

Bechtel

3000 Post Oak Boulevard
Houston, Texas 77056-6503

Mailing address: P.O. Box 2166
Houston, Texas 77252-2166

November 30, 1992

U. S. Department of Energy
Pittsburgh Energy Technology Center
Mail Stop 922-H
P. O. Box 10940
Pittsburgh, PA 15236

Attention: Mr. Swenam Lee
Project Manager

Subject: D.O.E. Coal Liquefaction
Base Line Design and System Analysis
Contract No. DE-AC22 90PC89857
Bechtel Job No. 20952
Task VI, Final Topical/Task Report
Letter No. BLD-120

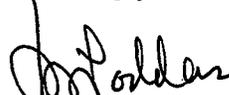
Dear Mr. Lee:

Task VI addresses the development of an ASPEN process simulation model training manual. The Task VI Topical/Task report documents the training manual.

The report consists of training material on ASPEN process simulation and ASPEN coal liquefaction kinetic reactor model. The four appendices included in this report addresses ASPEN process simulation model problem session and ASPEN coal liquefaction kinetic model problem session, in addition to file listings and various miscellaneous items.

Attached for your files are three copies of the subject report. As requested, one of these copies is bound in a loose leaf 3-ring binder for your desk use. Copies to other members of DOE, as required by the contract are sent directly to each of them.

Sincerely yours,



Syamal K. Poddar
Project Manager

Attachment

cc: Martin Byrnes, DOE/PETC
Robert Hamilton, DOE/PETC
A. Schachtschneider, AMOCO (2)
File

Gilbert V. McGurl, DOE/PETC
Joanne Wastek, DOE/PETC



Bechtel Corporation

The information and data contained in this report are the result of an economic evaluation and a preliminary design effort and because of the nature of this work no guarantees or warranties of performance, workmanship, or otherwise are made, either expressed or by implication.

PROCESS SIMULATION MODEL TRAINING MANUAL
TABLE OF CONTENTS

	<u>PAGE</u>
1. INTRODUCTION	1-1
2. EXECUTIVE SUMMARY	2-1
2.1 Task Overview	2-1
2.2 Model Overview	2-3
3. COMPUTER REQUIREMENTS	3-1
4. ASPEN/SP COMPUTER SIMULATION PROGRAM INTRODUCTORY COURSE	4-1
5. ASPEN PROCESS SIMULATION MODEL	5-1
5.1 Overview	5-1
5.2 Fortran Blocks and Fortran User Block Models	5-4
5.2.1 General Features	5-4
5.2.2 Process Calculations	5-6
5.2.3 Utilities Calculations	5-6
5.2.4 Capital Costs and Operating Labor	5-8
5.2.5 Error Checking and Warning Messages	5-9
5.2.6 Input Parameters	5-10
5.2.7 Management Summary Report	5-16
5.3 Simulation Models--Base Case	5-16
5.4 Executing the ASPEN Process Simulation Model	5-16
6. ASPEN COAL LIQUEFACTION KINETIC REACTOR MODEL	6-1
6.1 Overview	6-1
6.2 Introduction	6-1
6.3 Overall Methodology	6-2
6.4 Input Parameters	6-4
6.5 Results	6-6
6.6 Executing the Coal Liquefaction Kinetic Reactor Model	6-7

PROCESS SIMULATION MODEL TRAINING MANUAL
TABLE OF CONTENTS

	<u>PAGE</u>
APPENDICES	
A. ASPEN PROCESS SIMULATION MODEL PROBLEM SESSION . . .	A-1
B. FILE LISTINGS	B-1
C. MISCELLANEOUS ITEMS	C-1
D. ASPEN COAL LIQUEFACTION KINETIC REACTOR MODEL PROBLEM SESSION	D-1

1. INTRODUCTION

This presents the Task VI topical report. Task VI concerns the development of an ASPEN process simulation model training manual and presentation of a course on the use of ASPEN and the process simulation model.

The objective of this project is to develop a baseline design and computer simulation model for a coal liquefaction plant based on two-stage direct coupled catalytic reactor technology used at Wilsonville. Specifically, the scope of work calls for the development of:

1. A baseline design based on previous DOE/PETC results from the Wilsonville pilot plant and other engineering evaluations.
2. A cost estimate and economic analysis.
3. A computer model incorporating the above two steps over a wide range of capacities and selected process alternatives.

This model will enhance DOE's capability to assess coal liquefaction technology improvements in-house, thus avoiding costly and time-consuming evaluations by outside contractors.

The Task V Topical report documents the ASPEN process simulation model. A draft version of that report was used as reference material for the training course presented at the DOE facilities in Pittsburgh during the week of March 23, 1992. Therefore, much of the material contained in that report is not reprinted here.

Thus, this report summarizes the training presented at the DOE facilities in Pittsburgh during March, 1992.

2. EXECUTIVE SUMMARY

2.1 Task Overview

This report is the Task VI topical report. Task VI concerns the development of a training manual and a training course for the ASPEN/SP direct coal liquefaction process simulation model. The training course included a basic introductory course on the pc version of the ASPEN/SP process simulation program, an overview of the process simulation model, and instructions on the use and modification of the process simulation model. In addition, training and demonstrations were given on the use of the LOTUS 123 economic spreadsheet model.

The training course was completed before the process simulation model was finalized and delivered. Therefore, the examples and results presented during the course are not exactly those results which would be obtained with the final model. However, the methodology presented and results were representative enough for training purposes.

The three and one-half day introductory ASPEN/SP training course was based on the Simulation Sciences introductory ASPEN/SP course with modifications for use of the SPEXPRT system on personal computers and with examples and homework problems related to coal processing.

Table 2.1 contains a description of the individual subtasks as originally detailed in the Task I Management Plan. Some items were modified with the consent of or upon recommendation of the project manager as described below.

Subtask 6010 dealt with scheduling the training facilities and personnel. At the project managers request, training was conducted for one week at the DOE PETC facilities in Pittsburgh from March 23 through 27, 1992.

Subtask 6020 dealt with development of a training manual covering the required training items. Since most of the trainees did not have prior ASPEN experience, the three and one-half day introductory ASPEN/SP training course was included. The training manual for the ASPEN/SP introductory course consisted of copies of slides used in the presentation and printed copies of the homework problems and solutions. This material is not reproduced in this report.

Subtask 6030 concerned preparation of the draft topical report for Task VI, the training manual. This report without this section was the training manual used for training on the ASPEN/SP process simulation model and the LOTUS 123 economic spreadsheet model.

Subtasks 6040 and 6050 dealt with review and publication of the Task VI topical report, the training manual. A preliminary review of a draft of the Task VI topical report (the training manual) was done during the course, and publication was postponed until completion of the course.

Subtasks 6060 dealt with presentation of the training. The training session was conducted during the week of March 23 through 27 at the DOE - PETC facilities in Pittsburgh, Pa.

TABLE 2.1

TASK VI DESCRIPTION

Task VI concerns the development of a training manual, a training course for the process simulation model, and presentation thereof. The training course will include an overview of the system, modification of the reporting system, interfacing user models, modification of the chemical properties, use of the cost and economic modules, specifying flowsheets, specifying flowsheets, streams, components, properties, and convergence. Trainees will be instructed through the use of case study example problems.

Subtask Number	Subtask Title	Description
6010	Schedule training resources	Schedule training facilities and personnel.
6020	Develop training manual	A training manual will be developed covering the items mentioned in the above task description. If trainees have prior Aspen training (recommended) then the course content will be adjusted. PETC will be consulted regarding emphasis and content.
6030	Draft Topical Report for Task VI, the training manual	The training manual will be reviewed and available prior to the training course.
6040	Review Task VI	The draft topical report for Task VI will be reviewed with PETC.
6050	Finalize and issue Task VI topical report	The finalized topical report for Task VI will be issued.
6060	Conduct training	The training session, as described above, will be conducted.

2. Model Overview

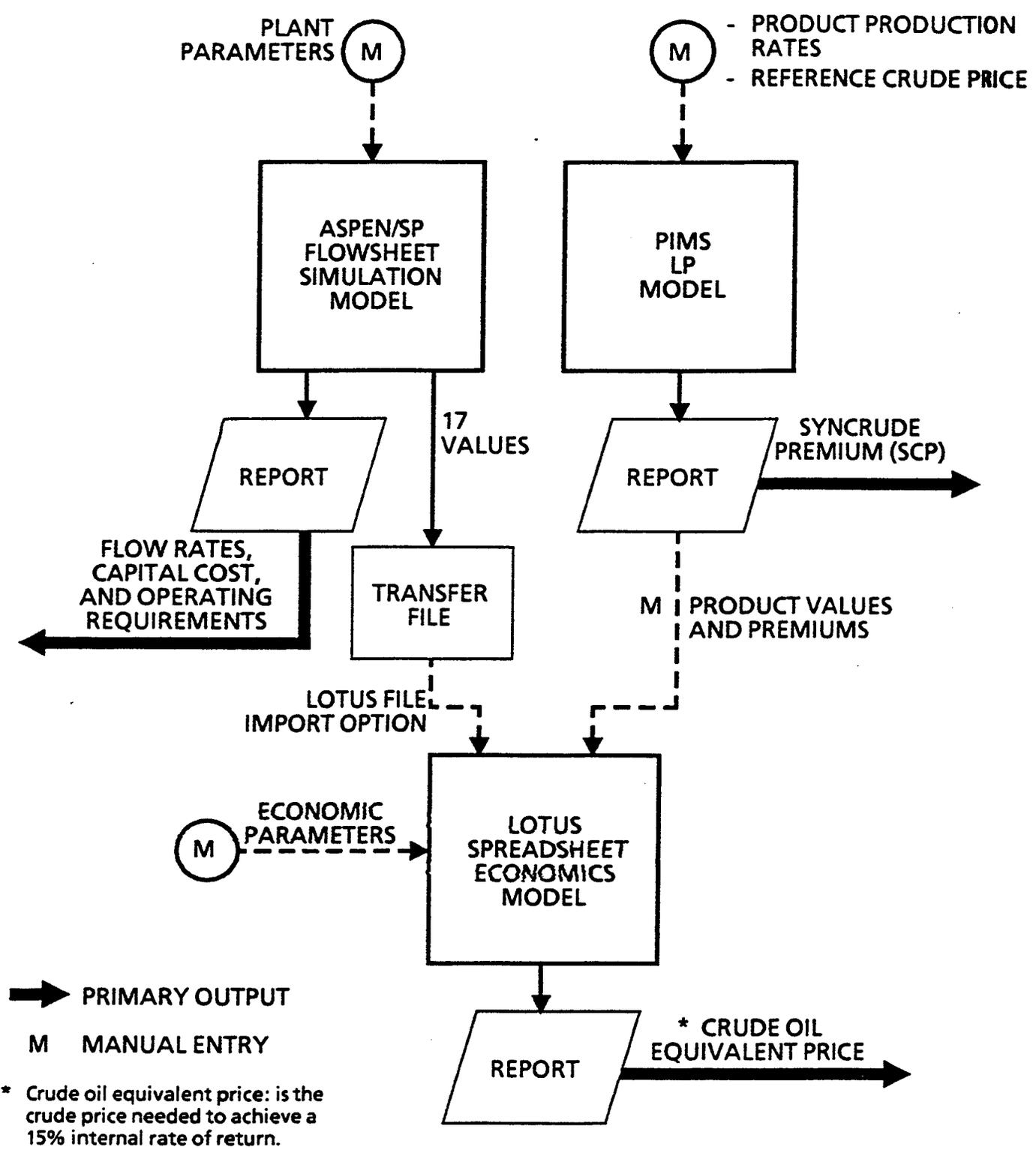
The ASPEN/SP flowsheet simulation model of the entire complex is the heart of the modeling system for the coal liquefaction complex. The complex is modeled in the ASPEN/SP framework using numerous Fortran user block models for the various individual plants. This is a research planning model that is designed to predict mass and utilities balances around the entire complex for predicting the inputs, outputs, and capital cost of the complex.

This model interacts with two other models as shown in Figure 2.1. Seventeen basic input values, output flows, capital cost and operator requirements are written to a transfer file for semi-automatic transfer to the LOTUS spreadsheet economics model. This spreadsheet model also requires the values of the products produced by the coal liquefaction complex. These values are obtained from a PIMS LP Model of a typical PAD II refinery and manually supplied to the spreadsheet model. Additional economic parameters, such as interest rates, expected inflation rates, etc., also have to be manually supplied to the spreadsheet model.

The spreadsheet model does a detailed year by year cash flow analysis of the complex and calculates an equivalent crude oil price to achieve a 15% internal rate of return.

Also, a separate ASPEN/SP flowsheet model of Plant 2, the coal liquefaction plant, has been developed for predicting the effects of selected operating variables and reactor performance on the performance and yields of the coal liquefaction reactors.

FIGURE 2.1
SIMPLIFIED USER INPUT - OUTPUT DIAGRAM
FOR COMPUTER MODELS USED IN
DIRECT COAL LIQUEFACTION STUDY



3. COMPUTER REQUIREMENTS

In order to run the ASPEN/SP computer program and the process simulation model, the following hardware and software are required.

Hardware Requirements

An IBM compatible personal computer with the following:

1. Intel 80386 or 80486 main processor
2. Intel 80387 math coprocessor if an 80386 computer
3. A minimum of 10 Mbytes of RAM
4. A minimum of 40 Mbytes of available hard disk space
5. VGA graphics capability
6. DOS, Microsoft or IBM Version 3.3 or later
7. A mouse, preferably a Logitech three button mouse, or a Microsoft compatible two button mouse

Software Requirements

For running ASPEN/SP, the ASPEN/SP software as provided by Simulation Sciences is required. Version 7, release 2 of ASPEN/SP was used to demonstrate the model.

The economics spreadsheet program was developed on LOTUS 123, Release 2.2. However, it should run on other spreadsheet programs that are compatible with LOTUS 123, Release 2.2 spreadsheet files since this is a two dimensional spreadsheet model with no macros.

In addition, an ASCII editor capable of viewing and editing files of up to 1 Mbyte in size is required. Version 4.0 of KEDIT by Mansfield Software Group, Inc. (P.O. Box 532, Storrs, Ct. 06268, 203-429-8402) was used in this course. However, any editor or word processing program capable of reading and writing large ASCII files could have been used.

For running the process simulation model of the baseline design, the following software files are required.

1. PLANTS.FOR - Fortran source code for the ASPEN user block models required for simulating the baseline design.
2. OTHERS.FOR - Additional Fortran source code required by the user block models in the above PLANT.FOR file.
3. DCLN.INP - The ASPEN/SP input file for simulating the baseline design for the Nth plant.

4. ASP.BAT - A batch file for running ASPEN/SP with the OTHERS.FOR file.
5. DCLRPT.BAT - A batch file for combining the individual plant summary report files together into a single management summary report file.
6. DCLSTART.REP - The cover page for the management summary report file that is produced by the DCLREP.BAT file.

For running the kinetic model process simulation of Plant 2, the following files are required.

1. USR2G.FOR - Fortran source code for the ASPEN user block model required for simulating the coal liquefaction reactors in Plant 2.
2. OTHERS.FOR - Additional Fortran source code required by the user block models in the above USR2G.FOR file. This is the same file as above.
3. T2V2S.INP - The ASPEN/SP input file for simulating the baseline design of the coal liquefaction reactors in Plant 2 .
4. ASP.BAT - A batch file for running ASPEN/SP with the OTHERS.FOR file.

For running the LOTUS 123 spreadsheet economics program, the following files are required.

1. BASENTH.WK1 - The LOTUS 123 economics spreadsheet input file.
2. DCL1.PRN - An output file generated by the ASPEN/SP coal liquefaction simulation model which contains the principal results that have to be transferred to the spreadsheet.

4. ASPEN/SP COMPUTER SIMULATION PROGRAM INTRODUCTORY COURSE

The first three days of training were dedicated to a introductory course on the use of ASPEN/SP on an IBM PC compatible computer. The course was presented an Amoco Chemical Corporation engineer who has taught this material several times. Some of the material used in the course was obtained from Simulation Sciences and was used with their permission. That material is not reprinted here.

The topics covered in this introductory ASPEN/SP course are shown in the first part of Table 4.1. The second part outlines the material covered in the final two days of the course.

Table 4.1

ASPEN/SP Coal Liquefaction Course

March 23 - 27, 1992
DOE - PETC
Pittsburgh, Pennsylvania

I. ASPEN/SP Introductory Course - 3 days

Basic Simulation Sciences ASPEN/SP Introductory Course taught by Steve Lythgoe covering

- A. Introduction
- B. General overview of ASPEN/SP input language
- C. Analysis/description of ASPEN/SP History and Report files
- D. Global specifications and keywords
- E. Components and physical properties, including solids
- F. ASPEN/SP stream structure, including solids
- G. Unit Operations - Mixers, Splitters, Flashes, Heaters, Pumps, Compressors and Reactors
- H. Unit Operations - Distillation
- I. Design-specifications and Fortran Blocks
- J. Case studies and optimization
- K. Convergence - Tear streams, convergence methods and sequencing
- L. Crude slicing and blending, pseudocomponents and characterization
- M. Costing

Each day will have a problem session.

II. Coal Liquefaction Simulation Model - 2 days

- A. ASPEN/SP Model
 - 1. Model structure
 - 2. Fortran block model structure
 - 3. Customized reports
 - 4. Other features
 - 5. Demonstration
 - 6. Hands-on operation - Practice problems and solutions
- B. Coal Liquefaction Kinetic Reactor Model - Design and Structure
- C. Economic Spreadsheet Model
 - 1. Design and Structure
 - 2. Hands-on operation - Studying "What-if" cases

5. ASPEN PROCESS SIMULATION MODEL

5.1 Overview

The coal liquefaction complex is modeled within the ASPEN/SP framework by input files which call Fortran user block models to simulate the various plants. This technique avoids supplying much greater amounts of input information required by the standard ASPEN/SP models, and shortens execution times of the simulations. This also avoids supplying process information required by the ASPEN/SP models that is not available for the proprietary plants in the complex (e.g., the ROSE-SR process).

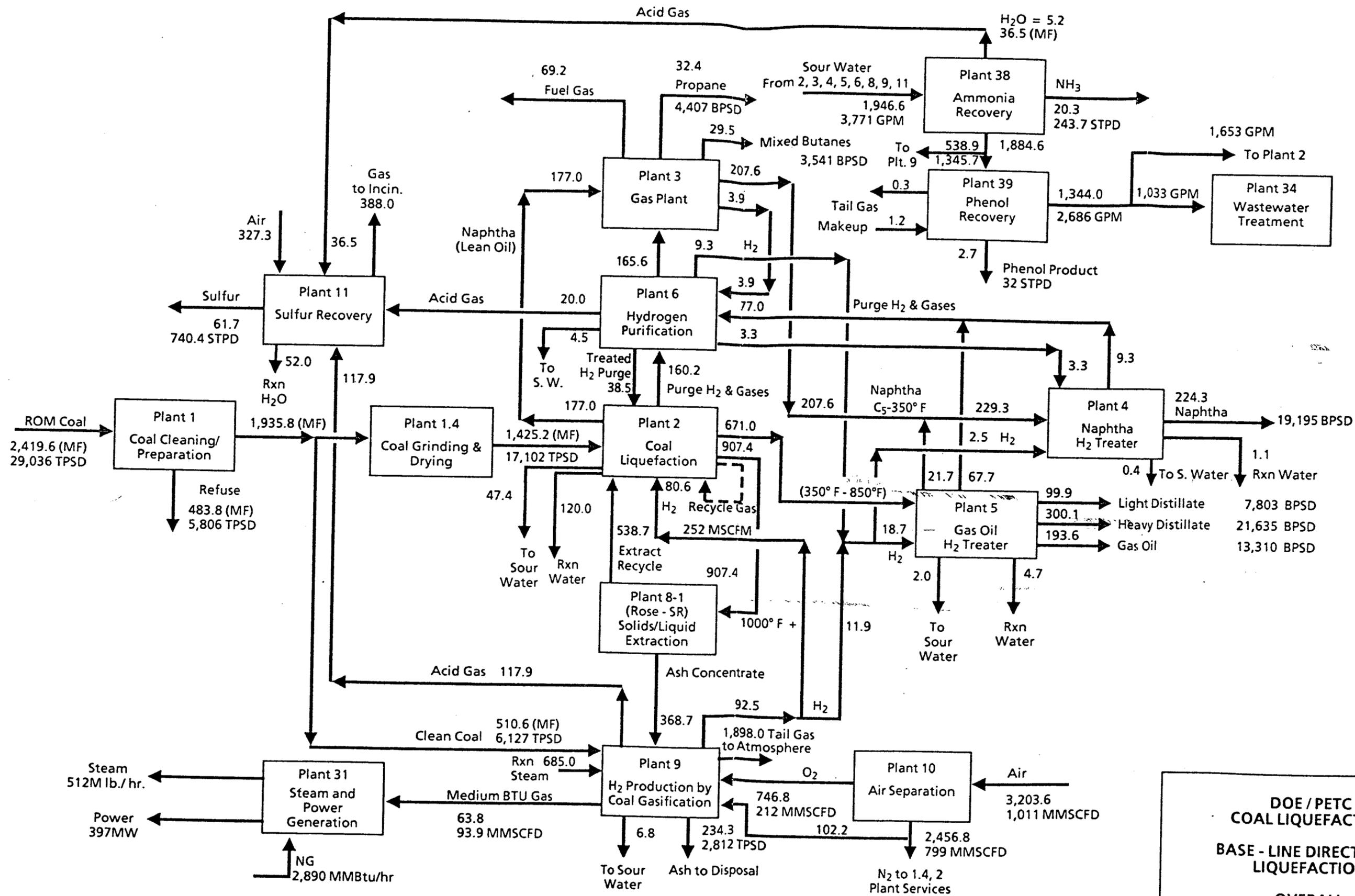
The user may simulate plants individually or in combination by specifying the input parameters required by the models, and modifying and/or combining input files to properly connect interplant streams. By setting only the appropriate input file parameters, output reports may be customized to include elemental balances, overall material balances, utilities requirements, capital and operating costs, and economic analyses for the individual plants, or for the entire complex. It should not be necessary to modify the Fortran user block models.

The plant models simply compute and report the product rates leaving a particular plant from the feed entering it. However, a separate ASPEN/SP input file and model for Plant 2 was developed that contains kinetic equations which compute the compositions and rates of the product streams, and the size requirements of the coal liquefaction reactors from the reaction conditions specified in the input file. Thus, this Plant 2 model can be used to obtain more detailed information on the coal liquefaction plant, and the results from the detailed Plant 2 simulation can be used to modify the overall block model for Plant 2 to study the effect on the entire complex.

Each plant model has the capability to branch to other Fortran routines containing algorithms which are common to all the plants. These subroutines calculate and save utilities requirements, capital and operating costs, operating labor requirements, etc. for each plant, and generate reports according to the input file instructions.

The ASPEN/SP program was modified to predict costs of individual pieces or groups of equipment as functions of capacity. This allows the total cost of each plant to be determined based on the duplicate equipment parameters set by the user. Another modification enabled ASPEN/SP to compute elemental balances in addition to its component balance capability.

Figure 5.1 shows the overall flowsheet of the base-line design for the coal liquefaction complex as taken from Volume I the Task II Topical Report. Figure 5.2 shows the overall flowsheet as modeled by the ASPEN process flowsheet simulation model.



**DOE / PETC
 COAL LIQUEFACTION
 BASE - LINE DIRECT COAL
 LIQUEFACTION
 OVERALL
 MATERIAL BALANCE
 Figure 5.1**

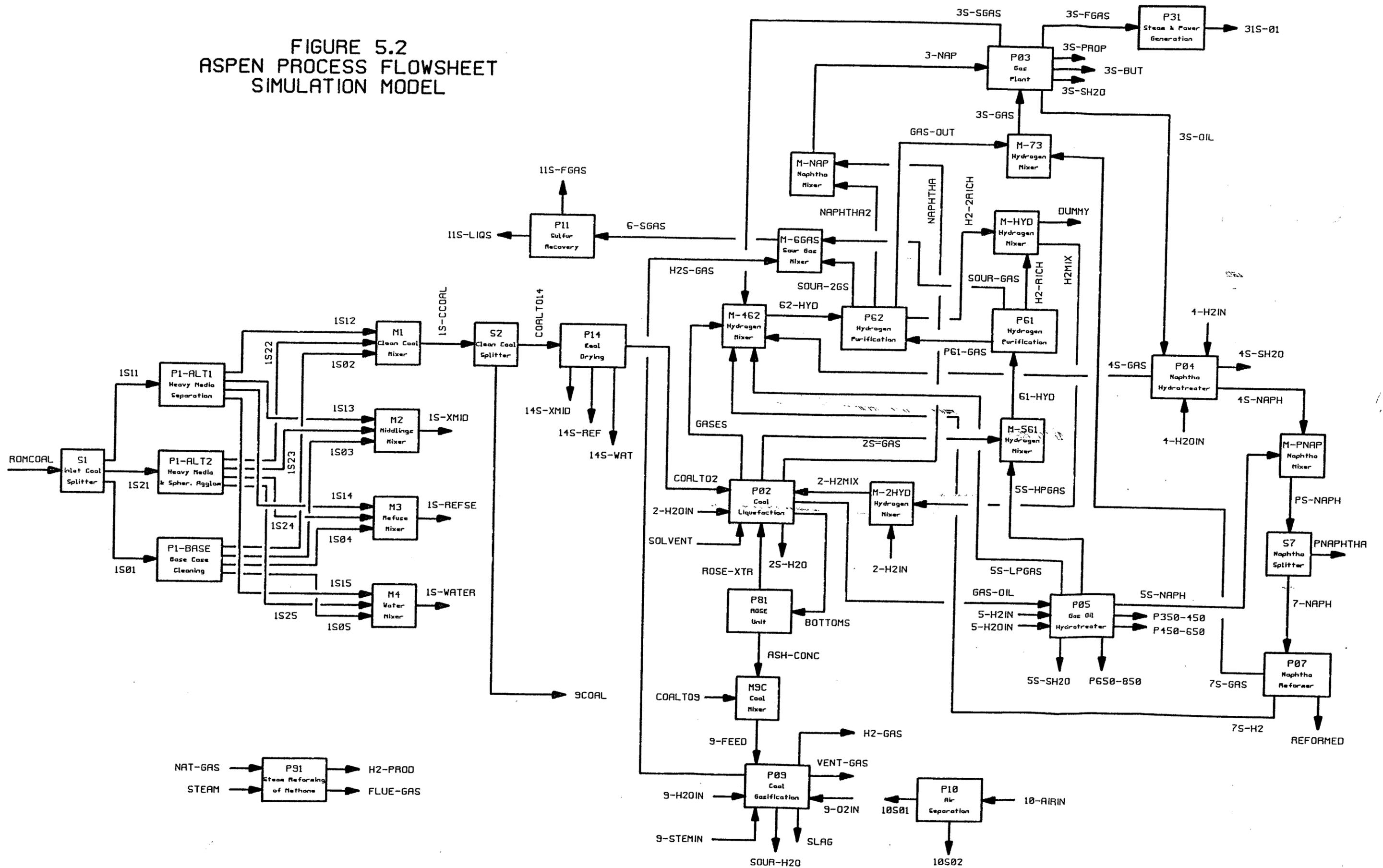
Revised 11/26/91

1291048-2

Notes:

1. Flow rates are in MLB/HR unless noted and on dry basis
2. Simplified water flow distribution diagram is shown on Figure 41.1
3. Minor streams including steam, water, sour water, and make-up amine are not shown on this diagram
4. Flow rates around plants #38, 39, 34 are shown on wet basis

FIGURE 5.2
 ASPEN PROCESS FLOWSHEET
 SIMULATION MODEL



5.2 Fortran Blocks and Fortran User Block Models

Fortran blocks allow the user to insert his own Fortran statements into the flowsheet computations within the ASPEN/SP framework. Among a large number of uses for these are feed forward control, interactive simulations, setting make-up stream flow rates, performing auxiliary calculations, generating data files for use by other parts of the simulation, and printing customized reports.

Fortran user block models are user-designed simulations that may be substituted for ASPEN/SP unit operation models, or to simulate processes not available within ASPEN/SP.

Both techniques are used extensively here to avoid supplying much greater amounts of input information required by the standard ASPEN/SP models, and to shorten execution times of the simulations. This also avoids supplying process information required by the ASPEN/SP models that is not available for the proprietary plants in the complex (e.g., the ROSE-SR process).

5.2.1 General Features

Each Fortran user block model contains equations which simulate the chemical reactions, separations, utilities requirements, etc., for a particular plant from the parameters specified in the input files. These equations require that certain streams and components be specified, consistent with that model's design. Streams and components that may be inadvertently omitted or set by a user, e.g. an ethane component not specified, or a flow of solids stipulated in the feed to the gas plant, will halt execution of the simulation and cause the appropriate error messages to be reported in the ASPEN/SP history file.

Each model contains the following sections:

1. Introductory description and comments
2. Common statements
3. Local variable declaration statements and descriptions
4. Parameter initialization
5. Input
6. Process calculations
7. Report

The parameter initialization and input sections set up the required information from the input stream(s) and calling parameters for use in the sections that follow it. The calculations section simulates this plant and calculates the output stream compositions and flow rates.

The report section is divided into three subsections, a stream report section, a utilities consumption section, and a capital cost section. By use of an integer input parameter, the user can control whether the whole user block summary report is printed, selected portions are printed, or if it is not printed.

Although each model was developed specifically for the direct coal liquefaction facility simulation, several features were included so that they may be easily adapted to and used in other ASPEN/SP simulations. Each model consists of one or more Fortran subroutines the name of which is limited to six characters, beginning with the letters USR followed by the plant number. A letter suffix is added if more than one subroutine is required. For example, the model for plant 10 is called USR10.FOR, and the first subroutine in it is named USR10A.FOR. The first subroutine in the plant 8.1 model would be named USR81A.FOR.

ASPEN/SP requires that all input and output streams to and from a model be of the same stream class. Each model has been programmed to work with an input stream consisting of a conventional component sub-stream and a second sub-stream of non-conventional components of ASPEN/SP stream class MIXNC or MIXNCPSD. However, those plant models which require only conventional components, such as the air separation plant, also will function correctly when the input stream or streams contain only one sub-stream of conventional components.

When a non-conventional component sub-stream is present, these plant models require that each non-conventional component have the following four component attributes, PROXANAL, ULTANAL, SULFANAL and AOXANAL. These component attributes must be specified in the above order for each non-conventional component in an ATTR-COMPS sentence, such as the one that follows for the non-conventional component COAL:

```
ATTR-COMPS COAL PROXANAL ULTANAL SULFANAL AOXANAL
```

When specific components are used in a plant model, the Fortran block model for that plant has been programmed to locate these components by name, up to a maximum of 100 conventional components. Therefore, they must be identified by the same name in the ASPEN/SP input file as used in the direct coal liquefaction facility simulation. If the model cannot locate a required component by name, an error message will be written to the history file and execution will be terminated.

For example, the Fortran block model of the air separation plant requires two key components, oxygen and nitrogen. Therefore, this model has been programmed to locate these components by searching the component list for these component names to determine their relative component numbers and save them in two local variables, KO2 and KN2. Thus, if this model is to be used in another simulation which uses a different component ordering, these components only have to be specified with the same names in the ASPEN/SP input file.

5.2.2 Process Calculations

The process calculations section in each Fortran user block differs depending on the plant being simulated. While any of the seventy REAL input parameters discussed in the following subsections may be changed by the user, only the first twenty are process-specific, i.e., values that the user may normally change in the input file specifications. These are reserved for process related items, such as conversions and separation ratios. Additional information on these parameters is provided in the subsections below which describe the individual plant models. The remaining REAL parameters control utilities consumptions, etc. and are not normally changed in the input files.

Each output stream leaving every Fortran user block model is set to a default temperature of 70 °F and a default pressure of 15 psia. These values can and should be changed to more appropriate values for the specific simulation by the use of a FLASH-SPECS sentence in the block paragraph which calls the user Fortran block model. Any outlet stream conditions specified in the FLASH-SPECS sentence will override the default values set in the Fortran user block model. For example, the following FLASH-SPECS sentence will set the outlet temperature of the FLUE-GAS stream to 110 °F and 50 psia and cause ASPEN/SP to calculate the appropriate properties (enthalpy, entropy, etc.) at these conditions.

```
FLASH-SPECS STRM = FLUE-GAS  KODE = 2  TEMP = 100  PRES = 50
```

5.2.3 Utilities Calculations

Since each of these plants is being modeled by a single Fortran user block model, little useful additional information can be gained by an enthalpy balance calculation around the entire plant. Instead, the models have been programmed to calculate the following eleven plant utilities requirements.

1. Power consumption in kilowatts
2. 900 psig / 750 F steam consumption in Mlbs/hour
3. 900 psig saturated steam consumption in Mlbs/hour
4. 600 psig / 720 F steam consumption in Mlbs/hour
5. 600 psig saturated steam consumption in Mlbs/hour
6. 150 psig saturated steam consumption in Mlbs/hour
7. 50 psig steam saturated consumption in Mlbs/hour
8. Fuel consumption in MM BTU/hour
9. Cooling water consumption in Mgal/hour
10. Process water consumption in Mgal/hour
11. Nitrogen consumption in MM SCF/hour of nitrogen

If desired, additional utility consumptions (or productions) can be added. Such additional utilities might be condensate, boiler feed water or a medium pressure steam.

Each plant's utility requirement is calculated as a linear function of its key flow rate. This may be either the total flow rate of a specific feed or product stream, or the flow rate of the major component in a specific feed or product stream. For example, the key flow rate for the coal cleaning plant is the clean coal product stream rate in Mlbs/hr, and the key flow rate for the hydrogen plants is the useable hydrogen production rate (flow rate of hydrogen in the hydrogen-rich product gas stream) in MM SCF/hr of hydrogen. Utilities requirements are calculated by Equation 5.1.

$$U_i = A_i + B_i * F_O \quad (\text{Eq. 5.1})$$

Where:

i = Subscript designating a specific utility in the above listed order

U_i = Consumption of utility i

F_O = Total key flow rate for all duplicate plants in appropriate units, such as MM SCF/hour or Mlbs/hour

A_i = Constant for the calculation of utility i

B_i = Constant for the calculation of utility i

The sign convention used for all utilities is that positive values represent utilities that are imported to (consumed by) the plant, and negative values represent utilities that are exported from (produced by) the plant.

The numerical values for the A_i and B_i parameters for each utility are input parameters to each Fortran user block model. The user supplied parameters for the utilities calculations are REAL parameters 21 through 42. REAL(21) and REAL(22) are the A and B constants for the power consumption, respectively. REAL(23) and REAL(24) are the A and B constants for the 900 psig / 750 F steam consumption, respectively. Similarly, REAL(25) and REAL(26) are for the 900 psig saturated steam consumption; REAL(27) and REAL(28) are for the 600 psig / 720 F steam consumption; REAL(29) and REAL(30) are for the 600 psig saturated steam consumption; REAL(31) and REAL(32) are for the 150 psig saturated steam consumption; REAL(33) and REAL(34) are for the 50 psig saturated steam consumption; REAL(35) and REAL(36) are for the plant fuel consumption; REAL(37) and REAL(38) are for the cooling water consumption; REAL(39) and REAL(40) are for the process water consumption; and REAL(41) and REAL(42) are for the nitrogen consumption.

All utility parameters must be on a consistent basis with the values for any unit specific parameters which are supplied for the process calculation section.

5.2.4 Capital Costs and Operating Labor

The ISBL field cost for each plant is calculated as a function of the key flow rate by Equations 5.2 through 5.4. The key flow rate may be either the total flow rate of a specific feed or product stream or the flow rate of the major component in a specific feed or product stream. For example, the key flow rate for the coal cleaning plant is the clean coal product stream rate in Mlbs/hr, and the key flow rate for the hydrogen plants is the useable hydrogen production rate (flow rate of hydrogen in the hydrogen-rich product gas stream) in MM SCF/hr of hydrogen.

$$\text{COST} = \text{FCOST} + (N - 1) * \text{SCOST} \quad (\text{Eq. 5.2})$$

$$\text{FCOST} = A + B * (F_o / (N * \text{RF}_o))^E \quad (\text{Eq. 5.3})$$

$$\text{SCOST} = F * \text{FCOST} \quad (\text{Eq. 5.4})$$

Where:

COST = Total ISBL field cost of all duplicate trains

FCOST = ISBL field cost of the first train

SCOST = ISBL field cost of each subsequent duplicate train after the first one

N = Total number of duplicate trains, including spares

F_o = Total key flow rate of all duplicate trains in appropriate units, such as MM SCF/hour or Mlbs/hour

RF_o = Reference key flow rate of a single train in appropriate units, such as MM SCF/hour or Mlbs/hour. This flow rate is used to scale the ISBL field cost of a single train as a function of train capacity

A, B, E and F = Constants for the calculation of the ISBL field cost of a single train as a function of train capacity

In the above ISBL field cost equation, constant A is the fixed ISBL field cost associated with a single train. The sum of constants A and B is the ISBL field cost of a single train of capacity RF_o . Thus, constant B is the variable ISBL field cost of a single train of capacity RF_o . Constant E is the train cost scaling exponent. Constant F is the cost reduction factor for the construction of duplicate trains after the first one.

The Fortran user block model will calculate the required number of duplicate trains or operating units in the plant from the total plant capacity and the specified maximum and minimum single train capacities. However, each Fortran user block model allows the user

to specify the number of operating duplicate trains as an input parameter. When this number is supplied, that value will be used, and the calculation of the number of duplicate operating trains will be bypassed.

When the maximum capacity of a single operating train within a plant is not specified (i.e.; a zero or negative value is supplied), the total ISBL field cost will be calculated based on a single train.

The numerical values for the plant costing parameters, number of duplicate operating trains, and number of spare trains are input parameters to each Fortran user block model. Parameter INT(3) is the specified number of duplicate operating trains, excluding spares, and parameter REAL(58) is the number of spare trains. If INT(3) has a value of zero, the number of duplicate operating trains will be calculated based on the specified maximum capacity of a single train. If INT(3) has a positive value, that value will be the number of duplicate operating trains that will be used to calculate the total ISBL field cost.

Parameter REAL(51) is the reference capacity of a single operating train for the calculation of the ISBL field cost, expressed as the key flow rate in MM SCF/hour or Mlbs/hour. Parameters REAL(52) and REAL(53), respectively, are the maximum and minimum capacities of a single operating train for which these costing parameters are applicable, expressed in the same manner as parameter REAL(51). Parameters REAL(54) through REAL(57) set the A, B, E and F parameters in equations 3.3 and 3.4 for the calculation of the total ISBL field cost of the plant as a function of capacity. The units of all REAL plant cost parameters, Mlbs/hr, etc., must be consistent with the REAL parameters specified for process calculations.

Operating labor costs are calculated as a linear function of the number of trains or plants. For example, if a single reactor train in Plant 2 requires seven operators per shift, then three trains would require three times as many operators.

5.2.5 Error Checking and Warning Messages

The Fortran user block models may contain some model specific error checking procedures and warning messages which may be printed in the user model report besides those described in the previous capital cost calculations section. In general, error checking procedures have been implemented to test for:

1. The required number of inlet streams
2. The required number of outlet streams
3. Missing required components
4. Solids present in input streams which should not contain them
5. Erroneous user supplied parameters

Whenever possible, appropriate corrections are made to allow the model to run. Appropriate error or warning messages are written to the history file and/or, if appropriate, to the plant summary report.

Warning messages will be printed in the cost section of the plant summary report if either the calculated capacity of a single train is below the specified minimum capacity, or if the calculated capacity of a single train is above the specified maximum capacity of a single train.

5.2.6 Input Parameters

The ASPEN/SP program allows values to be passed to and from Fortran user block models via parameters specified in the input files. There are two types of parameters, integer and real (floating point). The NINT= phrase of the PARAM sentence in the input file specifies the number of integer parameters, and the NREAL= phrase specifies the number real parameters. The values of the integer parameters are specified in the INT sentence, and the values of the real parameters are specified in the REAL sentence.

The Fortran user block model will calculate the required number of duplicate trains or operating units from the total plant capacity and the specified maximum and minimum single unit capacities. However, each Fortran user block model allows the user to specify the number of operating duplicate plants as an input parameter. When the number of operating duplicate plants is supplied as an input parameter, that value will be used, and the calculation of the number of operating duplicate plants will be bypassed.

When the maximum capacity of a single train or operating unit within a plant is not specified (i.e., a zero or negative value is supplied), the total plant cost will be calculated based on a single unit. Operating labor requirements are calculated as a function of the number of units in each plant.

Table 5.1 describes the input parameters which are common to all of the Fortran user block models. The models have at least four integer input parameters and up to 70 real input parameters. Additional information on these parameters is provided in the subsections below which describe the individual plant models.

All the Fortran user block models have four common integer input parameters, INT(1) through INT(4). The first integer parameter, INT(1), is the user block summary report control switch which controls the printing of the three sections of the user block summary report. When INT(1) has a value of zero, all three sections of the summary report are printed. When it has a value of one, only the stream report and utilities report sections are printed. When it has a value of two, only the stream report section is printed. When it has a value of three or more, the entire user block model summary report is not printed.

The second integer parameter, INT(2), is the user Fortran block summary report destination control switch. When INT(2) has a value of zero, the summary report will be written to the normal ASPEN/SP report file. When it has a value of one, the user block summary report will be written to a separate summary report file for each plant. This file name will begin with the letters DCL followed by some numbers and possibly some letters to identify the specific plant or option, and have a filespec of REP. Thus, the separate summary report file for Plant 1 is DCL01.REP; the separate report file for Plant 4 is DCL04.REP, and that for Plant 10 is DCL10.REP.

Table 5.1

General Fortran User Block Model Input Parameters

<u>Parameter</u>	<u>Description</u>
<u>Integer Parameters</u>	
INT(1)	User block summary report control switch. 0 => Write the complete user block summary report. 1 => Skip the capital cost portion of the summary report. 2 => Skip the capital cost and utilities portions of the summary report. 3 => Skip writing the entire user block summary report.
INT(2)	User block summary report destination control switch. 0 => Write the user block summary report to the normal ASPEN/SP output report file. 1 => Write the user block summary report to a separate user block output report file.
INT(3)	Number of operating duplicate trains, excluding spares. If INT(3) = 0, the minimum number of operating duplicate trains, excluding spares, will be determined so that the capacity of each train does not exceed the maximum train capacity specified by parameter REAL(52). If INT(3) > 0, the number of operating duplicate trains, excluding spares.
INT(4)	History file additional output control switch. 0 => Write no additional output to the history file. 1 => Write only the subroutine entry and exit messages to the history file. 2 => Write some additional output to the history file. 3-5 => Write some more additional output to the history file. Larger values will generate more additional output.
<u>Real Parameters</u>	
REAL(1)- REAL(20)	Model specific parameters. These parameter locations are reserved for items which are specific to each Fortran user block model, such as conversion, component distribution factors, etc.
REAL(21)	Constant factor for the power consumption, kw.
REAL(22)	Power consumption per CAP unit, kw/(CAP units).
REAL(23)	Constant factor for the 900 psig / 750 F steam consumption, Mlbs/hr.
REAL(24)	900 psig / 750 F steam consumption per CAP unit, (Mlbs/hr)/(CAP units).
REAL(25)	Constant factor for the 900 psig saturated steam consumption, Mlbs/hr.
REAL(26)	900 psig saturated steam consumption per CAP unit, (Mlbs/hr)/(CAP units).

- Continued on Next Page -

Table 5.1 (Continued)

General Fortran User Block Model Input Parameters

<u>Parameter</u>	<u>Description</u>
REAL(27)	Constant factor for the 600 psig / 720 F steam consumption, Mlbs/hr.
REAL(28)	600 psig / 720 F steam consumption per CAP unit, (Mlbs/hr)/(CAP units).
REAL(29)	Constant factor for the 600 psig saturated steam consumption, Mlbs/hr.
REAL(30)	600 psig saturated steam consumption CAP unit, (Mlbs/hr)/(CAP units).
REAL(31)	Constant factor for the 150 psig saturated steam consumption, Mlbs/hr.
REAL(32)	150 psig saturated steam consumption per CAP unit, of hydrogen (Mlbs/hr)/(CAP units).
REAL(33)	Constant factor for the 50 psig saturated steam consumption, Mlbs/hr.
REAL(34)	50 psig saturated steam consumption per CAP unit, (Mlbs/hr)/(CAP units).
REAL(35)	Constant factor for the plant fuel consumption, MM BTU/hr.
REAL(36)	Plant fuel consumption per CAP unit, (MM BTU/hr)/(CAP units).
REAL(37)	Constant factor for the cooling water consumption, Mgal/hr.
REAL(38)	Cooling water consumption per CAP unit, (Mgal/hr)/(CAP units).
REAL(39)	Constant factor for the process water consumption, Mgal/hr.
REAL(40)	Process water consumption per CAP unit, (Mgal/hr)/(CAP units).
REAL(41)	Constant factor for the nitrogen consumption, MM SCF/hr.
REAL(40)	Nitrogen consumption per CAP unit, (MM SCF/hr)/(CAP units).
REAL(42) -	
REAL(48)	Future use.
REAL(49)	Constant factor for the number of operators per day.
REAL(50)	Number of operators per day per operating train.
REAL(51)	Reference capacity of a single train as defined by the key flow rate in CAP units for the calculation of the ISBL field cost of a single train as a function of train capacity.
REAL(52)	Maximum size of a single train as defined by the key flow rate in CAP units.
REAL(53)	Minimum size of a single train as defined by the key flow rate in CAP units.
REAL(54)	Constant A in the ISBL field cost equation, the fixed capital cost of a single plant in MM \$.
REAL(55)	Constant B in the ISBL field cost equation, the variable cost of a single plant having the key flow rate specified in variable REAL(51) in MM \$.
REAL(56)	Constant E in the ISBL field cost equation, the plant cost scaling exponent.
REAL(57)	Constant F in the ISBL field cost equation, the cost reduction factor for the construction of duplicate trains after the first one.
REAL(58)	Number of spare trains.

- Continued on Next Page -

Table 5.1 (Continued)

General Fortran User Block Model Input Parameters

<u>Parameter</u>	<u>Description</u>
REAL(59) - REAL(70)	Future use.

NOTE: The plant capacity as used in the various calculations is defined as a key flow rate. This key flow rate may be either the total flow rate of a specific stream or the flow rate of the main component in a specific stream. This flow rate is expressed in an appropriate set of units such as MM SCF/hr, Mlbs/hr, or MM SCF/hr of hydrogen. In this generalized table, this set of units is called CAP units since the key flow rate item and appropriate units are not known.

Consequently, files DCL01B.REP, DCL01A1.REP and DCL01A2.REP are the separate plant summary report files for the three Plant 1 coal cleaning options with the DCL01B.REP file being used for the baseline design case and the A1 and A2 files being used for the two alternate cases.

The third integer parameter, INT(3), is the number of operating duplicate trains, excluding spares. When INT(3) has a positive value, it is the number of operating duplicate trains that will be used in the calculation of the total capital cost of the plant. When INT(3) is zero, the number of operating duplicate trains will be calculated based on the specified maximum train capacity given in parameter REAL(52).

The fourth integer parameter, INT(4), controls how much additional information is written to the history file for debugging purposes. When INT(4) has a value of zero, no information except any warning or error messages are written to the history file. When INT(4) has a value of one or greater, some additional information will be written to the history file. In general, the amount of information written to the history file increases as the value of INT(4) increases. Normally, INT(4) should be set either to zero so that no additional information is written to the history file, or to one so that only the master subroutine entry and exit messages are written to the history file.

The first twenty REAL (floating point) parameters, REAL(1) through REAL(20), are used to specify the conversions, component distributions, etc. necessary for the calculation of the output stream flow rates and compositions in each model.

The next thirty REAL parameters, (REAL(21) through REAL(50)), are used to calculate the utilities consumptions or productions for this plant as a linear function of the plant capacity expressed as the flow rate of a key stream.

The next 10 REAL parameters, REAL(51) through REAL(60), are used to calculate the number of duplicate operating units, the capacity of each, and the total capital cost of the entire plant.

The final 10 REAL parameters, REAL(61) through REAL(70), are reserved for future use, such as for calculating the manpower requirements and operating costs.

The models require that the ASPEN/SP input file contain some or all of the components shown in Table 5.2. However, the components may be present in any order, and any component may have a zero flow rate. The model will print a warning message and terminate execution if any of the required component(s) is not specified in the input file.

Table 5.2

ASPEN/SP Input File--Complete Components List

<u>ASPEN/SP Short Component Name</u>	<u>Full Component Name</u>
H2	Hydrogen
N2	Nitrogen
O2	Oxygen
H2S	Hydrogen sulfide
NH3	Ammonia
H2O	Water
CO	Carbon monoxide
CO2	Carbon dioxide
HCL	Hydrogen chloride
COS	Carbonyl sulfide
CH4	Methane
C2H6	Ethane
C3H8	Propane
IC4H10	Iso-butane
NC4H10	Normal butane
IC5H12	Iso-pentane
NC5H12	Normal pentane
T125	100-150 F material leaving Plant 2
T175	150-200 F material leaving Plant 2
T225	200-250 F material leaving Plant 2
T275	250-300 F material leaving Plant 2
T325	300-350 F material leaving Plant 2
T375	350-400 F material leaving Plant 2
T425	400-450 F material leaving Plant 2
T475	450-500 F material leaving Plant 2
T525	500-550 F material leaving Plant 2
T525	550-600 F material leaving Plant 2
T625	600-650 F material leaving Plant 2
T675	650-700 F material leaving Plant 2

- Continued on Next Page -

Table 5.2 (Continued)

T725	700-750 F material leaving Plant 2
T775	750-800 F material leaving Plant 2
T825	800-850 F material leaving Plant 2
T875	850-900 F material leaving Plant 2
T925	900-950 F material leaving Plant 2
T975	950-1000 F material leaving Plant 2
T1000+	1000+ F material leaving Plant 2
P125	Hydrotreated 100-150 F material
P175	Hydrotreated 150-200 F material
P225	Hydrotreated 200-250 F material
P275	Hydrotreated 250-300 F material
P325	Hydrotreated 300-350 F material
P375	Hydrotreated 350-400 F material
P425	Hydrotreated 400-450 F material
P475	Hydrotreated 450-500 F material
P525	Hydrotreated 500-550 F material

ASPEN/SP Input File--Complete Components List

ASPEN/SP Short
Component Name

Full Component Name

P575	Hydrotreated 550-600 F material
P625	Hydrotreated 600-650 F material
P675	Hydrotreated 650-700 F material
P725	Hydrotreated 700-750 F material
P775	Hydrotreated 750-800 F material
P825	Hydrotreated 800-850 F material
P875	Hydrotreated 850-900 F material
P925	Hydrotreated 900-950 F material
P975	Hydrotreated 950-1000 F material
P1000+	Hydrotreated 1000+ F material
REFORMAT	Reformate product from the naphtha reformer
L-SULFUR	Liquid Sulfur
COAL	Coal Feed
URCOAL	Unreacted Coal
SLAG	Slag from the Texaco Gasifier

NOTE: The last three components, COAL, URCOAL and SLAG are non-conventional components of ASPEN component type NC.

The models require that the input and output streams be Conventional, MIXNC, or MIXNCPD ASPEN/SP stream classes. In the ATTR-COMPS statement, required for the latter two stream classes, the items PROXANAL, ULTANAL, SULFANAL, and AOXANAL must be in the stated order. For example, any ATTR-COMPS statements in the input files must be of the form:

ATTR-COMPS COAL PROXANAL ULTANAL SULFANAL AOXANAL

Both ASPEN/SP and the Fortran user block models assume that the order shown is used.

5.2.7 Management Summary Report

As discussed in subsection 5.2.6, several levels of reporting can be selected by the user by setting integer parameters in the input files. These may include the standard ASPEN/SP stream reports, history reports, etc. A customized management summary report was designed for this project which lists for each plant the important streams and components, equipment costs, utilities and manpower requirements that may be of interest in evaluating various coal liquefaction scenarios.

5.3 Simulation Models--Base Case

The Task V report contains a process description and discussion of the Fortran user block model for each plant in the coal liquefaction complex. These discussions contain block diagrams for each plant which show the input and output streams that are handled by the simulation model. The calculation methods and required plant-specific input parameters that may be set by the user in the input file are discussed.

Because this material is contained in the Task V report, it is not repeated here.

5.4 Executing the ASPEN Process Simulation Model

The ASPEN/SP process simulation model of the coal liquefaction complex is executed as follows.

1. Enter ASPENSET to set up the ASPEN/SP system and place the computer in the ASPENSP\RUNS subdirectory. Once done, this step does not have to be repeated unless the computer has been rebooted.
2. All the required files must be either in the ASPENSP\RUNS sub- directory or the ASPENSP\BAT subdirectory. The required files are given in Section 3. If missing, copy PLANTS.FOR, OTHERS.FOR, and DCLN.INP into the ASPENSP\RUNS subdirectory. If missing, copy ASP.BAT, DCLRPT.BAT and DCLSTART.BAT into the ASPENSP\BAT subdirectory.
3. Compile the PLANTS.FOR file to create a PLANTS.OBJ file by typing
F77 PLANTS <Enter>
Once compiled, the file does not need to be recompiled unless the Fortran source code file, PLANTS.FOR, has been changed.
4. Compile the OTHERS.FOR file to create an OTHERS.OBJ file by typing
F77 OTHERS <Enter>
Once compiled, the file does not need to be recompiled unless the Fortran source code file, OTHERS.FOR, has been changed.

5. Execute the ASPEN/SP process simulation model by typing
ASP PLANTS <Enter>
and when prompted for the input file name enter
DCLN <Enter>

The ASPEN/SP process simulation program will now execute generating numerous output files. These will include several ASPEN/SP system generate files having the DCLN. filename. The model will also generate several DCL????REP files containing the block model summary reports. For example, the block model summary report for Plant 4 will be called DCL04.REP. In addition, the model will generate two other files called DCLSUM.REP and DCL1.PRN. The DCL1.PRN file is the file used to transfer the process simulation model results to the LOTUS spreadsheet economics model.

6. Execute the DCLRPT.BAT file to combine all the individual plant summary report files into the combined summary report file called ALL.REP file by typing
DCLRPT <Enter>
This ALL.REP file then may be viewed or printed, as desired.

6. THE COAL LIQUEFACTION KINETIC REACTOR MODEL

6.1 Overview

The kinetic-based reactor model predicts product yields and reactor sizes for the baseline design. Wilsonville Run 257-E results provided the basis for the model, for Illinois No. 6 bituminous coal liquefied in the two-stage Catalytic/Catalytic mode, using AMOCAT™-1C catalyst in each stage. Because no interstage separator was used in Run 257-E, first-stage liquid yields were estimated from earlier Wilsonville runs.

Resid conversion in each ebullated-bed reactor is modelled by first-order reaction rate expressions for a continuous stirred reactor (CSTR). The model accounts for the effects of resid recycle on conversion in each reactor, of thermal and catalytic reaction rates, of catalyst addition rates, and of recycle solvent boiling point compositions. The model also predicts liquid and gas yields, hydrogen consumption, and computes the overall elemental balances for each reactor. However, the capability for rigorous product quality predictions is significantly limited by lack of data from Wilsonville.

The model is also used to size the ebullated-bed reactors. This design capability includes detailed calculations for bed hydrodynamics, heat balances, reactor weight, and hydrogen partial pressure. This allows the determination of the number of reactor trains necessary for given coal processing requirements.

The model can thus be used as a research guidance tool for run planning, for economic evaluations of bituminous coal liquefaction processes, and with modifications, for studies of coal reactivity and catalysts.

Areas for future improvements include fine-tuning the model's liquid yield/quality predictions (e.g. based on Wilsonville Run 261 which used an interstage separator), accounting for the effects of hydrogen partial pressure on resid conversion and product yields/quality, and more rigorous coal conversion kinetics. The model might also be modified to handle the liquefaction of low rank coals, and the use of dispersed catalysts.

6.2 Introduction

The Bechtel/Amoco Base Line design study primarily focuses on the development of a base case design and cost estimates for a conceptual commercial plant for direct liquefaction of Illinois No. 6 bituminous coal. The base case technology is the Catalytic/Catalytic (C/C) two-stage process developed at the Wilsonville pilot plant. In this process, coal is liquefied in the presence of hydrogen and a hydrogen-donor solvent using two close-coupled ebullated-bed reactors filled with supported Ni/Mo hydrocracking catalyst. Similar to the H-Oil/LC-Fining technologies for conversion of petroleum resid, these ebullated-bed reactors facilitate coal plus resid conversion to 1000- °F liquids.

A kinetic model has been developed to predict resid conversion, including key product yields and hydrogen consumption, in each stage of the two-stage C/C process. The

calculations are performed for a given set of key operating conditions such as reactor temperature, coal space velocity, resid recycle rate, and catalyst addition rates. The model has been extended to estimate key reactor design parameters such as diameter and height, hydrogen partial pressure, ebullated-bed hydrodynamics, and heat balances. The key objective is to use the model as a research guidance tool for run planning and economic evaluations, including optimization of catalyst formulations and operating conditions.

In its current form, the model is designed to predict yields for Illinois No. 6 coal using AMOCAT™-1C catalyst in each stage. Depending on the availability of experimental data at operating conditions similar to those used in this study, the key model parameters can be modified to suit other bituminous coals and other supported catalysts.

6.3 Overall Methodology

The key calculation steps for the kinetic model are shown in Figure 6.1.

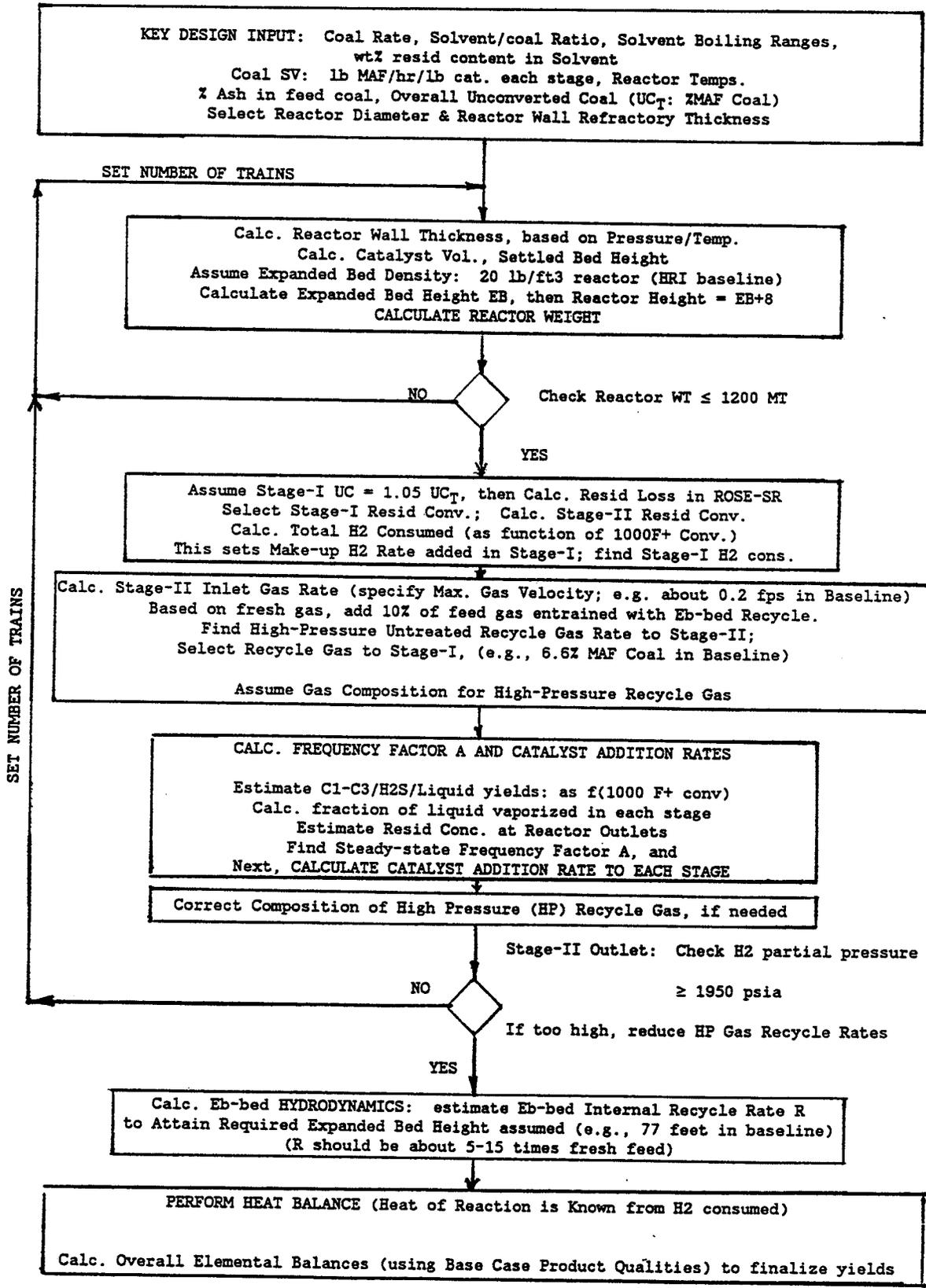
The steady-state catalyst addition rate for each reactor is predicted to obtain specific resid conversion in each stage. Key design parameters are reactor temperature, solvent/coal ratio, resid content of recycle solvent, coal space velocity (defined as lb moisture-ash free coal/hr/lb catalyst), boiling point distribution of 1000- °F solvent component, etc.). The key calculation steps are:

- Provide various design inputs such as coal rate, temperatures, coal SV, reactor diameter, stage I resid conversion, etc. Select number of reactor trains. Overall coal conversion is an input in the program. For Illinois No. 6 coal, overall coal conversion is typically 88-93% MAF coal.
- Calculate reactor weight based on catalyst volume and expanded bed density (design input, typically 20-26 lb/ft³ of expanded bed volume).
- Check reactor weight. If it is more than 1,200 MTons, change design parameters such as coal SV (if the model is being used for run planning) or number of trains (for case studies with conceptual commercial designs).
- If the reactor weight is about 1,200 MTons, check hydrogen partial pressure at the outlet of the second-stage reactor for the required overall resid conversions. This will require detailed estimates for liquid and gas flows in each stage.
- From coal conversion and ash content of feed coal, estimate resid loss with the ROSE-SR ash concentrate. Calculate overall resid conversion. Establish gas flow rates (make-up + recycle) for each stage. Hydrogen consumption is estimated as a function of 1000+ °F conversion.

FIGURE 6.1

C/C TWO-STAGE COAL LIQUEFACTION: KINETIC MODEL

Coal: Illinois No. 6 Coal, Catalyst: Amocat-1C (Each Reactor)



- Based on 1000°F+ coal conversion in each stage, calculate gas and liquid yields based on MAF coal. Using solvent recycle rate and composition, establish liquid flow rates to each stage. Next, calculate resid concentration at reactor outlet from vapor-liquid equilibrium estimations. Determine frequency factor "A" for each stage, and then estimate catalyst addition rates.
- Calculate H₂ partial pressure at Stage II outlet; it should be greater than 1950 psia. If it is significantly lower than 1950 psia, the gas recycle rates/distribution to each stage should be changed. This may require a change in the number of reactor trains if the gas velocities in each stage are too high (for example, more than 0.2 ft/sec).

If H₂ partial pressure is much higher than 1950 psia, reduce gas recycle rates.

- Next, check reactor fluid dynamics. Calculate ebullated-bed internal recycle rate to achieve the desired bed expansion (assumed in the design; in the base line design the bed height is 77 feet). Typically, the ratio of recycle rate/fresh liquid feed should be about 5-15.
- Perform heat balance for each stage, based on H₂ consumption and average bed temperature, and reactor flow rates. Estimate bed exotherm and inlet temperature of fresh feed (gas plus liquid mixture). Typically, bed exotherm should be within 15-40°F.
- Calculate overall elemental balances for each stage using product quality data from the base line design. Make minor adjustments in yields of C₁-C₃ gas make, water, or ash concentrate streams to achieve elemental balances.

A detailed discussion of the internal workings and equations used in the coal liquefaction kinetic reactor model is contained in the Task V report and is not repeated here.

6.4 Input Parameters

The kinetic model does not use all of the same input parameters that the other Fortran user block models use. Following is a list of the integer and real input parameters this model uses.

The five integer parameters and the functions are:

- INT(1) User block summary report control switch.
- 0 => Write the complete user block summary report.
 - 1 => Skip the capital cost portion of the summary report.
 - 2 => Skip the capital cost and utilities portions of the summary report.
 - 3 => Skip writing the entire user block summary report.

- INT(2) User block summary report destination control switch.
 0 => Write the user block summary report to the normal ASPEN/SP output report file.
 1 => Write the user block summary report to a separate user block output report file on logical unit 62 called DCL02.REP.
- INT(3) NOT APPLICABLE.
- INT(4) History file additional output control switch.
 0 => Write no additional output to the history file.
 1 => Write the only the subroutine entry and exit messages to the history file.
 2 => Write some additional output to the history file.
 3-5 => Write some more additional output to the history file. Larger values generate more intermediate output.
- INT(5) Reactor selection switch
 6 => First coal liquefaction reactor. (Yields are calculated in subroutine USR2R via a kinetic model for first stage reactor only. This model is called P2RX1.)
 7 => Second coal liquefaction reactor. (Yields are calculated in subroutine USR2R via a kinetic model for second stage reactor. It is assumed that input are the yields from P2RX1 plus the recycle stream 2S27. This model is called P2RX2.)

The twenty real parameters and the functions are:

- REAL(1) Percent coal conversion based on fresh MAF coal entering the coal liquefaction reactors
- REAL(2) Future use
- REAL(3) Resid yield in reactor I, %MAF
- REAL(4) Overall unconverted coal, %MAF
- REAL(5) Resid loss in ROSE unit, %MAF
- REAL(6) Coal SV, lb MAF coal/hr/lb catalyst
- REAL(7) Fixed carbon, WT% MF
- REAL(8) Reactor internal diameter stage I and II, ft
- REAL(9) Maximum reactor weight, 1322 short tons
- REAL(10) Reactor I temperature, deg F
- REAL(11) Reactor II temperature, deg F
- REAL(12) Stage I pressure, psia
- REAL(13) Stage II pressure, psia
- REAL(14) Maximum gas velocity, ft/sec
- REAL(15) Unconverted coal in stage 1, %MAF
- REAL(16) -
- REAL(20) Future use

6.5 Results

For the base line design, Table 6.1 shows the key reactor parameters predicted by the model.

Table 6.1

KINETIC MODEL: KEY RESULTS FOR BASE LINE DESIGN*

Reactor	I	II
ID, ft	15	15
Refractory Thickness, in.	6	6
Weight, Short Tons	1295	1295
Gas Velocity, fps	0.107	0.212
Total Liquid Velocity, fps	0.104	0.084
Bed Height, ft:		
Settled	43.6	43.6
Expanded	77.0	77.0
Recycle/Fresh Feed Ratio	6.1	3.3
Reactor Average Temp, °F	790	760
Bed Exotherm, °F	30	27

*Total coal rate: 15,140 t/day MAF, number of reactor trains: 5
Catalyst: average diameter, 0.83 inches, length, 0.240 inches,
and equivalent spherical diameter, 0.135 inches.

The reactor weight, gas/liquid velocities, ebullated-bed internal recycle rates, and bed exotherm data are well within the design guidelines. For example, for Stage II, HRI used a gas velocity of about 0.2 ft/sec (vs. 0.22 ft/sec predicted in the model).

Table 6.2 shows that the gas and liquid velocities are quite similar to those used in actual PDU-10 experiments for the H-Coal process (reference: Amoco Oil Company, Final Progress Report, "Study of Ebullated Bed Fluid Dynamics," DOE Contract DE-AC22-80PC30026).

Table 6.2

**TYPICAL GAS/LIQUID VELOCITIES AND BED EXPANSION
(EBULLATED-BED REACTORS USED FOR COAL LIQUEFACTION)**

HRI H-Coal Coal Data: PDU-10*

PDU Test	Liquid Velocity fps	Gas Velocity, fps	% Bed Expansion
1	0.119	0.070	74
2	0.045	0.071	59
3	0.085	0.065	59
4	0.046	0.065	59
5	0.102	0.066	104

*Reference: "Study of Ebullated Bed Fluid Dynamics," Amoco Oil Company, DOE Contract DE-AC22-80PC30026, Final Progress Report, July 1983.

6.6 Executing the Coal Liquefaction Kinetic Reactor Model

The ASPEN/SP coal liquefaction reactor kinetic model is executed as follows.

1. Enter ASPENSET to set up the ASPEN/SP system and place the computer in the ASPENSP\RUNS subdirectory. Once done, this step does not have to be repeated unless the computer has been rebooted.
2. All the required files must be either in the ASPENSP\RUNS sub- directory or the ASPENSP\BAT subdirectory. The required files are given in Section 3. If missing, copy USR2F.FOR, OTHERS.FOR, and T2V2S.INP into the ASPENSP\RUNS subdirectory. If missing, copy ASP.BAT the ASPENSP\BAT subdirectory.
3. Compile the USR2F.FOR file to create a USR2F.OBJ file by typing
F77 USR2F <Enter>
Once compiled, the file does not need to be recompiled unless the Fortran source code file, USR2F.FOR, has been changed.
4. Compile the OTHERS.FOR file to create an OTHERS.OBJ file by typing

F77 OTHERS <Enter>

Once compiled, the file does not need to be recompiled unless the Fortran source code file, OTHERS.FOR, has been changed.

5. Execute the ASPEN/SP process simulation model by typing
ASP USR2F <Enter>
and when prompted for the input file name enter
T2V2S <Enter>

The ASPEN/SP process simulation program will now execute generating numerous output files. These will include several ASPEN/SP system generate files having the T2V2. filename. The model will also generate two report files, DCL2R.REP and DCL2R_M7.REP, containing the reactor summary report information for the first and second reactors, respectively.

APPENDIX A
ASPEN PROCESS SIMULATION MODEL PROBLEM SESSION

ASPEN Process Simulation Model Problem Session

Starting with the base case simulation that you have just run, modify the input file to add a naphtha reformer to process the naphtha to produce a high octane gasoline blending component, additional light hydrocarbons and hydrogen. Call this new input file DCL2.INP. What are the major effects associated with this processing change?

ASPEN Process Simulation Model
Problem Session

Starting with the base case simulation that you have just run, modify the input file to add a naphtha reformer to process the naphtha to produce a high octane gasoline blending component, additional light hydrocarbons and hydrogen. Call this new input file DCL2.INP. What are the major effects associated with this processing change?

Solution

The flow splitter block S7 is used as a valve to switch the naphtha from the naphtha product stream (PNAPHTHA) to the reformer feed stream (7-NAPH). As implemented in the base case model, all the flow entering the S7 flow splitter is directed to the naphtha product stream by the FRAC sentence,

```
FRAC 7-NAPH 0.000
```

In the DCL1.INP file, locate the naphtha splitter block statement
BLOCK S7 FSPLIT

There are two ways switch all the flow to the naphtha reformer. The first is to comment out this FRAC statement by inserting a semicolon (;) in column 1 and removing the semicolon in column 1 from the previous FRAC statement which reads

```
FRAC PNAPHTHA 0.000
```

The other way is to replace the 0.000 in the FRAC 7-NAPH statement with a 1.000 to force all the flow to the naphtha reformer.

Save this input file as DCL2.INP. RUN ASPEN/SP with the ASP.BAT file using the DCL2.INP file. Below is a comparison of the results from this case and the base case.

	<u>With Reformer</u>	<u>Base Case</u>
ROM COAL FEED RATE, MTSD	28.257	29.035
COAL CLEANING REFUSE RATE, MTSD	5.651	5.807
ASH PRODUCTION RATE, MTSD	2.737	2.812
NATURAL GAS RATE, MMMBTU/SD	90.787	84.264
ELECTRICITY PURCHASE, MEGA-WH/SD	.000	.000
RAW WATER MAKE-UP, MMGSD	16.875	17.340
NAPHTHA PRODUCTION, MBSD	17.199	19.208
LT.DIST.PRODUCTION, MBSD	7.809	7.809
HVY.DIST. PRODUCTION, MBSD	21.648	21.648
GAS OIL PRODUCTION, MBSD	13.319	13.319
LIQUID PROPANE PRODUCTION, MBSD	4.821	4.411
MIXED BUTANES PRODUCTION, MBSD	3.756	3.544
SULFUR PRODUCTION, MTSD	.721	.741
NUMBER OF OPERATORS/BOARDMEN	426	415
TOT.INSTALLED CAPITAL, \$MM (E-YR)	3339.515	3491.598
Plant 9 H2 production, MM SCF/hr	16.03	17.19

The model shows that the naphtha production rate has decreased by 2009 bbl/day, but the naphtha that is now produced is a reformat, a high octane gasoline blending component. The propane production has increased by 410 bbl/day, and the butanes production has increased by 212 bbl/day. Because of the hydrogen produced in the naphtha reformer, the hydrogen produced in Plant 9 was reduced by 1.16 MM SCF/hr.

The above also shows that the coal rate has decreased by 778 tons/day and the natural gas rate has increased by 6.523 MMM BTU/day.

APPENDIX B
FILE LISTINGS

The ASP.BAT file

```
@ECHO OFF
REM Batch file to run ASPEN/SP and include the OTHERS.OBJ file in the
REM Fortran linking step.
REM %1 = Fortran user block file name.
REM
IF %1a == a GOTO NOARGS
IF EXIST %1.OBJ GOTO ASPEN
ECHO
ECHO
ECHO ASP cannot find the %1.OBJ file you specified.
ECHO Please check your input and try again.
ECHO
ECHO
GOTO END
:ASPEN
ASPEN %1 OTHERS
GOTO END
:NOARGS
ECHO
ECHO
ECHO ASP requires the Fortran user block model file name as an argument.
ECHO The correct format is as follows: ASP fn
ECHO
ECHO
:END
```

The DCLRPT.BAT file

```
@ECHO OFF
REM Batch file to combine all the individual plant summary reports
REM into a single file called ALL.REP, and optionally print this file
REM when the single calling argument is not blank.
REM
REM Use: Call this batch file by
REM DCLRPT [ ARG
REM When ARG is NOT blank, all the individual plant summary
REM reports will be printed.
REM
REM Prepared under DOE contract no. DE-AC22 90PC89857.
REM
REM Last revision - June 29, 1992.
REM
REM If an old ALL.REP file is present, delete it.
IF EXIST ALL.REP ERASE ALL.REP
REM
REM Heading page.
COPY ALL.REP+\ASPENSP\BAT\DCLSTART.REP ALL.REP > NUL
REM
REM The Summary Report Page.
IF EXIST DCLSUM.REP COPY ALL.REP+DCLSUM.REP ALL.REP > NUL
IF EXIST DCLSUM.REP ERASE DCLSUM.REP > NUL
REM
REM Plant 1 - Coal Cleaning and Preparation Plant - Baseline Case -
REM Coal Cleaning by Jigs for liquefaction.
IF EXIST DCL01B.REP COPY ALL.REP+DCL01B.REP ALL.REP > NUL
IF EXIST DCL01B.REP ERASE DCL01B.REP > NUL
REM
REM Plant 1 - Coal Cleaning and Preparation Plant - Alternate Case 1 -
REM Coal Cleaning by Heavy Media Separation for liquefaction.
IF EXIST DCL01A1.REP COPY ALL.REP+DCL01A1.REP ALL.REP > NUL
IF EXIST DCL01A1.REP ERASE DCL01A1.REP > NUL
REM
REM Plant 1 - Coal Cleaning and Preparation Plant - Alternate Case 2 -
REM Coal Cleaning by Heavy Media Separation and Spherical Agglomeration
REM for liquefaction.
IF EXIST DCL01A2.REP COPY ALL.REP+DCL01A2.REP ALL.REP > NUL
IF EXIST DCL01A2.REP ERASE DCL01A2.REP > NUL
REM
REM Plant 1 - Coal Cleaning and Preparation Plant - Baseline Case -
REM Coal Cleaning by Jigs for gasification.
IF EXIST DCL01G.REP COPY ALL.REP+DCL01G.REP ALL.REP > NUL
IF EXIST DCL01G.REP ERASE DCL01G.REP > NUL
REM
REM Plant 1.4 - Coal Grinding and Drying Plant
IF EXIST DCL01D.REP COPY ALL.REP+DCL01D.REP ALL.REP > NUL
IF EXIST DCL01D.REP ERASE DCL01D.REP > NUL
REM
```

- Continued on Next Page -

The DCLRPT.BAT file - Page 2

```
REM Plant 2 - Coal Liquefaction Plant.
IF EXIST DCL02.REP COPY ALL.REP+DCL02.REP ALL.REP > NUL
IF EXIST DCL02.REP ERASE DCL02.REP > NUL
REM
REM Plant 3 - Gas Plant.
IF EXIST DCL03.REP COPY ALL.REP+DCL03.REP ALL.REP > NUL
IF EXIST DCL03.REP ERASE DCL03.REP > NUL
REM
REM Plant 4 - Naphtha Hydrotreater.
IF EXIST DCL04.REP COPY ALL.REP+DCL04.REP ALL.REP > NUL
IF EXIST DCL04.REP ERASE DCL04.REP > NUL
REM
REM Plant 5 - Gas-oil Hydrotreater.
IF EXIST DCL05.REP COPY ALL.REP+DCL05.REP ALL.REP > NUL
IF EXIST DCL05.REP ERASE DCL05.REP > NUL
REM
REM Plant 6.1 - Hydrogen Purification by Membrane Permeation Plant.
IF EXIST DCL61.REP COPY ALL.REP+DCL61.REP ALL.REP > NUL
IF EXIST DCL61.REP ERASE DCL61.REP > NUL
REM
REM Plant 6.2 - Hydrogen Purification by Pressure Swing Absorption.
IF EXIST DCL62.REP COPY ALL.REP+DCL62.REP ALL.REP > NUL
IF EXIST DCL62.REP ERASE DCL62.REP > NUL
REM
REM Plant 7 - Naphtha Reformer Plant.
IF EXIST DCL07.REP COPY ALL.REP+DCL07.REP ALL.REP > NUL
IF EXIST DCL07.REP ERASE DCL07.REP > NUL
REM
REM Plant 8.1 - ROSE-SR Unit.
IF EXIST DCL81.REP COPY ALL.REP+DCL81.REP ALL.REP > NUL
IF EXIST DCL81.REP ERASE DCL81.REP > NUL
REM
REM Plant 8.2 - Fluid Coking Plant.
IF EXIST DCL82.REP COPY ALL.REP+DCL82.REP ALL.REP > NUL
IF EXIST DCL82.REP ERASE DCL82.REP > NUL
REM
REM Plant 9 - Hydrogen Production by Coal Gasification Plant.
IF EXIST DCL09.REP COPY ALL.REP+DCL09.REP ALL.REP > NUL
IF EXIST DCL09.REP ERASE DCL09.REP > NUL
REM
REM Plant 9.1 - Hydrogen Production by Natural Gas Reforming Plant.
IF EXIST DCL91.REP COPY ALL.REP+DCL91.REP ALL.REP > NUL
IF EXIST DCL91.REP ERASE DCL91.REP > NUL
REM
REM Plant 10 - Air Separation Plant.
IF EXIST DCL10.REP COPY ALL.REP+DCL10.REP ALL.REP > NUL
IF EXIST DCL10.REP ERASE DCL10.REP > NUL
REM
REM Plant 11 - Sulfur Plant.
IF EXIST DCL11.REP COPY ALL.REP+DCL11.REP ALL.REP > NUL
IF EXIST DCL11.REP ERASE DCL11.REP > NUL
```

- Continued on Next Page -

The DCLRPT.BAT file - Page 3

```
REM
REM Plant 31 - Utilities Plant.
IF EXIST DCL31.REP COPY ALL.REP+DCL31.REP ALL.REP > NUL
IF EXIST DCL31.REP ERASE DCL31.REP > NUL
REM
REM Plant 38 - Ammonia Recovery Plant.
IF EXIST DCL38.REP COPY ALL.REP+DCL38.REP ALL.REP > NUL
IF EXIST DCL38.REP ERASE DCL38.REP > NUL
REM
REM Plant 39 - Phenol Plant.
IF EXIST DCL39.REP COPY ALL.REP+DCL39.REP ALL.REP > NUL
IF EXIST DCL39.REP ERASE DCL39.REP > NUL
REM
REM Plant 31.1 & 31.4 - Fluidized Bed Combustor and Steam Turbine Gen.
IF EXIST DCLA6.REP COPY ALL.REP+DCLA6.REP ALL.REP > NUL
IF EXIST DCLA6.REP ERASE DCLA6.REP > NUL
REM
REM If there is an argument on the command line, print ALL.REP, else quit
IF %1. == . GOTO END
PRINT ALL.REP
:END
ECHO
```

The DCLSTART.REP File

The following file is copied to the beginning of the ALL.REP file by the DCLRPT.BAT file to provide a title page for the plant summary report file.

**U. S. DEPARTMENT OF ENERGY
PITTSBURGH ENERGY TECHNOLOGY CENTER**

**DIRECT COAL LIQUEFACTION BASELINE
DESIGN AND SYSTEMS ANALYSIS
CONTRACT NO. DEAC22 90PC89857**

PLANT SUMMARY REPORTS

APPENDIX C
MISCELLANEOUS ITEMS

APPENDIX C

Miscellaneous Items

This appendix contains the following two items.

1. The course schedule which was passed out on Monday morning, March 23, 1992, at the beginning of the course.
2. An outline for the use of the KEDIT full screen editor (Mansfield Software Group, Inc., P. O. Box 532, Storrs, Ct. 06268).
3. A listing of the PROFILE.KEX file which configures KEDIT for use as described in the previous outline.

ASPEN/SP Modeling Course

DOE-PETC Pittsburgh, Pennsylvania

March 23, 1992

8:30 am An Introduction to ASPEN/SP
9:30 am An Overview of ASPEN/SP Input Language
10:15 am Break
10:30 am ASPEN/SP History and Report Files
12:00 pm Lunch
1:00 pm Global Specifications
1:45 pm Simulation Strategy
2:00 pm Components and Physical Properties
2:30 pm Break
2:45 pm Components and Physical Properties continued
4:00 pm Problem Session #1

March 24, 1992

8:30 am Flowsheets and Streams
10:00 am Unit Operations 1 -- General
10:15 am Break
10:30 am Unit Operations 1 continued
11:30 am Unit Operations 2 -- Distillation
12:00 pm Lunch
1:00 pm Unit Operations 2 continued
2:00 pm Unit Operations 3 -- Reactors
2:30 pm Break
2:45 pm Unit Operations 3 continued
3:30 pm Problem Session #2

March 25, 1992

8:30 am Design Specifications and FORTRAN Blocks
10:15 am Break
10:30 am Design Specifications and FORTRAN Blocks continued
10:45 am Case Studies and Optimization
12:00 pm Lunch
1:00 pm Calculation Sequencing and Convergence
2:30 pm Break
2:45 pm Problem Session #3

March 26, 1992

8:30 am Crude Slicing, Blending and Pseudocomponents
10:15 am Break
10:30 am Costing
11:45 am General ASPEN/SP Wrap Up
12:00 pm Lunch

1:00 pm Process Simulation Model
o Overall Philosophy
o Overall Description
o Block Descriptions
2:30 pm o Block Descriptions (continued)
o Running Baseline Design

March 27, 1992

8:30 am o Process Simulation Model Options
o Optional Case Study
10:15 am Break
10:30 am Reactor Kinetic Model
12:00 pm Lunch
1:00 pm Reactor Kinetic Model (continued)
o Running Baseline Design Case
2:15 pm Break
2:30 pm Lotus Spreadsheet Economics Model
o Description
o Example cases
o Running what-if cases
4:00 pm Adjournment

OUTLINE FOR USE OF KEDIT FULL-SCREEN EDITOR

- I. Starting KEDIT
 - A. New files
 - 1. K <ENTER>, then it prompts for fn.ext
 - 2. K fn.ext <ENTER>
 - B. Existing files
 - 1. Start the same as above
 - 2. KEDIT brings a working copy of the file into memory
- II. Screen layout
 - A. ID line - top line
 - 1. Name of the file
 - 2. Line and column position
 - 3. Number of lines in the file
 - 4. Number of changes since last saved
 - B. Command line - second line
 - 1. Contains a small arrow
 - 2. Issue commands with <ENTER> key
 - 3. <HOME> key moves cursor to command line
 - 4. Displays information and error messages
 - C. Scale line - third line
 - 1. Displays column numbers
 - D. Current line - fourth line
 - 1. Highlighted
 - 2. Commands usually start operation at this line
 - E. Status line - bottom line
 - 1. After first keystroke copyright notice changes to
 - 2. Version number
 - 3. Number of files being edited
 - 4. Information on memory usage
 - 5. Time
 - F. File area
 - 1. Between the scale line and status line
 - 2. Text displayed between top of file and end of file lines
- III. Important keys and their functions
 - A. <HOME> key
 - 1. Moves the cursor to the command line
 - 2. Executes pending prefix commands (cursor may be repositioned as in the add line command)
 - B. <ENTER> key
 - 1. Executes commands on the command line
 - 2. Moves cursor to first column of prefix area of next line in file area
 - C. <RIGHT>/<LEFT>/<UP>/<DOWN> arrow keys
 - 1. Moves cursor in prefix area and file area
 - 2. Wraps to next line
 - D. <TAB>/<SHIFT+TAB> keys
 - Moves cursor to the start of the next/previous field
 - E. <PAGE UP>/<PAGE DOWN> keys
 - Moves display one screen up or down
 - F. <CTRL+PAGE UP>/<CTRL+PAGE DOWN> keys
 - Moves to top or bottom of file
 - G. <END> key
 - Moves the cursor to the end of the line
 - H. <ESC> key
 - Restores a modified line to its original condition if the cursor still is on that line (undo function)

IV. Important command line commands and their functions

- A. SET NUM ON/SET NUM OFF
Places/removes line numbers in the prefix area
- B. GET fn.ext
Brings a copy of fn.ext into working copy following the current line
- C. SET FILEID fn.ext
Changes reference to disk file fn.ext for saving
- D. nn
Moves current line down nn lines
- E. :nn
Makes line number nn the current line
- F. L/string/
Locates next occurrence of string and makes that line the current line
- G. C/string1/string2/n m
Changes m occurrences of string1 to string2 on n lines beginning with the current line (default=1, *=all)

V. Adding new lines

- A. F2 adds a blank line below cursor or current line
- B. From the prefix area
 1. Use A, to add a single line or An, where n=number of lines
 2. Press <HOME> key to execute

VI. Correcting typing mistakes

- A. Type over
- B. Use <DELETE> key to delete character under the cursor
- C. Use <INSERT> key to insert characters in front of the cursor

VII. Copying existing lines

- A. Use Cn, where n=number of lines, in the prefix area to mark
 1. Use an F, for following, or a P, for preceding, in the prefix area to mark where the copied lines will be placed
 2. Press the <HOME> key to execute
- B. Use CC, in the prefix area to mark the first and last lines of a group to be copied
 1. Use an F, for following, or a P, for preceding, in the prefix area to mark where the copied lines will be placed
 2. Press <HOME> key to execute

VIII. Deleting existing lines

- A. Use Dn, where n=number of lines, in the prefix area to mark. Press <HOME> key to execute
- B. Use DD, in the prefix area to mark the first and last lines of a group to be deleted. Press <HOME> key to execute

IX. Moving existing lines

- A. Use Mn, where n=number of lines, in the prefix area to mark
 1. Use an F, for following, or a P, for preceding, in the prefix area to mark where the moved lines will be placed
 2. Press <HOME> key to execute
- B. Use MM, in the prefix area to mark the first and last lines of a group to be moved
 1. Use an F, for following, or a P, for preceding, in the prefix area to mark where the moved lines will be placed
 2. Press <HOME> key to execute

- X. Saving files and ending a KEDIT session
 - A. Move the cursor to the command line with <HOME> key
 - B. Use SAVE to save the working copy to disk and continue the KEDIT session
 - C. Use FILE to save the working copy to disk and exit KEDIT
 - 1. If the file is new, the working copy is saved to disk
 - 2. If the file already exists, the working copy overwrites the disk copy and replaces it
 - 3. KEDIT session ends and screen display returns to DOS prompt
 - D. Use QQ to quick quit without saving and exit KEDIT
 - 1. If the file is new, it is not saved to disk
 - 2. If the file already existed, or was saved, the working copy is discarded and the disk version remains unchanged
 - 3. KEDIT session ends and screen display returns to DOS prompt

FUNCTION KEYS

- F1 - Edit the KEDIT.HLP help file
- F2 - Add a blank line below the cursor
- F3 - Quick Quit - End the KEDIT session without saving
- F4 - Move cursor to next tab column
- F5 - Cursor line becomes current line
- F6 - Redisplay last command line
- F7 - Split line at cursor position
- F8 - Join following line at cursor position
- F9 - Reissue last command
- F10 - Page down
- F11 - Page up
- F12 - File - Save working copy to disk and end KEDIT session

ATTACHMENT II
THE PROFILE.KEX FILE

```
* Simple PROFILE.KEX file executed at the start of each KEDIT
* session to SET screen colors, layout, and other options and
* DEFINE special key assignments
*
'set attributes 2 15 112 120 14 14 15 15 7 14 7 7 15 7 2 14'
'set prefix on left'
'set cmdline top'
'set curline 4'
'set scale on 3'
'set autosave 20'
'set beep on'
'set wrap on'
'set keyboard enhanced'
'set arbchar on `~'
'define F7 split aligned'
'define F8 join aligned'
'define F10 forward'
'define F11 backward'
'define F12 file'
```

APPENDIX D

ASPEN COAL LIQUEFACTION KINETIC REACTOR MODEL PROBLEM SESSION

ASPEN Coal Liquefaction Kinetic Reactor Model
Problem Session

1. Starting with the baseline simulation, how would the reactor operations change if the average diameter of the catalyst particles is changed from 0.083 inches to 0.031 inches? Predict the required changes in the "ratio of liquid recycle to fresh feed" in each reactor in order to maintain the same expanded catalyst bed as the baseline design (77 feet). Do the "bed exotherms" change?
2. For the baseline design, what are the effects of changing the temperature of the coal slurry preheater outlet stream (stream 2S4) to 530 F (vs. 570 F in the baseline design), and of changing the temperature of the recycle gas preheater outlet stream (stream 2S10) to 1020 F (vs. 1050 F)? Based on these new figures, what is the estimated average bed temperature in the first stage? What is the predicted reactor outlet temperature? Compare these numbers with those predicted by the reactor heat balance model.

ASPEN Coal Liquefaction Kinetic Reactor Model
Problem Session

1. Starting with the baseline simulation, how would the reactor operations change if the average diameter of the catalyst particles is changed from 0.083 inches to 0.031 inches? Predict the required changes in the "ratio of liquid recycle to fresh feed" in each reactor in order to maintain the same expanded catalyst bed as the baseline design (77 feet). Do the "bed exotherms" change?

Solution:

Important: Make a back up copy of the USR2G.FOR and T2V2S.INP files of the base case for future use because these problems require changing these files.

The catalyst particle size (d_p) is defined as element 8 in vector C. Therefore, the value for this item has to be changed from 0.083 to 0.031 in the Fortran code in file USR2G.FOR. At the beginning of Subroutine USR02C, there is a DATA statement which initializes the items in the C vector. Change the eighth item from 0.083 to 0.031. This also requires changing the equivalent spherical diameter (d_s) as calculated from the following equation.

$$d_s = \sqrt[3]{\frac{3}{2} d_p^2 L_p}$$

For this design, $L = 0.24$ inches. Thus, for a d_p of 0.031 inches, the calculated d_s is 0.0702 inches. Change the tenth item in the C vector from 0.1354 to 0.0702. Recompile the USR2G.FOR file by typing "F77 USR2G <Enter>" to create a new USR2G.OBJ file. Rerun ASPEN using the same T2V2S input file.

The decreased catalyst particle size requires a reduction in the eb-bed liquid recycle ratio (in each stage) to maintain the same bed expansion. For Stage I, the ratio of "recycle to fresh feed" decreases from 6.12 to 4.90; the bed exotherm is increased from 29.5 to 34.9 Fahrenheit degrees (for an average bed temperature of 790 F). Similar trends also are observed for the second stage.

2. For the baseline design, what are the effects of changing the temperature of the coal slurry preheater outlet stream (stream 2S4) to 530 F (vs. 570 F in the baseline design), and of changing the temperature of the recycle gas preheater outlet stream (stream 2S10) to 1020 F (vs. 1050 F)? Based on these new figures, what is the estimated average bed temperature in the first stage? What is the predicted reactor outlet temperature? Compare these numbers with those predicted by the reactor heat balance model.

Solution:

Restore the original USR2G.FOR Fortran source code file to the ASPENSP/RUNS and compile it by typing "F77 USR2G <Enter>" to restore the original USR2G.OBJ file.

The slurry preheater outlet stream temperature is controlled by the outlet temperature specified for HEATER BLOCK 2L-101, and the recycle gas preheater outlet stream temperature is controlled by the outlet temperature specified for HEATER BLOCK 2L-102. In the T2V2S.INP input file, change the specified outlet temperature for HEATER BLOCK 2L-101 to 530 from 570, and change the specified outlet temperature for HEATER BLOCK 2L-102 to 1020 from 1050. Rerun ASPEN using this revised T2V2S.INP file.

Inspection of the results shows that the estimated average bed temperature in Stage I decreases from 825.9 in the base case to 791.9 F (vs. 790 F assumed in the kinetic model), and the outlet temperature decreases from 841.5 to 806.3 F (vs. 804.9 F predicted by the heat balance model). Thus, the model can be used to predict the required preheater outlet temperatures to achieve a desired reactor temperature.