				
CBASE1		X				
HYDCAL				X		
BLOCK DATA	X	X				X
CONAPI	X	X		X	X	X
ISTN				X		
UBASE			X			X
INITB		X		X		X
UNTREP				X	X	
UNTENR			X	X	X	
BLDARY	X					X
BLENDF	X					X
SSORTI	X					X
BLDREP	X					X
BPROP	X					X
SSORT	X					X
BMAX	X					X
MATCLC				X	X	X
INITV	X	X		X		

Common Block/	INAME	MATCAL	TITLER	UB1	UB2	UB3	UB4	UB5	UB6
Subroutine									
REFMOD (Main)	X	X	X	X	X	X	X	X	X
ECON	X		X						
CBASE									
CBASE1									
HYDCAL									
BLOCK DATA	X	X	X	X	X	X	X		X
CONAPI	X			X	X	X	X		
ISTN									
UBASE				X	X	X	X	X	X
INITB								X	
UNTREP	X		X						
UNTENR	X								
BLDARY	X	X		X	X	X	X	X	X
BLENDF	X								
SSORT1	X								
BLDREP	X		X						
BPROD	X								
SSORT	X								
BMAX	X								
MATCLC	X	X		X	X	X	X	X	
INITV		X		X	X	X	X		X

Common Block/	PAGER	EBAL	HYDROG	OBAL	INITB	ECONOM
Subroutine						
REFMOD (Main)	X	X	X	X	X	X
ECON	X				X	X
CBASE						
CBASE1						
HYDCAL						
BLOCK DATA	X	X		X		X
CONAPI						
ISTN						
UBASE						
INITB	X	X		X	X	
UNTREP	X			X		
UNTENR	X	X				
BLDARY			X			
BLENDF						
SSORT1						
BLDREP	X				X	
SSORT						
BMAX						
MATCLC			X	X	X	
INITV						

3.2 Description of Labeled Common Blocks

BLEND - This common block contains all of the blend property arrays for the jet fuel, distillate and residual fuel oil blends. This block also contains the blend volumes, compositions and the number of blend components.

CB - This common block contains all of crude assay properties, the specified crude volumes, and the total number of crudes in the data base.

HTCOM - Btu conversion factors are contained in this common block. HCON(1) = Btu per lb of steam; HCON(2) = Btu per lb fuel gas; HCON(3) = Btu/kWh; HCON(4) = Btu per lb hydrogen. This block also contains the calculation of the Btu per day content of the total refinery oil feed.

ISTNUM - This common block contains the array of active internal stream numbers pertinent to a given calculation and also the total number of these streams.

LENDEN - This common block contains the specific gravity of the first thirteen streams which correspond to distinct hydrocarbon species such as propane and propylene.

IB - This common block contains unit capacities, stream dispositions between alternate units, process unit severities, blending stock purchases, byproduct sales volumes and blend specifications - all of which are initialized in subroutine INITB.

INAME - This common block contains the array of crude oil names, product stream names and process unit names - all of which are used for reporting purposes.

MATCAL - This common block contains the volumetric (BPD) and weight flow (pound per hour) rates of all feed and intermediate process unit streams.

TITLER - This common block contains the current case run alphnumeric title.

UB1, UB2, UB3 - These common blocks contain the physical properties of process unit feed and product streams. These include specific gravity; sulfur, nitrogen and hydrogen contents; and viscosities for a portion of the process units. Also included are the process unit fractional yields.

UB4 - This common block contains the remaining stream viscosities; intermediate stream clear and leaded octane values and the differential specific gravities between process unit feed and product streams.

UB5 - This common block contains the limiting catalytic cracker gas oil conversion values and the limiting catalytic cracker platformate clear octane values which mark the severity range.

UB6 - This common block contains the special light and heavy kerosene properties which are pertinent to jet fuel blending. These include heat of combustion, PNA*, smoke and freeze points. This common block also contains the differential PNA values between process units feed and product streams as a function of hydrotreating severity.

PAGER - This common block contains the page number indicator and the report indicator IREP which controls the level of detail which is reported.

EBAL - This common block contains the oil refinery energy usage accumulators for steam, fuel, power and hydrogen.

HYDROG - This common block contains the calculated hydrogen contents for all the process unit internal streams. The hydrogen content is calculated as a function of specific gravity and mean boiling point, unless otherwise specified.

OBAL - This common block contains accumulators for the sulfur, nitrogen and hydrogen contents of all oil refinery feed and intermediate streams, as well as the mass accumulator. These are used to calculate the refinery mass, sulfur, nitrogen and hydrogen balances.

INITB - This common block contains oil refinery process unit feed and key product volumes. These are initialized in subroutine INITB before each case run calculation.

ECONOM - This common block contains all process unit fixed and variable costs; feed and product values; the refinery stream factor; scale factors used in the calculation of process unit investment costs; the capital investment carrying charge; and the cost of electricity.

---

* PNA refers to the weight percent of paraffins, naphthenes, and aromatics

4.0 FUNCTION STATEMENT DESCRIPTIONS

A. MAIN PROGRAM

BFPF (FREPT)	The conversion from freezing point (°F) to blending index value
FREP (BIFRP)	The conversion from blending index value to freezing point (°F)
CS1(X)	Conversion from 42 gallon barrels to cubic meters
CS2 (X)	Conversion from pound per hour to kilogram per second
CS3 (X)	Conversion from cubic feet to cubic meters

B. SUBROUTINE BLDARY

BFPF (FREPT)	The conversion from freezing point (°F) to blending index value
FREP (BIFRP)	The conversion from blending index value to freezing point (°F)
TAPI (X)	The conversion from specific gravity to API

C. SUBROUTINE BPROP

BFPF (FREPT)	See above
FREP (BIFRP)	See above

D. SUBROUTINE MATCLC

TAPI (XXX)	Conversion from specific gravity in API gravity
TSPGG (YYY)	Conversion from API gravity to specific gravity

5.0 PROGRAM VARIABLE DESCRIPTIONS

The following sections provide descriptions of the symbolic variables appearing in labeled common blocks and local data statements. The elements contained in the dimensioned stream related arrays, such as STR, are in the order given in Exhibit 5-Internal Refinery Stream and Process Identifiers -page 73 of Volume I (NASA CR-135333). Jet fuel, distillate fuel oil and residual fuel oil blend component arrays, such as VOL and API, contain elements in the order of the fuel blending components description for the 47 possible components as given in Section 2.1 of this volume under the description of subroutine BLDARY. Fuel blend arrays relating to the total jet fuel and fuel oil blends, such as VT and AP, contain elements in the order given under the Section 2.1 description of BLENDF, which enumerates 19 possible fuel blends in the sequence in which they are entered into the arrays.

5.1 Input Variables

All input variables are fully described in Volume I (NASA CR-135333) on pages 22 thru 54. Further description would be redundant. The input data variable names described are the same as the program symbolic names.

5.2 Additional Variables Appearing in Common

The following common variables are not input variables and are described below under their respective labeled common block. The variable type is indicated: R is real; I is integer; RA is real array; and IA is integer array variable.

A. COMMON/BLEND/

VARIABLE	TYPE	DESCRIPTION
VOL	RA	Array containing volume (BPD) of each jet fuel, middle distillate and residual fuel oil blending component.
API	RA	Corresponding specific gravity.
NIT	RA	Corresponding weight percent nitrogen content.
SUL	RA	Corresponding weight percent sulfur content.
VIS	RA	Corresponding viscosity blending index value @ 210°F.
HDR	RA	Corresponding hydrogen content in weight percent.
FRT	RA	Corresponding freezing point in degrees F.
PAR	RA	Corresponding paraffin content, weight percent.
NAP	RA	Corresponding naphthene content in weight percent.
ARO	RA	Corresponding aromatic content in weight percent.
SPT	RA	Corresponding smoke point in millimeters.
HTC	RA	Corresponding heat of combustion in BTU per pound.
NST	IA	Corresponding stream name identifying reference number.
NUN	IA	Corresponding identifying reference number for the process unit producing the stream.
VT	RA	The array containing the total volume of each of the possible 19 blends.

VARIABLE	TYPE	DESCRIPTION
AP	RA	The corresponding specific gravity of each of the blends.
NI	RA	Corresponding weight percent nitrogen content.
SU	RA	Corresponding weight percent sulfur content.
VI	RA	Corresponding viscosity blending index at 210°F.
HD	RA	Corresponding weight percent hydrogen content.
FR	RA	Corresponding blend freezing point in degree F.
PA	RA	Corresponding weight percent paraffins of each blend.
NA	RA	Corresponding weight percent naphthenes of each blend.
AR	RA	Corresponding weight percent aromatics of each blend.
SP	RA	Corresponding smoke point of each blend in millimeters.
HT	RA	Corresponding heat of combustion of each blend in BTU per pound.
PCT	RA	Total percentage volume of each blend. This will equal 100.0 with a negligible round-off discrepancy.
COMP (I,J)	RA	The volume percent of the I'th component in the J'th blend.
NBC	I	The total number of blend components. Set at 47.

B. COMMON/CB/

VARIABLE	TYPE	DESCRIPTION
NC	I	Total number of potential data base crudes, set at 35.

C. COMMON/HTCOM/

VARIABLE	TYPE	DESCRIPTION
HCON	RA	The heat content of steam, fuel gas, electricity and hydrogen, respectively. Expressed in BTU per pound, except for electricity in BTU/kWH.
BTUPDT	R	Total refinery heat content input in BTU per day.

D. COMMON/ISTNUM/

VARIABLE	TYPE	DESCRIPTION
ISTR	IA	The array of stream identification code numbers which are currently active in the program calculation.
NSTOT	I	The total number of active streams within array ISTR.

E. COMMON/LENDEN/

VARIABLE	TYPE	DESCRIPTION
SPGLE	RA	The array containing the specific gravity of light and components.

F. COMMON/INAME/

VARIABLE	TYPE	DESCRIPTION
CN	RA	The array containing the data base crude oil names.
SNAMES	RA	The array containing the process unit stream names.
UNAMES	RA	The array containing the process unit names.

G. COMMON/MATCAL/

VARIABLE	TYPE	DESCRIPTION
STR	RA	The array containing the BPD volume of each refining stream.
STC	RA	The array containing the volume of petroleum based crude oil streams.
STRS	RA	The array containing the volume of shale oil crude unit streams.

STRC	RA	The array containing the volume of coal oil crude unit streams.
STHK	RA	The array for kerosene hydrotreater feed and product streams.
STCO	RA	The array for fluid coker feed and product streams.
STVB	RA	The visbreaker stream array.
STCCG	RA	The fluid catalytic cracker stream array for virgin gas oil feed.
STCCC	RA	The fluid catalytic cracker stream array for coker gas oil feed.
STCCX	RA	The fluid catalytic cracker stream array for total combined feed.
STTCC	RA	The thermal cracker stream array.
STHYGG	RA	The gas oil hydrocracker stream array for virgin gas oil feed.
STHYGC	RA	The gas oil hydrocracker stream array for coker gas oil feed.
STHYGX	RA	The gas oil hydrocracker stream array for toal combined feed.
STGDG	RA	The gas oil desulfurizer stream array for virgin gas oil feed.
STGDC	RA	The gas oil desulfurizer stream array for coker gas oil feed.
STGDX	RA	The gas oil desulfurizer stream array for total combined feed.
STDDL	RA	The distillate desulfurizer stream array for light cycle oil feed.
STDDD	RA	The distillate desulfurizer stream array for virgin distillate desulfurizer.
STDDX	RA	The distillate desulfurizer stream array for total combined feed.

STDHD	RA	The distillate hydrocracker stream array for distillate feed.
STDHL	RA	The distillate hydrocracker stream array for light cycle oil feed.
STDHX	RA	The distillate hydrocracker stream array for total combined feed.
STREF	RA	The catalytic reformer stream array.
STBI	RA	The butane isomerizer stream array.
STAL	RA	The alkylation unit stream array.
STPO	RA	The polymerization unit stream array.
STH2	RA	The hydrogen plant stream array.
STSKL1	RA	The shale oil hydrotreater stream array for light kerosene range feed.
STSKH1	RA	The shale oil hydrotreater stream array for heavy kerosene feed.
STSKX1	RA	The shale oil hydrotreater stream array for combined feed.
STCKL1	RA	The coal oil hydrotreater stream array for light kerosene range feed.
STCKH1	RA	The coal oil hydrotreater stream array for heavy kerosene feed.
STCKX1	RA	The coal oil hydrotreater stream array for combined feed.
STSGH1	RA	The shale oil gas oil hydrotreater stream array.
STCGH1	RA	The coal oil gas oil hydrotreater stream array.

All of the above MATCAL common variables have companion variables beginning with W rather than S. These are the corresponding streams expressed in mass flow (pounds per hour) as opposed to volume flow (barrels per day).

H. COMMON/ECONOM/

VARIABLE	TYPE	DESCRIPTION
DIFF	R	The net refinery fuel which must be purchased in BFOE per day.

I. COMMON/PAGER/

VARIABLE	TYPE	DESCRIPTION
IPAGE	I	The current report page number.

J. COMMON/EBAL/

VARIABLE	TYPE	DESCRIPTION
SVBTU	RA	The total refinery energy consumption of steam, fuel, power and hydrogen, respectively, expressed in BTU per hour.
SVBTUS	RA	The above in joules per second.
SVFOE	RA	The above in barrels FOE per hour.
SVPCT	RA	The above as a percentage of total refinery heat content input.

K. COMMON/HYDROG/

VARIABLE	TYPE	DESCRIPTION
HYDVAL	RA	The hydrogen content in weight percent of each refinery stream.

L. COMMON/OBAL/

VARIABLE	TYPE	DESCRIPTION
SVSUL	RA	The total refinery sulfur by stream in pounds per hour.
SVNIT	RA	The total refinery nitrogen by stream in pounds per hour.
SVHYD	RA	The total refinery hydrogen by stream in pounds per hour.
SVWGT	RA	The total mass by stream in pounds per hour.

5.3 Local Variables Appearing in Data Statements

The key local variables appearing in data statements are described below and the subroutine in which they are defined is identified.

SUBROUTINE	VARIABLE	TYPE	DESCRIPTION
Main Program	CON1	R	Conversion factor, pounds of water/ 42 gal barrel @ 60F=349.788.
ECON	RPLEX	RA	Nelson Complexity points on graph of complexity vs. offsites cost.
ECON	OFFSP	RA	Nelson offsite costs expressed as a percentage of total refinery investment.
ECON	CON1	R	Conversion factor, cubic meters/42 gallon barrel = 0.158987.
ECON	CON2	R	Cubic meters/cubic foot = 0.02832.
ECON	CON3	R	Gallons/cubic foot = 7.48052.
ECON	CON4	R	Barrels/cubic foot = 0.1781076
ECON	GALS	R	Conversion factor, gallons/barrel=42.0
ECON	UNTXWF	RA	Nelson Complexity factors for each refinery process unit in order of Exhibit 5, p. 75, Volume I.
HYDCAL	BPI	RA	Array of API Technical Data Book mean boiling points taken from nomograph correlation of carbon-to-hydrogen ratio as a function of API and mean boiling points.
HYDCAL	BLDMBP	RA	Array of jet fuel and fuel oil mean boiling points (in order of VT array).
HYDCAL	STRMBP	RA	Array of fuel oil blending component mean boiling points (in order of VOL array).
HYDCAL	HYDLE	RA	Array of light end components carbon-to-hydrogen ratios.

SUBROUTINE	VARIABLE	TYPE	DESCRIPTION
HYDCAL	APII	RA	Array of API gravities corresponding to the BPI array.
HYDCAL	CHR	R	Array of carbon-to-hydrogen ratios corresponding to the BPI array.
UNTENR	BFOE	R	Conversion constant, BTU per barrel FOE = 6.05 million.
UNTENR	CON1	R	Pounds of water per 42 gallon barrel @ 60°F = 349.788.
UNTENR	CON2	R	Kg/second per pound/hour = 1.25997 E-04.
UNTENR	CON3	R	Joules/kg per BTU/pound = 2326.0.
UNTENR	CON4	R	Joules/second per BTU/hour = 0.29307.
UNTENR	CON5	R	Joules per BTU @ 60°F = 1054.68.
BLDARY	BLDMBP	RA	Same as BLDMBP in HYDCAL.
BLDREP	CON1	R	Cubic meters per 42 gallon barrel = 0.1589873.
BLDREP	CON2	R	Density of water @ 60°F = 999.04 kg/cubic meter.
BLDREP	CON3	R	Joules/kg per BTU/pound =2326.0.
MATCLC	CON1	R	Pounds water per barrel @ 60°F = 349.788.
UNTREP	CON1	R	Pounds of water per 42 gallon barrel = 349.788.
UNTREP	CON2	R	Kg/second per pound/hour = 1.25997E-04.
UNTREP	CON3	R	Density of water, at 60°F = 999.04 Kg per cubic meter.

6.0 DESCRIPTION OF PROGRAM FILES

The data bases for crude oil assay data, process unit yields, stream properties and economic data are self-contained within the Computer Model For Refinery Operations. Therefore, the program is not interfaced with external data base files and the use of files is limited to the standard input/output files and small temporary disk files which are purged after run termination. These files are described below:

Logical File Number	Type	Function (1)
5	Card Reader	Program input stream
6	Printer	Printed program output
17	Disk	Store user directed crude oil assay data base changes for the duration of the run (entered under reader card &CDATA).
18	Disk	Store process unit data base changes entered under header card &UDATA.
16	Disk	Store process unit data base changes entered under header card &UDATA1.
19	Disk	Store card images for the current run problem entered under header card &PDATA.
20	Disk	Store the above information on File 20 if the run problem corresponds to a base case.

(1) All files are accessed from the main program only, with the exception of File 6 which is referenced from the main program and from the report subroutines.

Files 16, 17, and 18 are reread in the main program in order to overlay data base values stored within subroutines CBASE, CBASE1 and UBASE. Files 19 and 20 are used in tandem. The base case problem input is stored on File 20 and the subject problem changes are stored on File 19. File 19 is reread following a read of file 20. Therefore, base case changes are not additive from subject case to subject case, but are always made with reference to the starting base case of a case study sequence. For a stand alone case, only file 19 is used.

7.0 PROGRAM SIZE LIMITATIONS

The Computer Model For Refinery Operations requires approximately 400K bytes of storage on the IBM 360/67 computer and about 225K words of storage on the CDC 6600 computer. Essentially all of the dimensioned array space reserved in the program is utilized. The key array limitations are outlined below:

ITEM	MAXIMUM
Number of refinery process streams	66
Number of refinery process units	20
Number of crude oils (all types)	35
Number of jet fuel and fuel oil blending components (total for all blends)	50
Number of distinct jet fuel plus distillate and residual fuel oil blends	20
Total number of items of crude oil assay information (individual cut fraction yields, properties, etc.)	57
Number of hydrotreater severity levels for each shale and coal oil process units	3
Number of purchased fuel oil blending stocks	4

8.0 CONCLUDING REMARKS

This report has presented detailed systems and programming documentation for The Computer Model For Refinery Operations. The report is Volume III of three volumes covering the description, application, and documentation of the refinery calculation program. This volume is intended to be used in conjunction with Volume I and II and with the program Fortran listing. The information represents a detailed description of all program subroutines, common blocks, program function statements, data statements and program files used during run execution. The preceding volumes (NASA CR-135333) and NASA CR-135334) are available from the NASA Project Manager. Computer tapes can be purchased through the Computer Software and Management Information Office (COSMIC), 112 Barrow Hall, University of Georgia, Athens, GA 30602, under the number LEW-13047.