COMPUTER-AIDED INDUSTRIAL PROCESS DESIGN

The ASPEN Project

First Annual Report
for the period
June 1, 1976 to May 30, 1977

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Department of Chemical Engineering and
Energy Laboratory
Massachusetts Institute of Technology
Cambridge, Massachusetts 02139

Date Submitted: June 15, 1977

PREPARED FOR THE UNITED STATES
ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION
FOSSIL ENERGY PROGRAM

Under Contract No. E(49-18)-2295 Task No. 9

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TABLE OF CONTENTS

ABSTRACT

Work during the first year of this contract concentrated on acquiring the project staff, development of a prototype simulator, the simulation of three coal conversion processes, a survey of software for acquisition, the development of a preliminary physical property subsystem, and the setting up of an advisory committee consisting of industrial government and university representatives. The prototype simulator, PLEXSYS II has been completed and is now being used in the simulation of the IGT HYGAS process, the Conoco CO_2 Acceptor process and the Exxon Donor Solvent process. Simulations of the HYGAS process and the CO_2 Acceptor process will be completed in August, 1977. Negotiations are under way with Exxon to release the proprietary data necessary to complete the simulation of the Donor Solvent process. The preliminary physical property subsystem incorporating properties of coal is being used in conducting these simulation studies. The software survey has been completed. The programs surveyed are now being evaluated for possible acquisitions. Negotiations will be conducted with holders of proprietary software for release of their programs to the ASPEN project. An advisory committee, consisting of representatives from 28 companies, 8 universities and 6 government laboratories has been formed to aid in the design of the system.

A list of seven reports and/or papers published during the year is included.

I. OBJECTIVE AND SCOPE OF WORK

The objective of this project is to develop a computer based process simulator and economic evaluation system for use in the engineering of fossil energy conversion processes. The system has been named ASPEN (Advanced System for Process Engineering). It will provide the U.S. Energy Research and Development Administration (ERDA) with a rapid, efficient, and consistent means of performing its process evaluation functions.

For a process such as coal gasification or liquefaction, ASPEN will be capable of performing detailed material and energy balances, equipment sizing, and economic evaluation. It will be designed to meet the specialized requirements of fossil energy conversion processes, including an extensive data base for coal physical properties, compatibility with conversion reactor models currently available and/or being constructed, and the capability of handling streams of solids.

The scope and specific objectives of the project are to:

1. Develop a prototype simulator and demonstrate the ability to simulate three specific fossil fuel conversion processes of interest to ERDA (HYGAS, Donor Solvent, and CO_2 Acceptor).
2. Develop a system structure of ASPEN with the necessary flexibility to model the different process configurations encountered in fossil energy process development

and to allow insertion of proprietary programs and data for use by industry

3. Develop a physical property subsystem that will calculate the properties important in modeling fossil energy processes. It will have an associated data base for coal physical properties.
4. Develop a unit operations subsystem which will have process models for all major types of equipment used in fossil fuel conversion processes.
5. Develop a cost estimation and economic evaluation subsystem that will compute capital investment, operating costs, and profitability of proposed designs.
6. Develop a data regression subsystem that will utilize experimental data to compute coefficients in correlations for physical properties.
7. Acquire existing industrial programs and data and modify them for incorporation into ASPEN. This will avoid the need to redevelop existing, standard routines for modeling unit operations, physical properties, and other calculations.
8. Demonstrate the capabilities of ASPEN by simulating a number of benchmark problems.

II. SUMMARY OF PROGRESS TO DATE

The work under Contract No. E(49-18)-2295 Task No. 9 is organized into eight reporting tasks. Summaries of work accomplished in these tasks appear in this section, for the period June 1, 1976 to May 31, 1977.

The year's work has resulted in the publication and/or presentation of the following reports, theses etc.:

Evans, L. B., B. Joseph, and W. D. Seider, "Computer-Aided Industrial Process Simulation and Design." Paper presented at the Conference on Mathematical Modeling of Coal Conversion Processes, Washington, D.C., November 1976. Available in Report No. CONF-761104, Energy Research and Development Adminstration, Washington, D.C.

Evans, L. B., B. Joseph, W. D. Seider, "System Structures for Process Simulation," accepted for publication in the AlChE Journal.

Evans, L. B., W. D. Seider, "The Requirements of an Advanced Computing System for Chemical Process Engineering," Chemical Engineering Progress, 72, 6 (1976).

Joseph, B., L. B. Evans and W. D. Seider, "The Use of a Plex Data Structure in Process Simulation," submitted for publication to Computers and Chemical Engineering, Pergammon Press. Also presented at the National Meeting of the AlChE, Kansas City, Missouri, April 1976.

Peterson, J. N., "Survey of Software for Computer-Aided Chemical Process Design," M.S. Thesis, Department of Chemical Engineering, Massachusetts Institute of Technology, January 1977.

Seider, W. D., B. Joseph, E. G. Wong, and L. B. Evans, "Routing of Calculations in Process Simulation," Paper presented at the 69th Annual Meeting of the AiChE, Chicago, Illinois, November 1976.

Wong, E. G., "Routing of Estimation Methods for Calculation of Physical Properties." M.S. Thesis, Department of Chemical Engineering, Massachusetts Institute of Technology, June 1976.

The following are task-by-task summaries of progress during the past year.

TASK 1, DEVELOPMENT OF PROTOTYPE COMPUTER SIMULATOR AND SIMULATION OF SPECIFIC FOSSIL ENERGY PROCESSES

During the past year the prototype simulator, PLEXSYS II, was programmed and is now in operation. The plex structure has proved to be a very flexible arrangement for modeling the different types of unit operations present in coal conversion operations. Preliminary experiments showed that the extra computing effort required to store and access information from the plex is not excessive. The prototype has demonstrated the use of plex structure in FORTRAN as an alternative to fixed array storage.

Simulation of the HYGAS coal gasification process is now being completed. All the unit modules required to complete the simulation have been prepared. These include two alternate models for the gasification reactor and the methanation reactor. A program prepared by the University of West Virginia has been adopted for sizing the acid gas removal section of the plant.

Modeling of the Exxon Donor-Solvent process has begun. Progress has been hampered by the lack of published literature on the process and restrictions on access to Exxon's proprietary data. A meeting was held between Exxon, ERDA and MIT representatives in May to discuss the release of

proprietary information to MIT. Negotiations are currently underway with Exxon to release some of the proprietary data on the process under a secrecy agreement.

The simulation of the CO_2-Acceptor process is also scheduled for completion during the next quarter using a combination of PLEXSYS II and FLOWTRAN. Contacts with the Conoco Coal Development Company were made to obtain pilot plant data and programs developed by Conoco to model the process. The simulation of the process is being carried out in two stages. The preliminary section of the plant involving solids handling such as crushing and grinding will be modeled using PLEXSYS II whereas the gas clean up operations will be simulated in FLOWTRAN. By combining the two simulators we can overcome the deficiency of FLOWTRAN in dealing with solids. Programs for gasification and dolomite regeneration were obtained from Conoco and are being converted for use with PLEXSYS II simulation.

TASK 2, DEVELOPMENT OF ASPEN SYSTEM STRUCTURE

An advisory committee consisting of representatives of industry, government, and universities was formed to guide development of ASPEN and to insure that it will meet the needs of the ultimate users.

A list of preliminary design criteria for ASPEN has been prepared. A questionnaire based on the criteria is being sent out to all members of the Advisory Committee to

get feedback from the industry users of computer software. During the next quarter, a list of functional specifications of the systems will be drawn up based on the results of the survey. A meeting of the Users/Use Interface Subcommittee of the Task Force on System Design will be held in August. Negotiations are underway with a software company, SOFTECH, to obtain assistance in the design of the system.

TASK 3, DEVELOPMENT OF PHYSICAL PROPERTY SUBSYSTEM AND DATA BANK

During the past year, a preliminary version of the physical property subsystem was developed. In addition, methods for calculating phase and chemical equilibrium were investigated under a subcontract with the University of Pennsylvania.

The preliminary physical property subsystem (PPS), designed for PLEXSYS II, is being used in the simulation of three coal conversion processes. The PPS incorporates ideas of routing and modularity which are needed in ASPEN. Programs for simulating properties of coal are included. Modules for calculating properties of gases, liquids and coal have been implemented. A report on the physical property system is being prepared and will be submitted separately to ERDA along with this stand alone PPS. All programs in the system were tested against experimental data available in the literature or when experimental data was not available, compared with FLOWTRAN results.

The coal properties estimation modules incorporated in this PPS are based on the Coal Conversion Systems Technical Data Book being prepared by IGT.

Under the subcontract, different methods for calculating phase and chemical equilibria were surveyed. Better implementation of existing methods and new methods were investigated. A number of example problems were selected from literature to study the effectiveness of this technique.

TASK 4, DEVELOPMENT OF UNIT OPERATIONS SUBSYSTEM

A list of unit operations modules required by ASPEN has been assembled and complete descriptions of the data required to specify them, methods of calculation, etc. are being prepared. The list will form the basis for deciding which modules need to be acquired, which programmed in house, and which are not essential to ASPEN. Work on this task is not scheduled to begin until the second year.

TASK 5, DEVELOPMENT OF COST ESTIMATION AND ECONOMIC EVALUATION SUBSYSTEM

The existing cost estimation and economic evaluation programs are being analyzed to better define the capabilities required in ASPEN. Among those being analyzed are ECONOMIST, PROVES, CHEEP, PEPCOST and CEDA. However, work on this task is not scheduled to begin until the second year.

TASK 6, DEVELOPMENT OF DATA REGRESSION SUBSYSTEM

Work on this task is not scheduled to begin until the second year.

TASK 7, ACQUISITION OF PROPRIETARY SOFTWARE AND MODIFICATION FOR USE IN ASPEN

Acquisition of software has proceeded on two parallel paths. The first subtask was to acquire a base simulator which will provide basic capabilities for simulating vapor - liquid processes. Programs of potential interest to ASPEN were identified. Negotiations are currently underway to acquire a simulator which will provide ASPEN with the capability to do simulations of processes involving vapor - liquid streams. This will assure that ASPEN will be built on current technology and will not duplicate work that has already been accomplished by private industry. The base simulator will also provide ERDA and its contractors with an immediate tool which can be used to simulate parts of energy conversion processes involving only liquids and gases.

The second subtask was concerned with identifying software which may provide modules to be incorporated into the integrated ASPEN system. An extensive survey of industry, universities and commercial software houses was conducted to identify programs that were of potential use to ASPEN. More than 500 letters were sent out. About 210 returns

have been processed so far and over 440 commercial, university and proprietary programs were identified. A meeting of the Task Force on Software Evaluation was held at M.I.T. on May 2 and 3, 1977 to screen out programs of inferior quality or programs that were irrelevant to the project. The project staff is currently evaluating the programs that were screened to better identify their scope and capabilities. The programs have been divided into five categories to aid in the evaluations, namely: heat exchangers and reactors, separation processes, physical properties, cost estimation and economic evaluation programs and miscellaneous unit operations including mathematical routines.

TASK 8, INTEGRATION, TESTING, AND DOCUMENTATION OF ASPEN SYSTEM

Work on this task is not scheduled to begin until the second year.

Program schedules for the eight reporting tasks appear in the pages directly following.

PROGRAM SCHEDULE

Revised 6/1/77

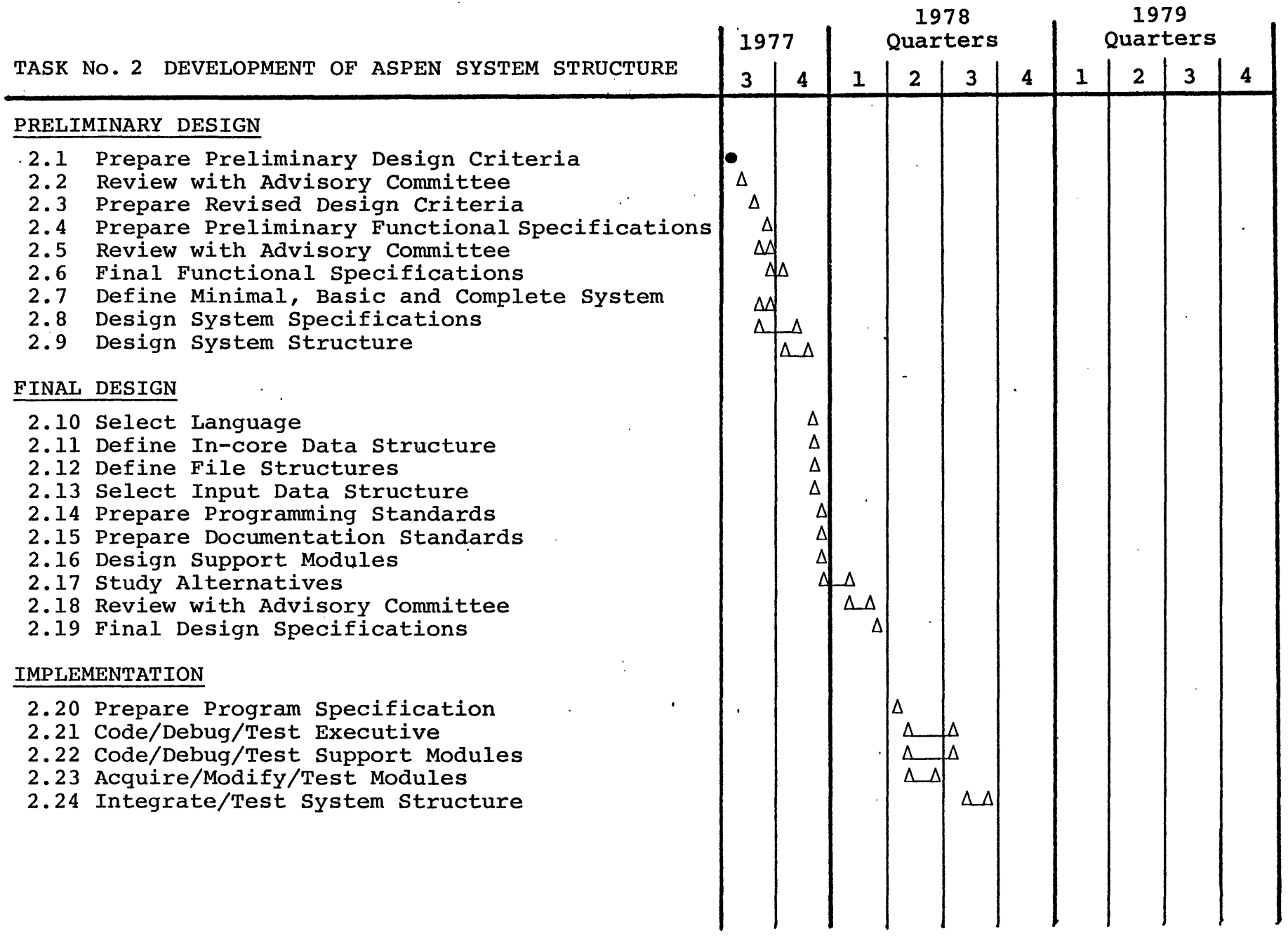
TASK No. 1 DEVELOPMENT OF PROTOTYPE SIMULATOR AND SIMULATION OF FOSSIL ENERGY PROCESSES	1977		1978 Quarters				1979 Quarters			
	3	4	1	2	3	4	1	2	3	4
1.1 Develop Prototype Simulator										
a. Design Prototype	●									
b. Code/Debug/Test	●									
c. Document System	●									
1.2 Select Processes to be Simulated	●									
1.3 Obtain Data on Processes	Δ									
1.4 Develop Models for Process Units	Δ	Δ								
1.5 Perform Sinulation Studies		Δ	Δ							
1.6 Prepare Reports		Δ								

● Task already completed

Δ Signifies beginning or end of activity

PROGRAM SCHEDULE

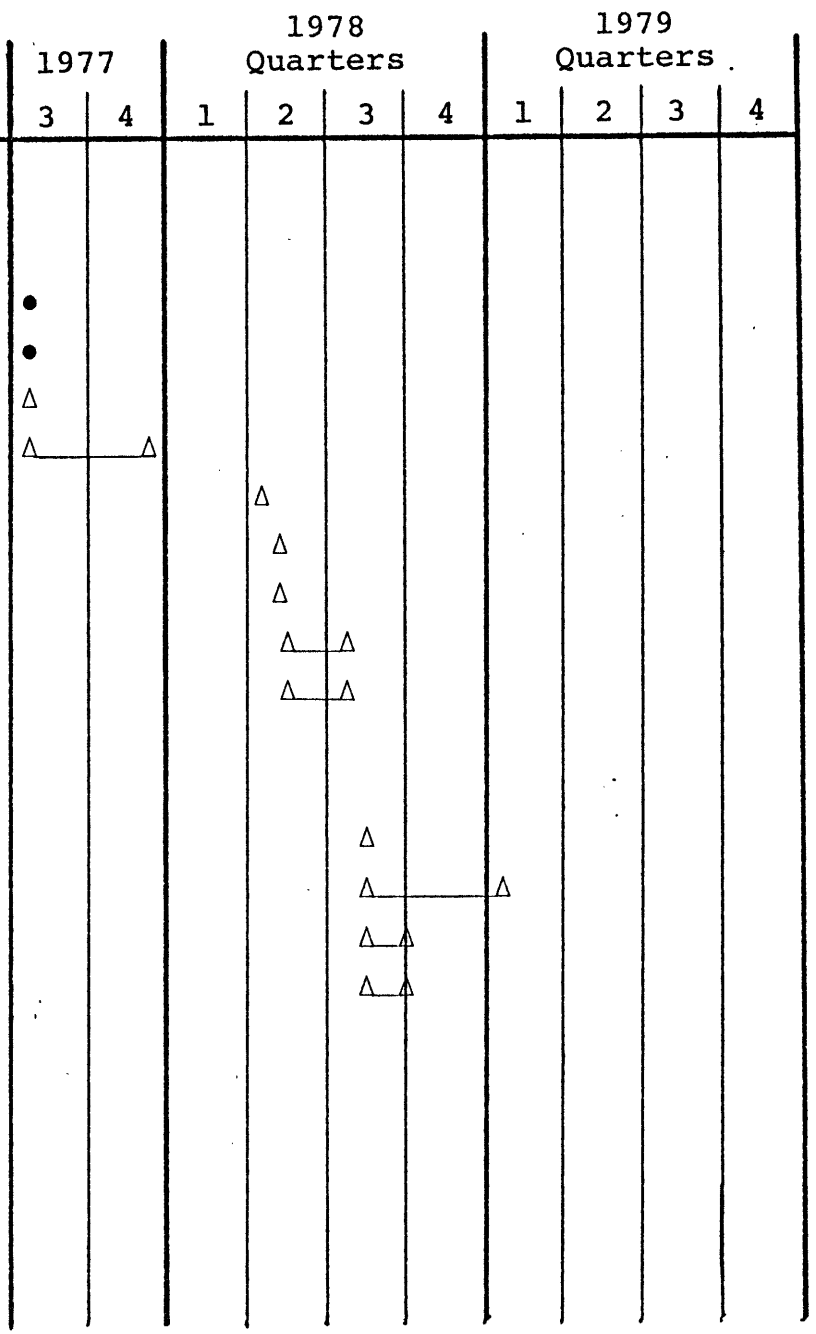
Revised 6/1/77



PROGRAM SCHEDULE

Revised 6/1/77

TASK No. 3 DEVELOPMENT OF PHYSICAL PROPERTY SUBSYSTEM AND DATA BANK



BASIC SYSTEM

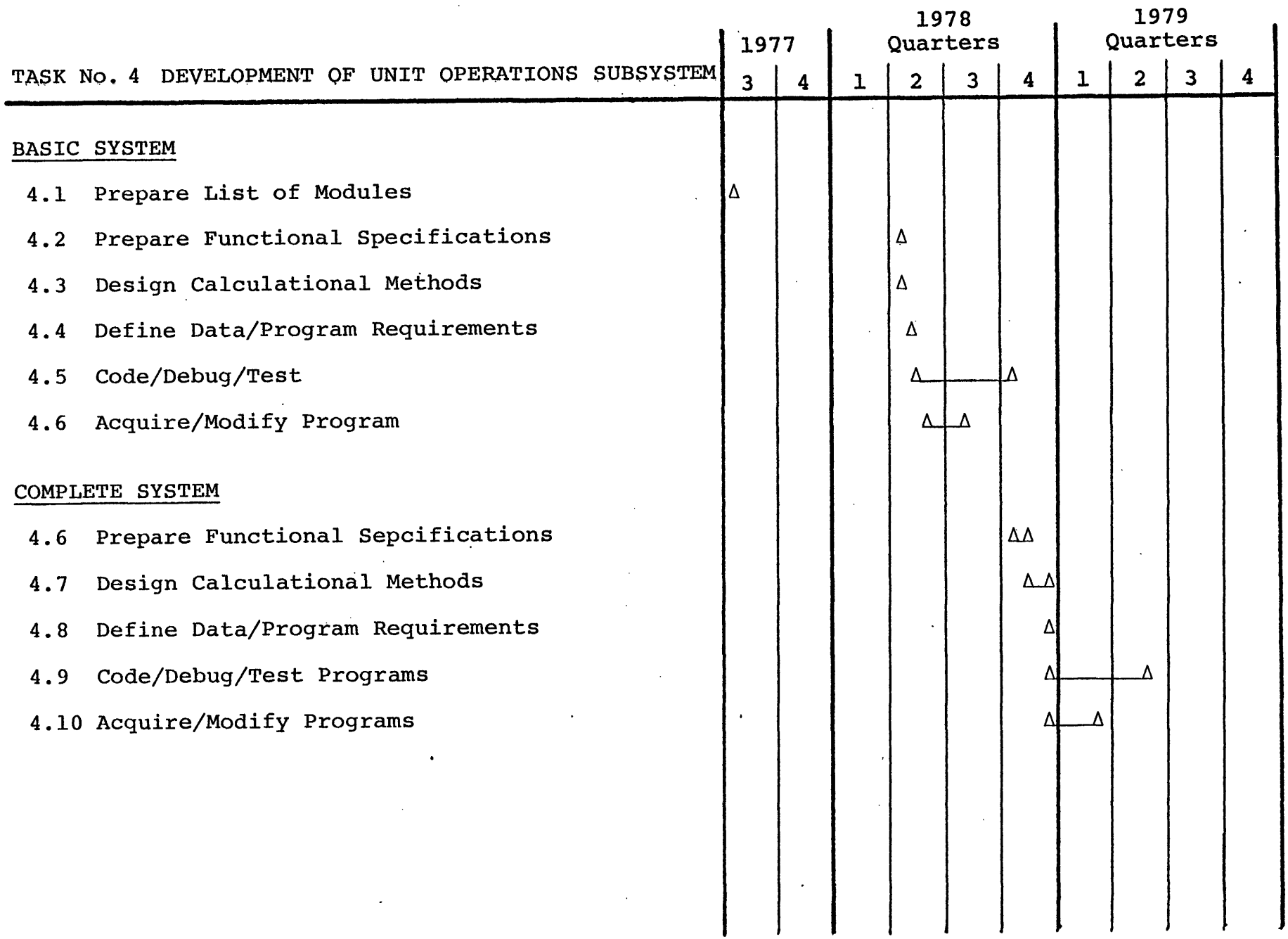
- 3.1 Design Preliminary Physical Property Subsystem for PLEXSYS II
- 3.2 Implement/Test Subsystem
- 3.3 Deliver Preliminary Subsystem
- 3.4 Study Properties of Coal and Solids
- 3.5 Prepare PPS Specifications
- 3.6 Prepare List of Modules
- 3.7 Define Data Base Requirements
- 3.8 Code/Debug/Test Program
- 3.9 Modify Data Base

COMPLETE SYSTEM

- 3.10 Prepare Program Specifications
- 3.11 Code/Debug/Test Modules
- 3.12 Acquire/Modify/Test Modules
- 3.13 Acquire/Modify Data Base

PROGRAM SCHEDULE

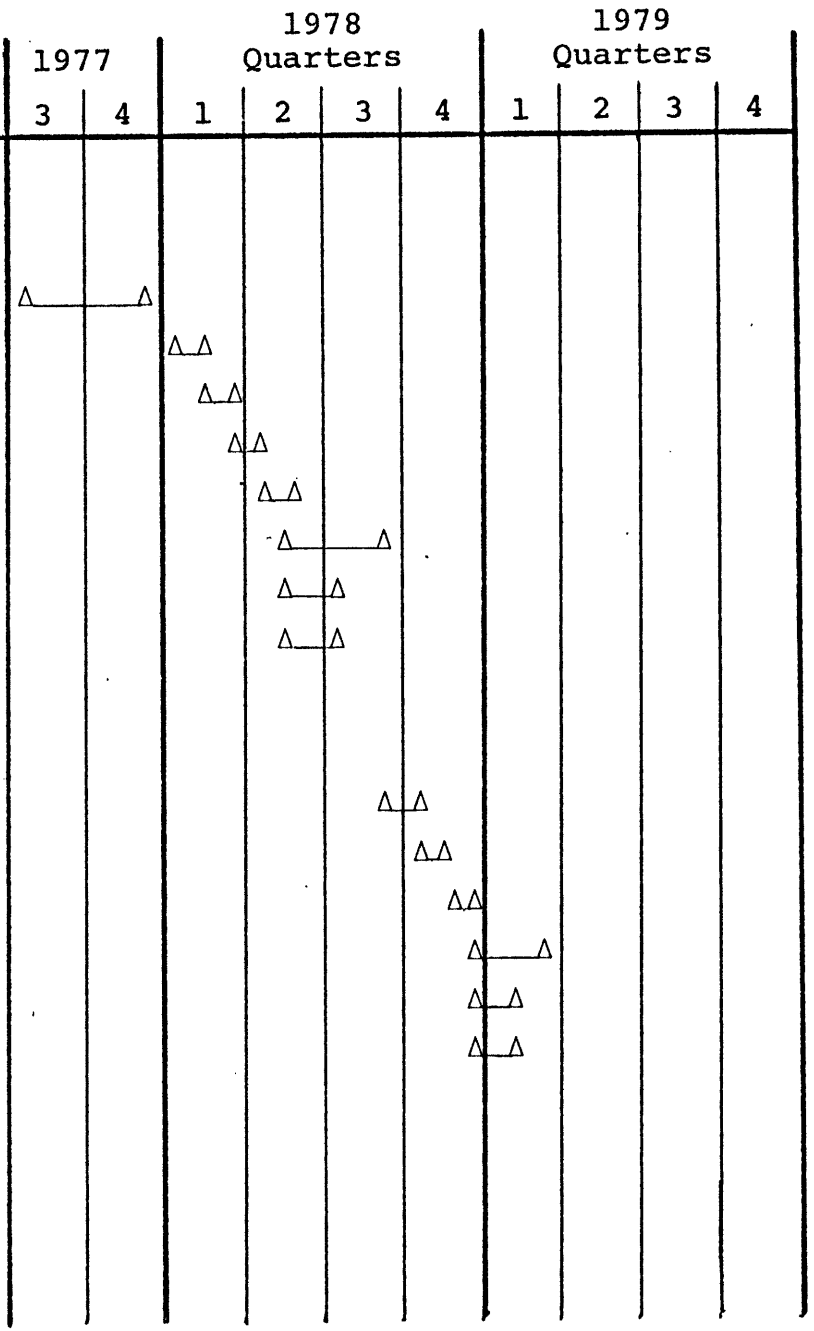
Revised 6/1/77



PROGRAM SCHEDULE

Revised 6/1/77

TASK No. 5 DEVELOPMENT OF COST ESTIMATION AND ECONOMIC EVALUATION SUBSYSTEM



BASIC SYSTEM

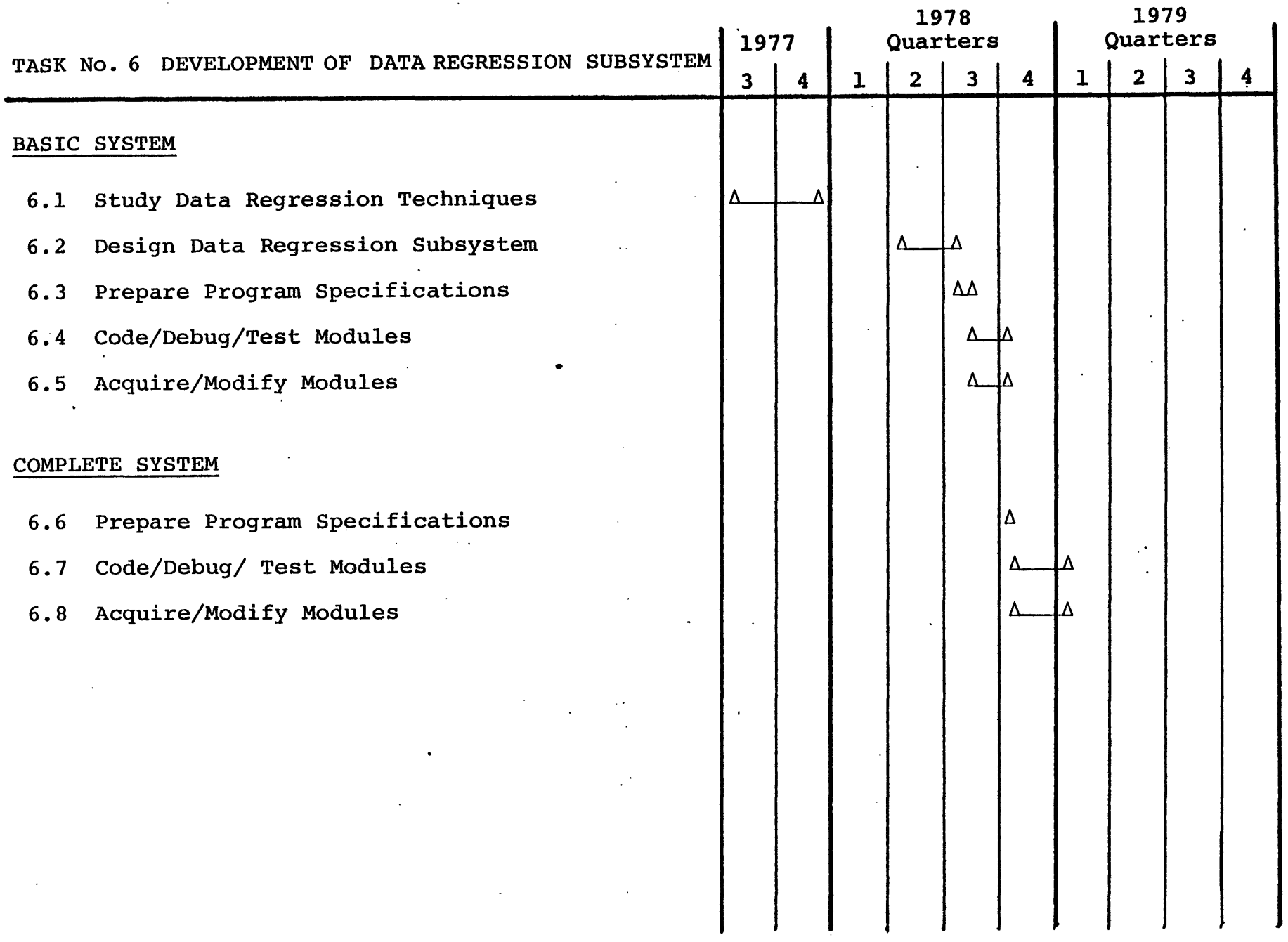
- 5.1 Study Cost Estimation and Economic Evaluation Methods
- 5.2 Prepare Functional Specifications
- 5.3 Design Calculational Methods
- 5.4 Define Data and Program Requirements
- 5.5 Design Programs
- 5.6 Code/Debug/Test Modules
- 5.7 Acquire/Modify Modules
- 5.8 Acquire/Modify Date Base

COMPLETE SYSTEM

- 5.9 Design Calculational Methods
- 5.10 Define Program/Data Requirements
- 5.11 Design Programs
- 5.12 Code/Debug/Test Modules
- 5.13 Acquire/Modify Modules
- 5.14 Acquire/Modify Data Base

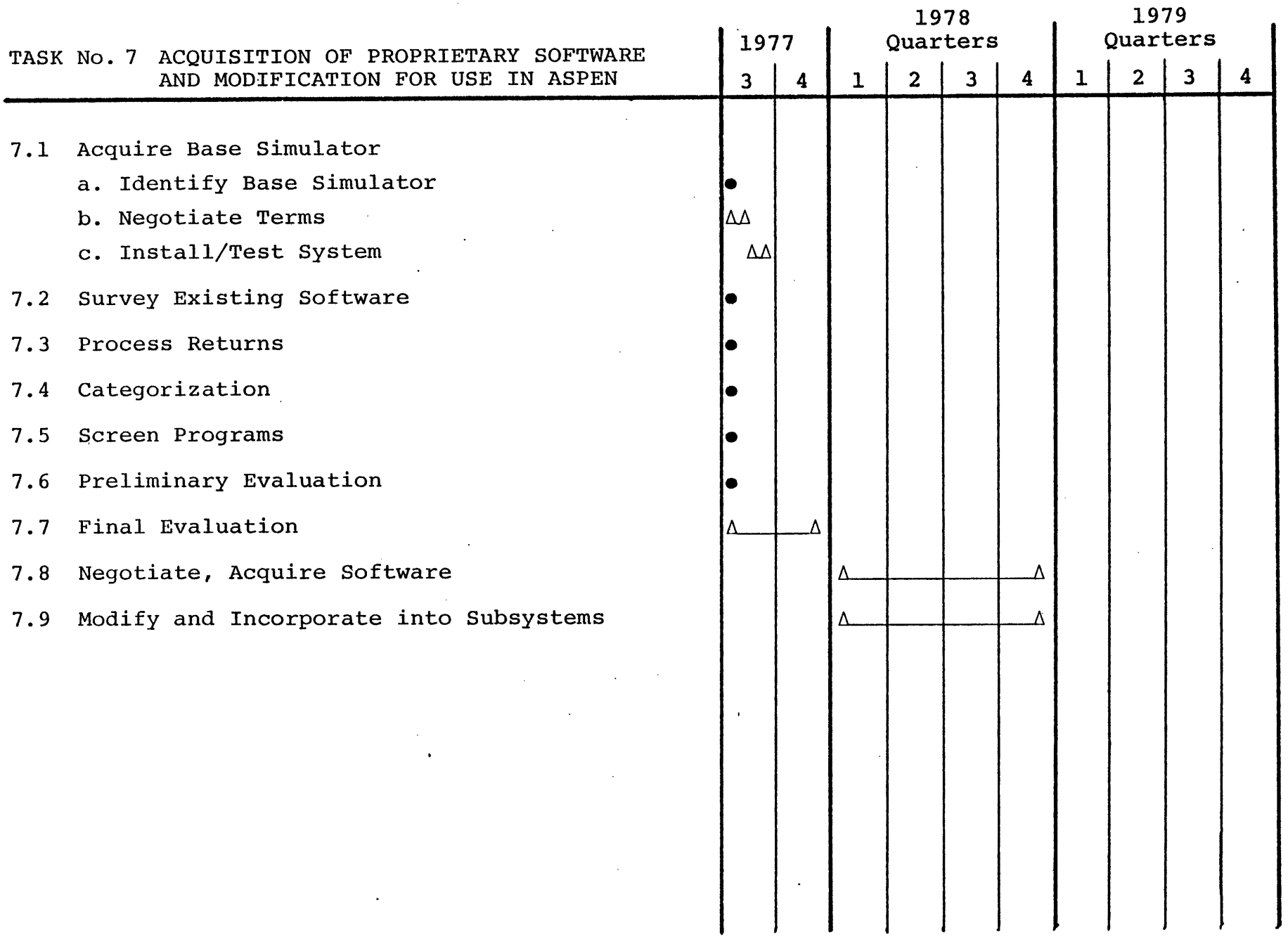
PROGRAM SCHEDULE

Revised 6/1/77



PROGRAM SCHEDULE

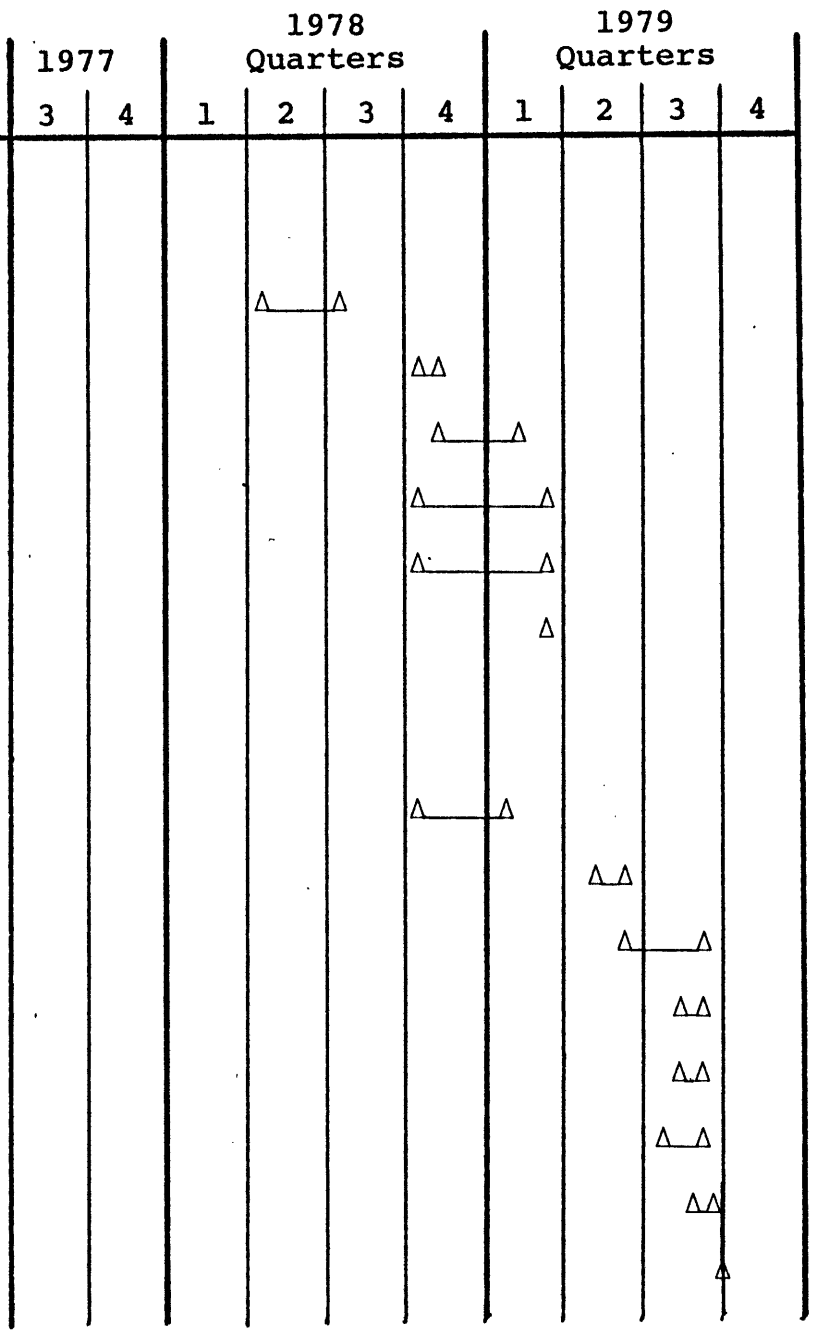
Revised 6/1/77



PROGRAM SCHEDULE

Revised 6/1/77

TASK No. 8 INTEGRATION, TESTING, AND DOCUMENTATION OF ASPEN SYSTEM



BASIC SYSTEM

8.1 Prepare Benchmark Problems for Testing

8.2 Run Benchmark Problems

8.3 Update System

8.4 Prepare User's Manual

8.5 Prepare System Manual

8.6 Release Minimal System

COMPLETE SYSTEM

8.7 Prepare Benchmark Problems for Testing

8.8 Run Benchmark Problems

8.9 Update System

8.10 Update User's Manual

8.11 Update System Manual

8.12 Prepare Educational Material

8.13 Review with Advisory Committee

8.14 Release Complete System

III. DETAILED DESCRIPTION OF TECHNICAL PROGRESS

TASK 1, DEVELOPMENT OF PROTOTYPE SIMULATOR AND SIMULATION OF SPECIFIC FOSSIL ENERGY PROCESSES

One of the major tasks for the first year of the project was the development of a prototype process simulator to test new concepts in process simulation needed to model fossil energy processes. The prototype simulator, named PLEXSYS II, is being used to simulate three coal conversion processes: The IGT HYGAS Process, the Exxon Donor-Solvent Process, and the Conoco Coal Development Corporation CO_2-Acceptor Process.

1.1 DEVELOPMENT OF PLEXSYS II

The basic system programs for PLEXSYS II were developed for and implemented during the second quarter of the project. The unique aspect of PLEXSYS II is the use of a plex data structure to store information regarding a process.

In current simulators, data are stored in fixed arrays, usually residing in common in FORTRAN programs. This structure leads to inflexibility, because the designer of the system must know all variables of interest at the time the system is designed. It becomes difficult to incorporate new types of variables without altering the layout of data in COMMON and changing every routine that was defined on the basis of the original layout.

In a plex structure, first proposed by Ross (1961), information is stored in blocks of contiguous storage locations known as beads. Beads of any length are created dynamically from a pool of free storage as needed during execution of the program. They are referenced and linked together by means of pointers. Beads may contain integer values, real values, Boolean values, character strings, and pointers intermixed as needed to describe an element of the model.

A paper has been prepared by Evans, et al. (1976) describing the use of a plex data structure for process simulation. It was included in the First Quarterly Progress Report.

A major question regarding the plex data structure is whether the extra computing effort required to store and access information in the plex will be excessive. To answer the question the first version of PLEXSYS (referred to as PLEXSYS I) was developed. It implemented the plex data structure with the FORTRAN programming language. A comparison was made on two example processes to compare the effectiveness of the plex data structure with traditional fixed-array structures. The results of these studies are described in a paper by Joseph et al. (1976) which was also included in the First Quarterly Report.

For a typical process involving a flash and recycle, there was a 20% increase in execution time. However this is not a serious limitation considering the flexibility offered by the data structure. It is possible to use a combination of the traditional fixed array data structure with the plex structure retaining the advantages of both. These and other possible data structures will be explored in the design of ASPEN. The use of plex data structure makes it easier to develop modular programs that are reusable and can be adopted to solve new types of problems. The plex structure also permits easy specification of the routes of computations when building block routines call upon other routines and choices exist at each level. Only a single argument is required when calling routines. This is discussed in greater detail in a paper by Seider et al. (1976) which is included in the First Quarterly Progress Report. These ideas have been implemented in PLEXSYS II.

While PLEXSYS I was excellent for determining the computing efficiency of alternate data structures and the effort required to interface programs with the plex, it is of limited use for process simulations. The limitations result from a very limited set of available physical properties and limited capabilities for data management.

The second version of the simulator, referred to as PLEXSYS II, is being used for the prototype simulation of the three fossil energy processes.

PLEXSYS II consists of two major parts: (1) The Plex Data Management System (PDMS) and (2) the Generalized Plex Building Routine (BUILD) for building a plex data structure from free-format commands on data cards. An associated set of physical property routines has also been developed and is discussed separately under Task 3.

Details of PLEXSYS II are discussed in two working reports of the project: PLEXSYS II User's Manual and PLEXSYS II System Manual.

The unit operations blocks required for the simulation of the coal conversion processes are being developed as they are needed. The system is being constantly modified to meet the new requirements as these pilot plant simulations proceed.

1.2 SIMULATION OF THE HYGAS PROCESS

The HYGAS coal gasification process developed by the Institute of Gas Technology (IGT) was the first of the three processes selected for study using PLEXSYS II. A pilot plant of the process has been constructed and operated by IGT. The objective of this study is to demonstrate the

feasibility of computer simulation of the coal conversion processes by comparing the simulation results with pilot plant data.

Figure 1.1 shows a schematic of the IGT pilot plant. There are many variations to the process. The one selected for study is the steam - oxygen process for which operating data has been reported by IGT. Figure 1.2 shows the major reactions taking place in the process. Figure 1.3 shows the block flow diagram showing the major computational blocks, the streams and stream classes involved in the process. There are eleven different classes of streams in the process, each one distinguished by the components and phases present. The components in each stream class are listed in Table 1.1.

In addition to specifying the stream class, it is also necessary to specify the stream type. In the HYGAS process there are six types of streams (liquid, solid, vapor, solid/liquid, and liquid/vapor). The type of each stream is indicated in Figure 1.1. The variables required to represent each type of stream are listed in Table 1.2.

Work during the past year has concentrated on modeling and programming the blocks required to do the simulation. A brief description of the blocks that have been completed is given below:

HTR - Block to simulate the high temperature reactor. Two different programs were written to model this block. The first one uses a kinetic model for gasification reported by

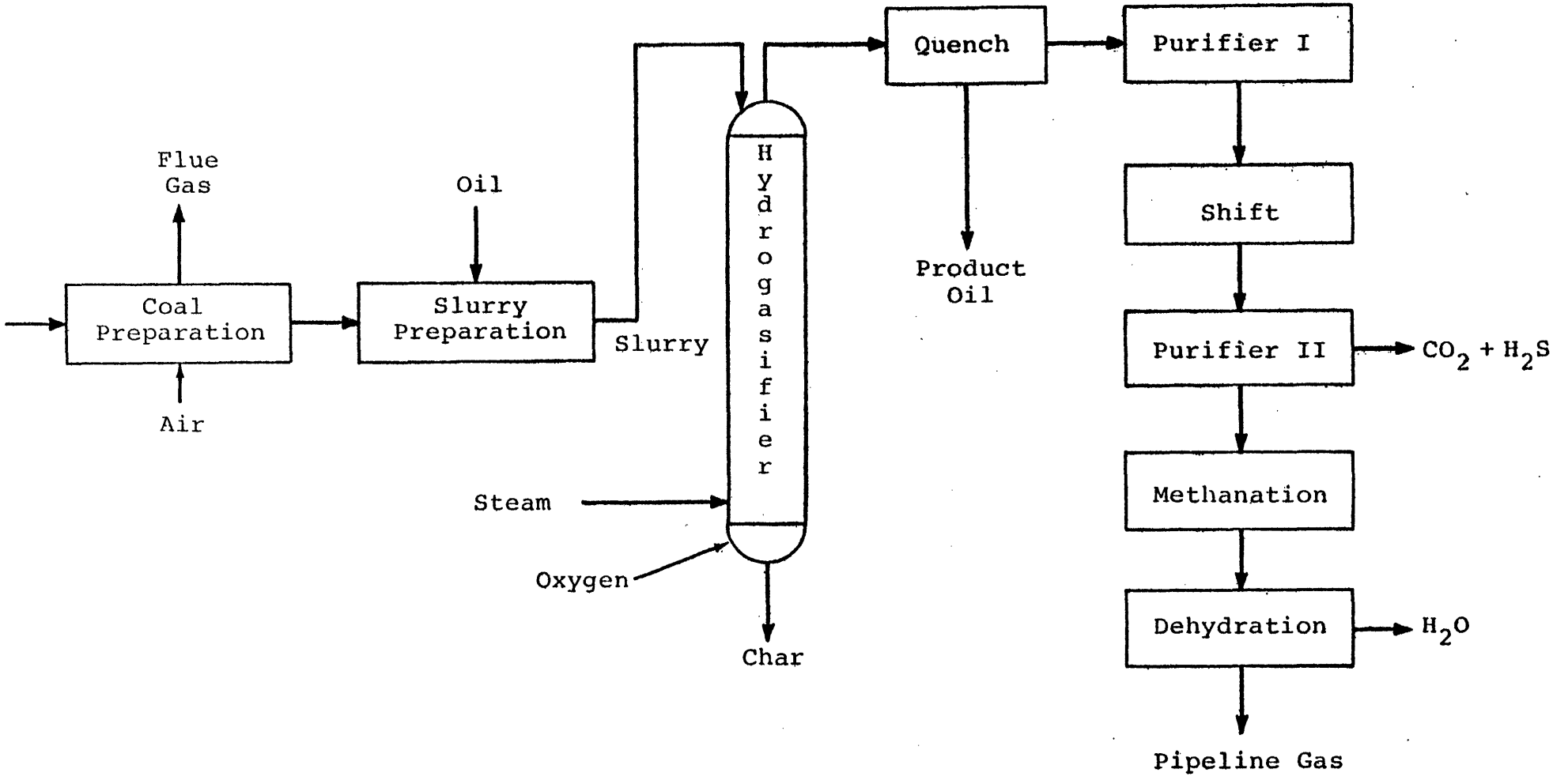


Figure 1.1 Schematic Diagram of the HYGAS Process

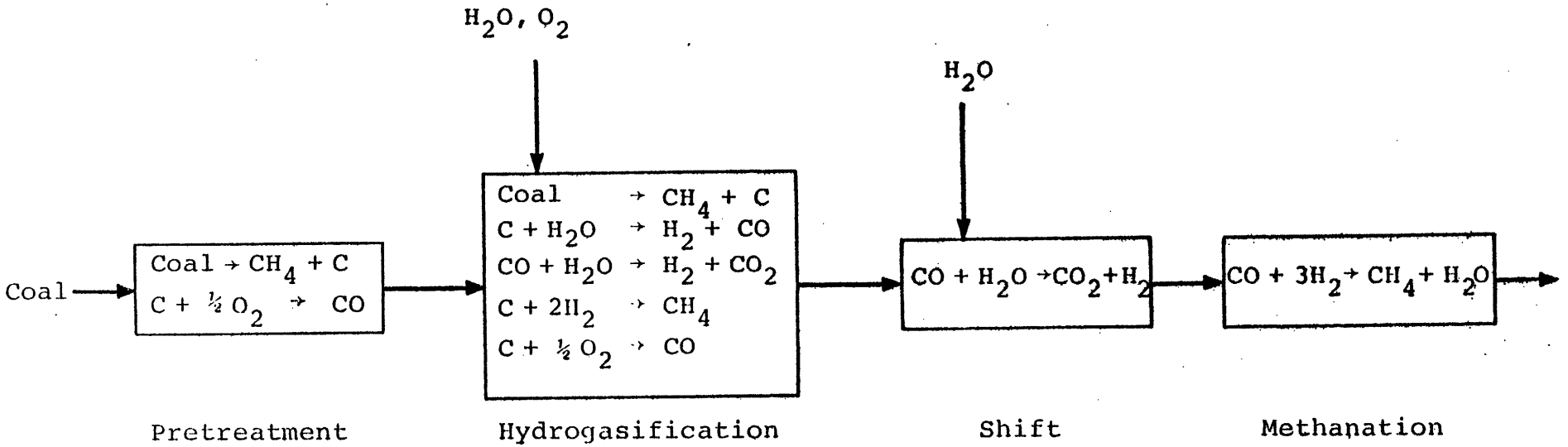


Figure 1.2 General Gasification Scheme

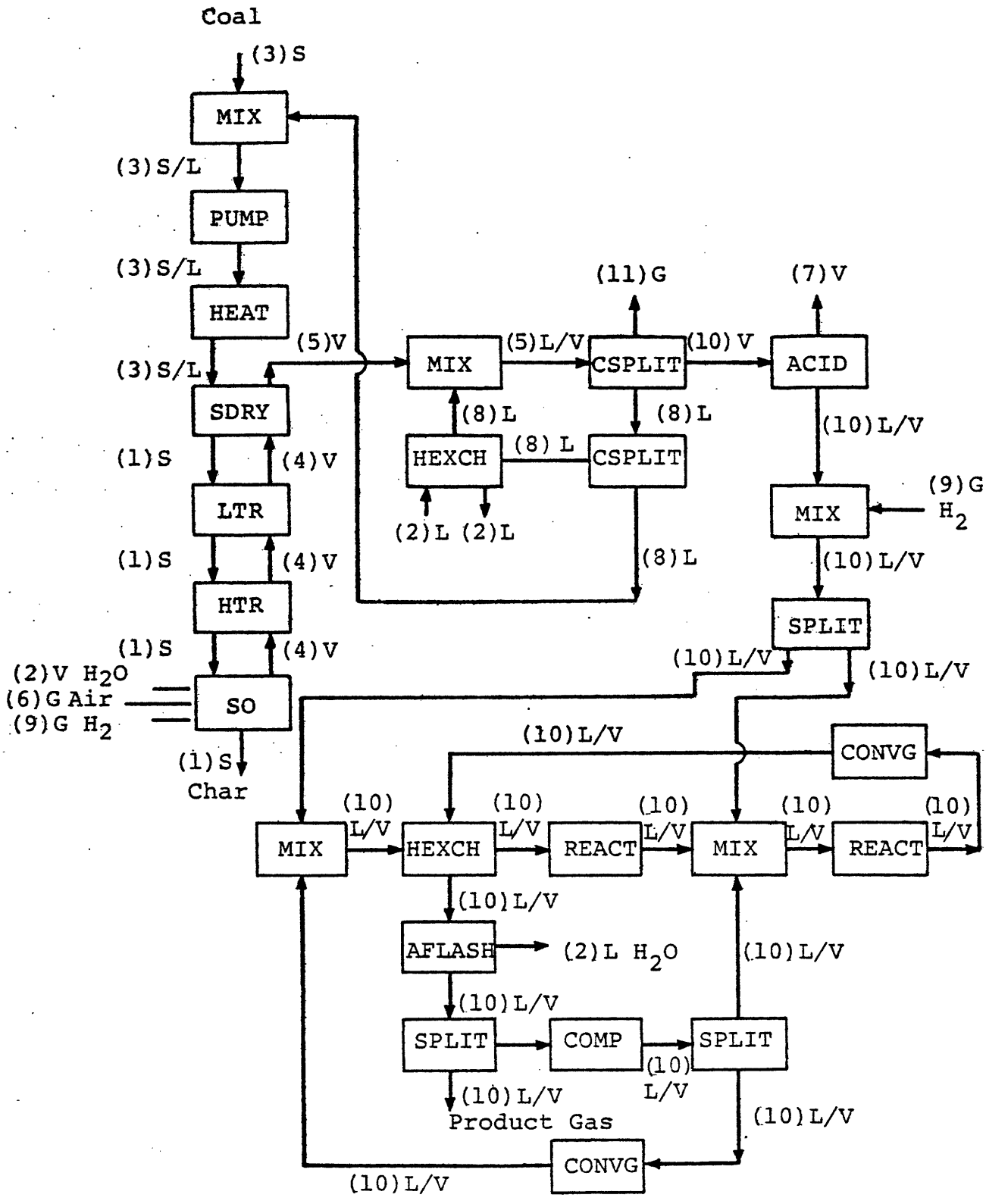


Figure 1.3 Flow Diagram of the HYGAS Process Showing Stream Classes and Types

TABLE 1.1

Chemical Components for Stream Classes in the HYGAS Process

Number	Name of Stream Class	Example of Stream	Components Present
1	ONE	Coal feed	CV*, CB*, H, N, O, S, Ash
2	TWO	Water feed	H_2O
3	THRE	Coal/toluene slurry	CV, CB, H, N, O, S, Ash/H_2O toluene
4	FOUR	Gasifier outlet	CO, CO_2, CH_4, H_2, H_2O, N_2, O_2, NH_3, H_2S
5	FIVE	Slurry Drier overhead	CO, CO_2, CH_4, H_2, H_2O, N_2, NH_3, H_2S, toluene
6	SIX	Air feed	O_2, N_2, H_2O
7	SEVN	Acid gas concentrate	CO_2, H_2S, H_2O
8	EGHT	Bottoms from gas-liquid separator	H_2O, toluene
9	NINE	Hydrogen feed	H_2
10	TEN	Product gas	CO, CO_2, CH_4, H_2, H_2O, N_2
11	ELEV	Ammonia effluent	NH_3

* CV and CB refer to Volatile carbon and Base carbon in the coal.

TABLE 1.2

Variables Used to Describe Each Stream Type in the HYGAS Process

Stream Type	Solid	Liquid	Vapor	Solid/Liquid	Liquid/Vapor
Variables	TEMP	TEMP	TEMP	TEMP	TEMP
	PRES	PRES	PRES	PRES	PRES
	ENTH	ENTH	ENTH	ENTH	ENTH
	TFLO	TFLO	TFLO	TFLS	TFLO
	MOFR	MOFR	MOFR	MFRS	PMFR
				TFLL	
				MFRL	

TEMP = Temperature

PRES = Pressure

ENTH = Enthaly flow

TFLO = Total flow rate, moles

MOFR = Pointer to bead containing mole fractions

VF = Fraction vapor

TFLS, TFLL = Total flow rate respectively of solid and liquid, moles

MFRS, MFRL = Pointers respectively to beads containing mole fractions of solid and liquid phases

IGT. This program involves considerable trial and error calculations and is hence slow to execute. Details of the model are given in the Second Quarterly Report. The second model is based on an approach to equilibrium and is more approximate. This model would also be used for the steam oxygen reactor.

SPLIT - The SPLIT subroutine is a simple stream splitter which can accomodate any specified number of outlet streams. No physical property routines are needed as both the mass and enthalpy flow rates of the outlet streams are fractional values of the inlet quantities, and the temperature and pressure are unchanged.

CSPLIT - The CSPLIT subroutine is a model of idealized isothermal separation process which places specified fractions of specified or 'key' components from an inlet stream into an 'overhead' stream while putting the remainder of the inlet stream into a 'bottoms' stream. For instance, the routine could simulate a drying process in which some fraction, say 90% of the inlet stream's water flow is to be removed to an overhead stream. The temperature and the pressure are unchanged, and the enthalpy and entropy changes are to be calculated and reported. The inlet and outlet streams are allowed to be of different types.

CPUMP - The CPUMP subroutine simulates a centrifugal pump, and can operate in either a design mode of calculating the required pump horsepower given the inlet and outlet stream

conditions and the pump efficiency, or in a simulation mode, calculating the outlet stream pressure specified as a parameter to the model. The stream classes of inlet and outlet streams are required to be identical. A check is made in the design mode to see that the outlet pressure has not been specified less than the inlet pressure. If so, an error message is printed and the outlet pressure set equal to the inlet pressure. The enthalpy of the outlet stream will be calculated.

CCOMP - The CCOMP subroutine simulates an adiabatic multi-step compression in either the design or simulation mode. When operating in the simulation mode, the routine uses the specified power and number of stages to calculate the outlet temperature and pressure. In the design mode, with the outlet stream pressure specified, the power requirement and number of stages are calculated. This routine uses physical property routines to determine the density, heat capacity, and enthalpy of gas stream.

CNTL - A control unit, CNTL, has been implemented to control a stream variable (referred to by stream pointer and variable name) by adjusting an equipment parameter (referred to by unit pointer and parameter name).

CONVG - A stream convergence block using the bounded Wegstein method unit has been written and tested. This block checks convergence of the stream's temperature, pressure, total flow rate, and motal flow rates.

HEXCH - Three heat exchanger blocks, using different specifications, have been prepared. HEXCH1 is a model of a counter-current exchanger with the input streams, the area, and the overall coefficient known. HEXCH3 is a heat requirement block which gives the inlet and outlet temperatures of a stream, calculates the heat requirement Q. HEXCH4 is a counter-current exchanger for which the inlet temperatures and one outlet temperature are specified. No phase changes are allowed in any of these blocks. A sizing block will be written to calculate the area given the overall coefficient and using the Q found in the simulation phase.

IFLASH - An isothermal flash block, IFLASH, has been prepared to make flash calculations in the presence of light or heavy components which always remain in vapor or liquid phase respectively. This block uses the half interval method as the equation solver. The heat requirements are also calculated.

METH - Two blocks have been prepared for modeling the methanation reactors. The first, XTENT, assumes the extent of reaction for the methanation reaction and calculates the outlet stream composition and temperature. The second, METH, solves the differential equations for the heat and mass balance of a packed-bed catalytic reactor, using reaction rates reported by IGT. The XTENT block will be used in the simulation of the methanation section, whereas the METH block will be used in sizing the reactors.

MIX - Three stream mixing routines have been prepared. MIX1, to be used in the methanation section, combines gas streams and calculates the outlet temperature assuming no heat losses. MIX2 combines a coal stream and the recycle toluene stream. MIX3 combines a gas stream and a liquid stream.

ACID GAS REMOVAL - For the simulation phase of our modeling effort, a CSPLIT block will be used for the acid gas removal before the methanation section. The CSPLIT block, described earlier, allows specified components to be split out of a stream, and has been modified to operate at a specified outlet temperature. The sizing phase of the model will utilize a group of blocks to model the packed-bed absorption and regeneration towers. These blocks have been prepared from the diglycolamine acid gas removal program of Wen (1972).

SDRY - A model of the slurry drier bed of the HYGAS gasification reactor has been written. Given a heat loss rate, and the inlet streams of slurry and LTR product gas, it calculates the temperature of operation and the composition of the outlet streams.

HEAT - A heat-requirement block has been written to model the slurry heater unit. This block is similar in function to HEXCH3, but handles the more complex coal slurry stream.

The next step is the simulation of sections of the process. The first section to be simulated will be the

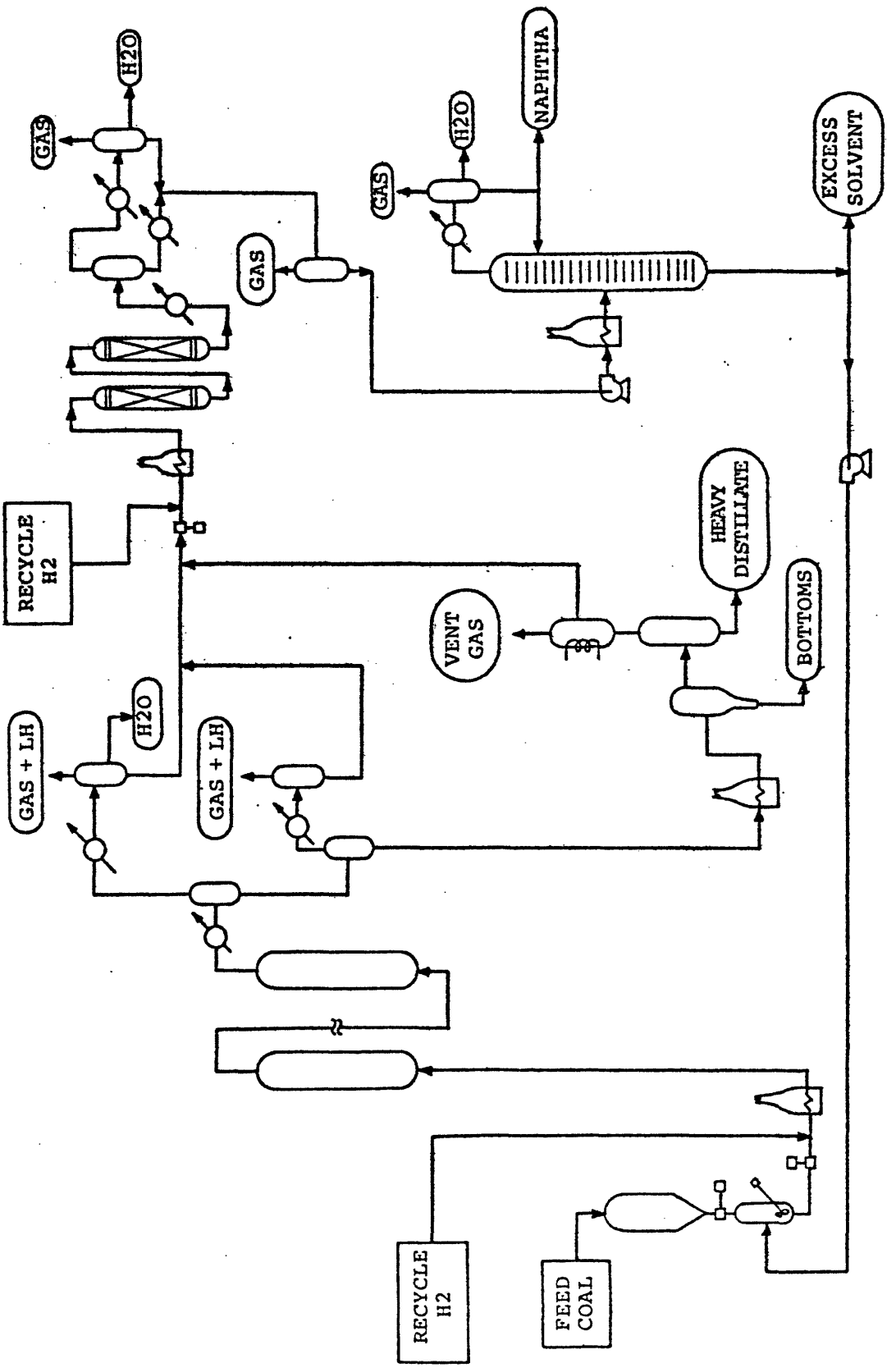


Figure 1.4 Flow Diagram for EDS

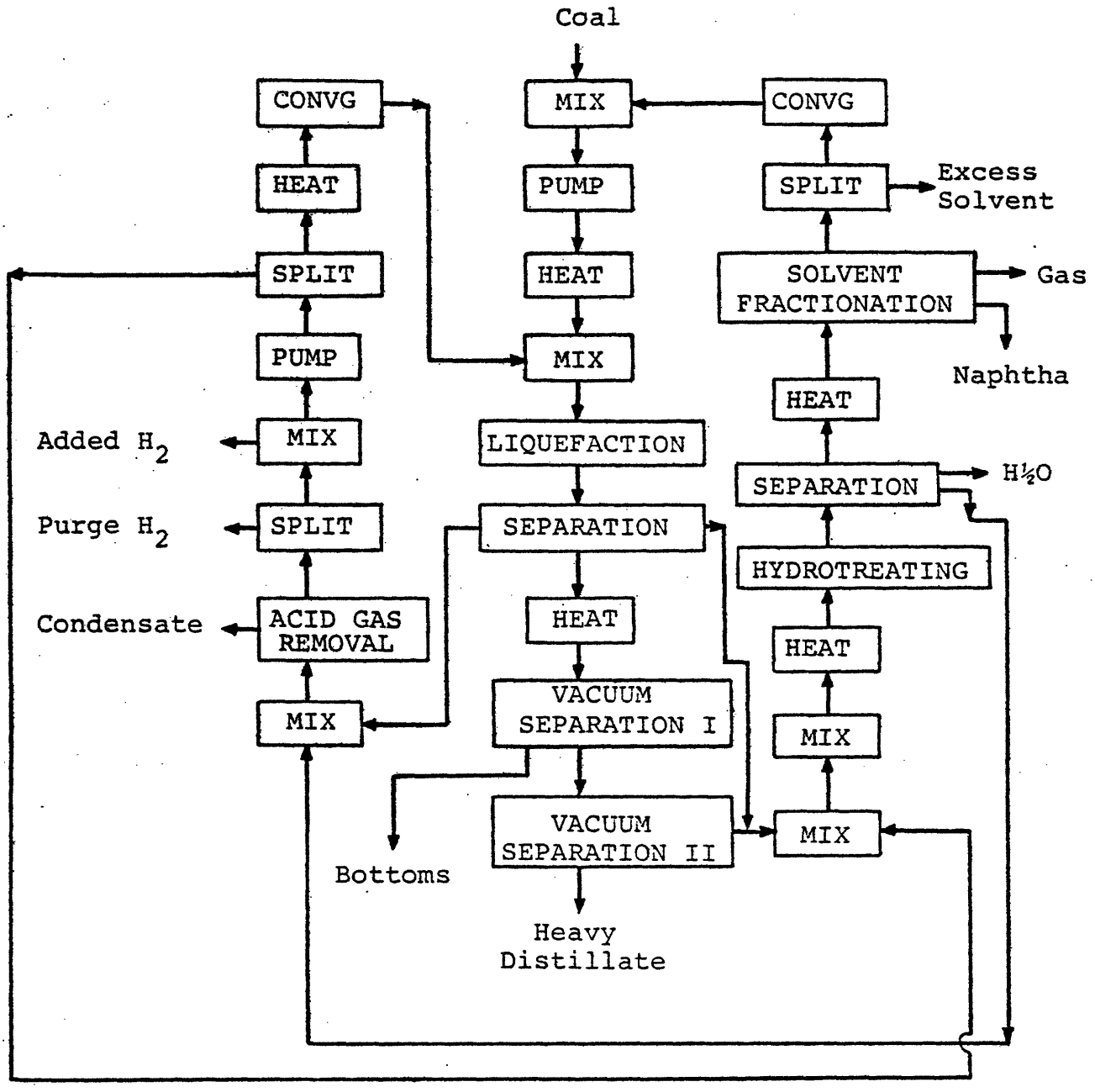


Figure 1.5 Information Flow Diagram for Simulation of Exxon Donor Solvent Process

methanation section. Next the quenching section will be simulated followed by the gasification section.

1.3 SIMULATION OF THE EXXON DONOR-SOLVENT PROCESS

The Exxon Donor-Solvent Process is a coal liquefaction process utilizing molecular hydrogen in addition to a hydrogenated solvent as the hydrogenating vehicle. The major advantage of the process is that it can be operated at relatively low pressures (100 bar) as compared to conventional processes which operate at 200 bars and above. It also separates the catalytic hydrosection step from the liquefaction reaction.

Exxon has been conducting bench-scale research on the process since 1966. In July, 1975, 1 ton/day pilot plant was completed and put in operation. A flow sheet of the process is shown in Figure 1.4 and a block diagram for simulation is shown in Figure 1.5.

In addition to blocks developed for the HYGAS process the various units required the EXXON Donor Solvent Process are listed below:

MIXING UNITS - these combine several streams into one outlet stream. They can be classified according to the number and type of phases present. In this process we have mixing units that handle the following phases: G/G, G/L, L/L, L/S, G/L,S (L = liquid, G = gas, S = solid).

SEPARATION UNITS - these separate a multiphase stream into different streams with different phases.

VACUUM FLASH UNITS - these separate the different components by the increased volatility at a reduced pressure. A model of gas/liquid/solid equilibrium is required.

SOLVENT FRACTIONATION UNIT - this separates the regenerated solvent into different streams of different boiling range. A Wang-Henke multicomponent distillation algorithm will be used for the modeling.

HYDROTREATING REACTOR - this rehydrogenates the spent solvent using molecular hydrogen. The model for this reactor is a fixed bed catalytic reactor.

LIQUEFACTION REACTOR - this carries out the central reaction of coal liquefaction using a catalyst. The model for the reactor would depend on the knowledge of the exact type of reactor used in the pilot plant.

The modeling of the process has been hampered by the lack of access to data collected by Exxon. To overcome this difficulty a meeting between Exxon representatives, ERDA personnel and ASPEN staff members was held in May at the Exxon Research Engineering Company in Florham Park, New Jersey. It was concluded that M.I.T. Would be required to enter into a secrecy agreement with Exxon in order to protect the proprietary data essential to carry out the simulation. The modeling effort at Exxon was also discussed. Currently a legal agreement is being worked out to obtain the data directly from Exxon.

Current work is being carried out with the available (published) data. Two areas are being investigated. First, the applicability of FLOWTRAN to simulate those parts of the process involving only liquids and gases. Secondly the ability of current thermodynamic property estimation techniques to predict properties of coal derived liquids is being studied.

1.3.1 Properties of Coal Derived Liquids

No correlations are available in the literature to predict the properties of coal derived liquids which are complex mixtures of a large number of hydrocarbon components. The synthetic crude produced from coal contains a higher percentage of cyclic compounds than natural crude. In the absence of any data, it appears the best method would be to use the methods applicable to petroleum fractions.

Accordingly, the coal liquid can be characterized by breaking it up into a number of boiling fractions and then using the petroleum correlations to predict the properties of each of these cuts. In order to validate this approach it is necessary to obtain some experimental data such as vapor liquid equilibrium data. It is expected that Exxon will be able to provide the necessary data and guidance in predicting physical properties.

1.3.2 FLOWTRAN Simulation of the EDS Process

A part of the Exxon Donor-Solvent (EDS) process has been simulated using the FLOWTRAN process simulator. The liquid was divided into ten boiling fractions and properties of each cut was generated using the petroleum correlation built into FLOWTRAN VLE program.

The part of the process (not involving solids) which was simulated using FLOWTRAN is shown in Figure 1.6. This represents the solvent separation section of the pilot plant. Figure 1.7 shows the FLOWTRAN Block diagram. In all cases, the simplest of the FLOWTRAN blocks were used in the simulation. No comparison with actual pilot plant data can be provided since the latter is not available until the secrecy agreement with Exxon is signed.

1.4 SIMULATION OF THE CO_2-ACCEPTOR PROCESS

(This simulation is being carried out at the University of Pennsylvania under a subcontract.)

The CO_2-Acceptor process for coal gasification is being developed by the Conoco Coal Development Company. A pilot plant of the process has been operated at South Dakota.

A flow sheet of the CO_2-Acceptor process is shown in Figure 1.8. Raw lignite from the mine is trucked to the lignite storage and handling section, a system of conveyors which transport coal among storage areas. The lignite is sent to the pretreatment section where it is crushed, dried,

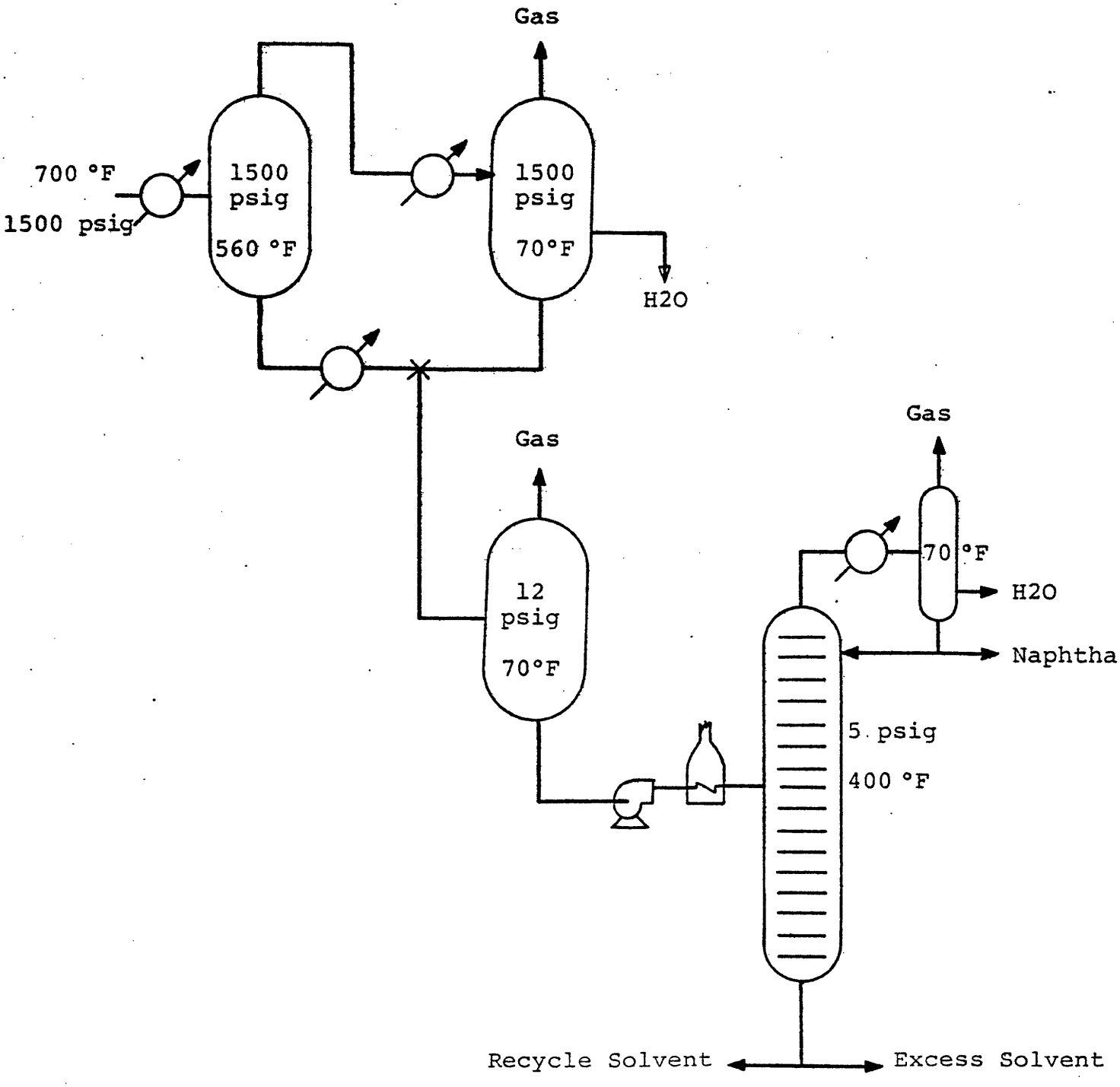


Figure 1.6 Process Flowsheet

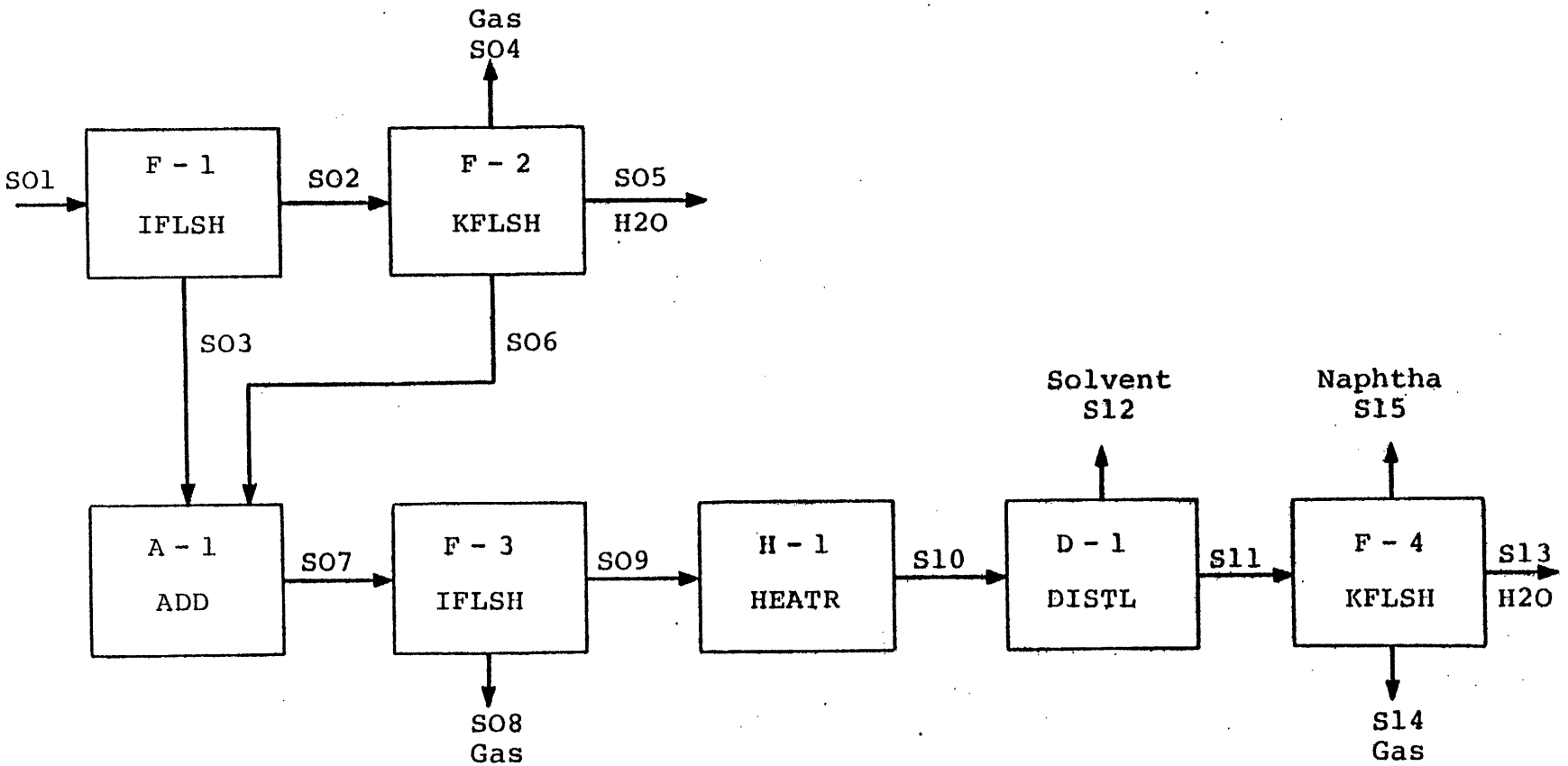


Figure 1.7 FLOWTRAN Unit Blocks

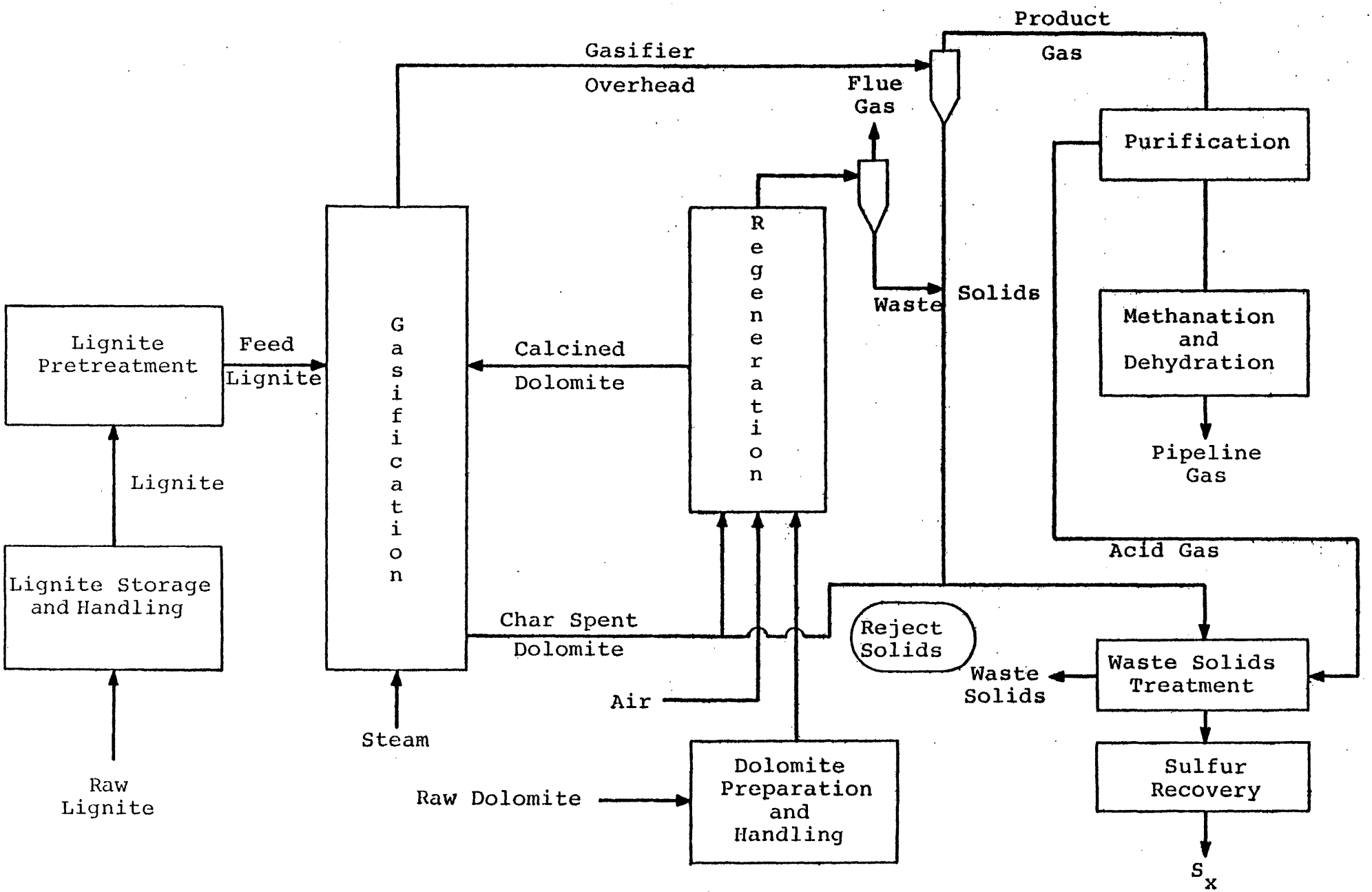


Figure 1.8 Schematic Diagram of the CO_2-Acceptor Process

and preheated. It is fed to the gasifier where it reacts with steam in the presence of calcined dolomite. Dolomite absorbs CO_2 and H_2S in the gasifier and produces a hydrogen rich product low in H_2S. Spent dolomite is regenerated to drive off CO_2 by burning char in the regenerator. Since H_2S is not recovered during regeneration, some spent dolomite is removed for sulfur recovery. Hence, make-up dolomite is added from the dolomite preparation and handling section. Waste solids (principally ash) are removed from the gasifier and regenerator overhead streams, combined with reject dolomite, and sent to the waste solids treatment section. Here, spent dolomite is reacted with CO_2 to release H_2S which is sent to the sulfur recovery section. Product gas from the gasifier is purified to remove CO_2 and H_2S and sent to the methanation and dehydration sections. Since CO_2 is absorbed by dolomite in the gasifier and H_2 is produced, a process for shift conversion is not necessary.

We are currently modeling the lignite pretreatment and gasification processes.

1.4.1 Description of the Lignite Pretreatment and Gasification Processes

The following description of these processes parallels that in ERDA Report, ERDA-76-58, FE-2083-7.

The lignite pretreatment section of the process includes grinding, drying and preheating. A block flow diagram for the

pretreatment section is shown in Figure 1.9. Lignite from storage is fed to receiving hoppers and from there to the primary crusher where it is reduced to less than one inch. Crushed lignite is transported to hot gas swept hammer mills where it is ground to less than one eighth inch. Hot flue gas from the furnace is mixed with overhead recycle gas to maintain the mill inlet temperature at 600°F and reduce the moisture content of lignite from 40 to 20 percent. After gases are cleaned in cyclones, some lignite is sent to furnaces for combustion and the remainder proceeds to flash dryers, where it is contacted with hot flue gas and its moisture reduced to 5 percent. Finally, at 200°F lignite is sent to a fluidized bed preheater where it is heated to 500°F and remaining moisture removed. The preheated lignite is then transported to the gasification process.

The block flow diagram for the gasification flowsheet is shown in Figure 1.10. Preheated lignite is fed to fluid bed gasifiers by lock hoppers. Calcined dolomite from regenerators and steam are added and gasification takes place at 1550°F and 150 psig. The dolomite: (1) carries heat to the gasifier, (2) absorbes CO_2 by the exothermic reaction:

$$MgO \cdot CaO + CO_2 \rightarrow MgO \cdot CaCO_3$$

and (3) absorbs H_2S by the reaction:

$$MgO \cdot CaO + H_2S \rightarrow MgO \cdot CaS + H_2O$$

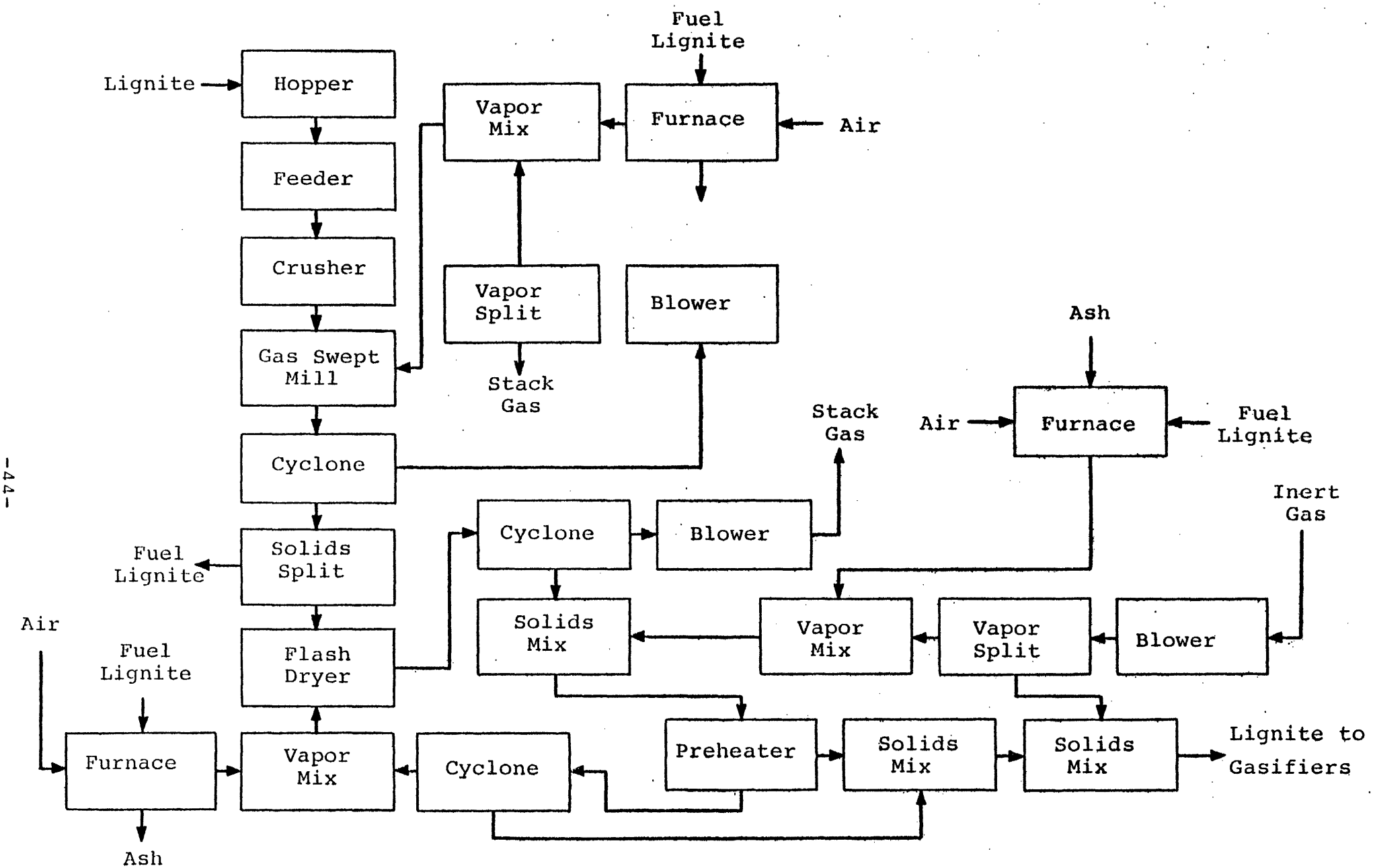


Figure 1.9 Computational Blocks in Pretreatment Section

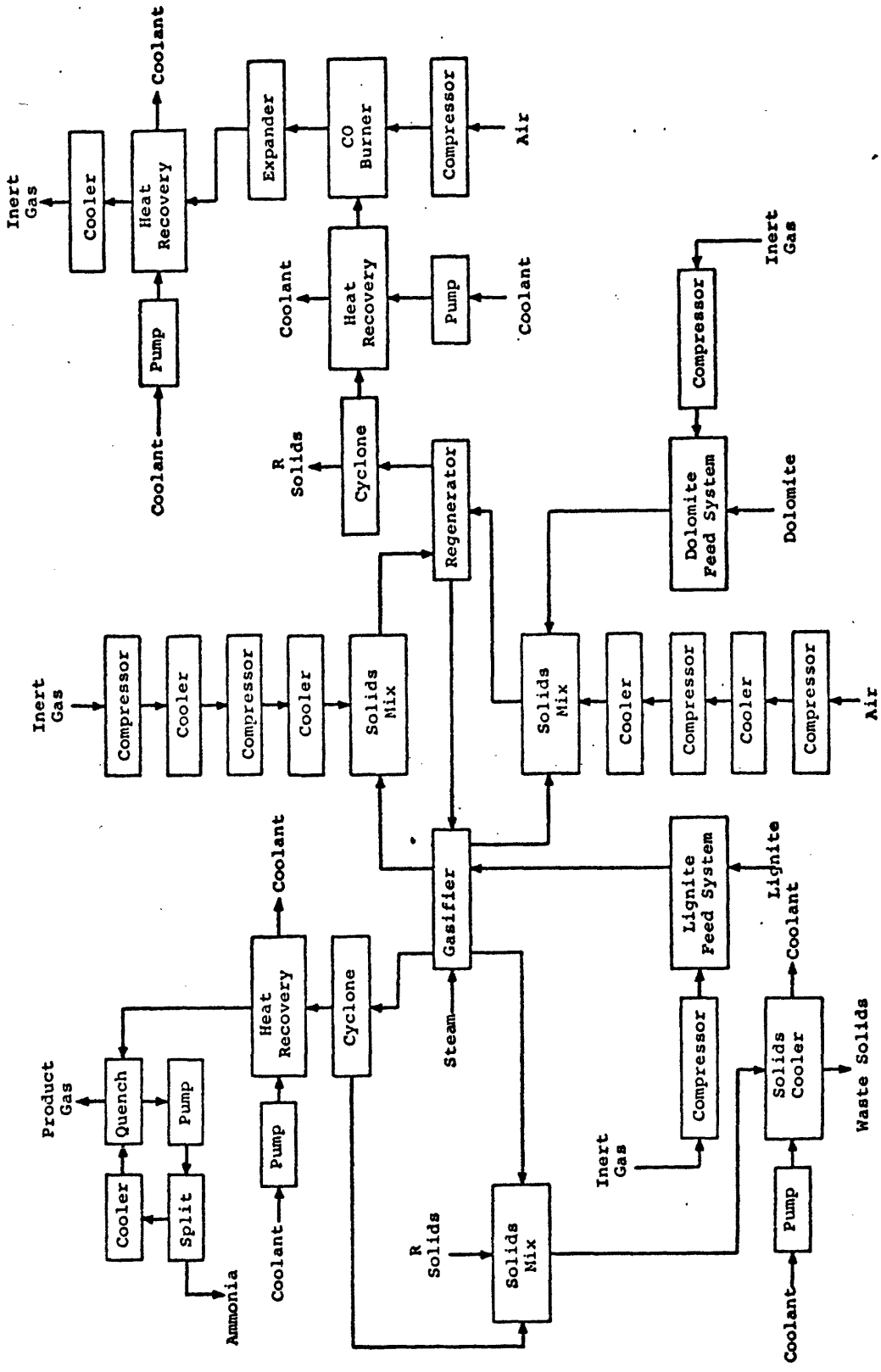


Figure 1.10 Computational Blocks in Gasification Section

Note that absorption of CO_2 in the gasifier forces the water gas shift reaction,

$$CO + H_2O \rightleftharpoons CO_2 + H_2$$

to the right, and eliminates the need for a separate shift conversion process. Spent dolomite is transported to regenerators where CO_2 is removed at 1859°F with heat supplied by burning char. Entrained ash and dolomite are separated from the regenerator off gas in cyclones. The remaining gas is sent to an energy recovery section where waste heat is recovered, residual carbon monoxide is burned, and power is recovered in gas expanders. The gasifier product gas passes through a cyclone, waste heat boiler and a quench tower where ammonia is removed. The cooled product gas at 230°F is sent to the purification section.

1.4.2 Work Accomplished

An early step in modeling the CO_2-Acceptor Process involved preparation of information flow diagrams that show process units for which computer models are required. These diagrams are illustrated in Figures 1.9 and 1.10. The work has concentrated on preparing models for process units that handle solids such as the crusher, gas swept hammer mill, cyclone, gasifier, and regenerator. It is planned to use existing programs to model process units involving vapors and liquids, wherever feasible.

To minimize efforts, the use of FLOWTRAN was explored for simulation of process units involving the vapors and liquids. PLEXSYS would represent the data structure for the entire pretreatment and gasification sections. Programs for simulation of process units involving solids would incorporate this data structure, while data for process units involving vapors and liquids would be converted to a form compatible with FLOWTRAN building-blocks. Also, programs to estimate properties of vapors and liquids within FLOWTRAN would be called from programs to model solids-handling equipment, such as driers.

A short period was devoted to determining the feasibility of using PLEXSYS with the FLOWTRAN system, after which it was decided to proceed with this promising approach. Details of the Job Control Language to link PLEXSYS routines with FLOWTRAN will be worked out during the simulation period in July and August.

A model to simulate milling was completed in May. It predicts the particle size distribution of the product stream and the energy requirements of the mill. Specifications are characteristics of the input stream, the mill breakage function, the selection function, and the classification function. For details of the solution method, see Perry's Handbook (1973) and the paper by Masson and Sligar (1974).

A model to simulate drying of solid particles has been completed. It involves simultaneous heat and mass transfer within spherical particles. The model is similar to that developed by Mcintoch (1976).

Dr. Joseph Maskew of Conoco, at Library, Pennsylvania, provided a copy of his computer program (in the BASIC language) to model the gasifier and regenerator. This model is expected to be suitable for use in our simulation. The program will be converted to FORTRAN and the plex data structure incorporated.

1.5 WORK FORECAST

The prototype simulator PLEXSYS II will continue to be updated to meet the requirements of the three simulations. An updated version of the User's manual and Systems manual will be issued in the next quarter to document all the changes made. Input/output facilities and debugging features will be improved to facilitate the simulations.

1.5.1 Simulation of the HYGAS Process

This work is planned to be completed in the next quarter. The immediate goal is to complete simulation of sections of the plant before simulating the integrated pilot plant. After the simulation has been completed, the effect of important process variables on product yield will be studied. Sizing blocks will be written for major pieces of equipment. A separate report describing the simulation will be issued.

1.5.2 Simulation of the Exxon Donor-Solvent Process

Negotiations with Exxon will continue during this quarter to obtain the proprietary process data under a secrecy agreement. FLOWTRAN simulation studies will be continued for those sections of the plant not involving solids. Investigations on the physical property estimation of coal derived liquids will continue over the next quarter.

1.5.3 Simulation of the CO_2 Acceptor Process

The development of models for the Cyclone Separator, Furnace, Flash Drier and Preheater, Gasifier and Regenerator will be carried out in the next quarter. The simulation of the entire process is expected to be completed in August, 1977.

TASK 2, DEVELOPMENT OF ASPEN SYSTEM STRUCTURE

2.1 WORK ACCOMPLISHED

An advisory committee consisting of representatives of industry, government, and universities was formed to guide development of ASPEN and to insure that it will meet the needs of the ultimate users. A list of names of members of this committee is given in Table 2.1. The first meeting was held on December 13, 1976.

Three task forces of the advisory committee were formed to assist with specific aspects of the project. These are:

(1) Task Force on System Design - will make recommendations regarding design criteria for the system and proposed approaches. It will review the work on the project staff as the system design emerges.

(2) Task Force on Software Evaluation - will help to identify existing software and devise means of comparative evaluation for potential use in the system.

(3) Task Force on Benchmark Problems - will consider the ultimate end use of the system and devise benchmark problems typical of those the system will be expected to solve. The problems will guide development of the system and serve as tests of it when completed.

Other task forces may be needed and will be created on an ad hoc basis. The task forces may draw upon the project staff to assist them in their work.

Each of the task forces met separately as working groups and prepared preliminary reports which were included in the Third Quarterly Progress Report.

A list of preliminary design criteria has been prepared and is being sent out to all members of the Advisory Committee in the form of a questionnaire shown in Figure 2.1. The objective is to get as much input as possible from industry (the ultimate user of ASPEN) early in the design stage so that ASPEN, when developed, would meet both industry's and ERDA's needs.

We have engaged the services of Softech, Inc., a software consulting company, to aid in the development of the system. We are in the process now of preparing a subcontract to Softech. Softech will bring extensive experience in the design and implementation of large software systems. The specific tasks to be assigned are: (1) Help determine the functional requirements of the system. (2) Provide assistance in the design of the system. (3) Assist in the examination of software products proposed for acquisition (4) Help establish an appropriate design environment and (5) Provide assistance in project planning and scheduling.

2.2 WORK FORECAST

The questionnaire replies from the members of the Advisory Committee will be analyzed. Based on the conclusions, the system specifications will be drawn up. A meeting of the

Committee on User/Use Profile of the System Design Task Force will be held in August in order to discuss the functional specifications and its impact on the user.

The implementation of the system structure will begin in the second quarter of the second year.

TABLE 2.1

ASPEN PROJECT

Task Force Membership

Review of System Design

Michael Tayyabkhan, Mobil (Chairman)
Malcolm C. Beaverstock, Foxboro
Jay C. Brubaker, Union Carbide
Brice Carnahan, University of Michigan
W. M. (Mac) Clarke, Olin
William D. Daley, Allied Chemical
Robert S. Davis, TRW
Carlos W. DiBella, Bureau of Mines
Robert D. Dodge, Fluor
Roger L. Gariepy, Air Products and Chemicals
Wilbur B. Johnson, DuPont
Dwight L. Johnston, Shell
Richard S. H. Mah, Northwestern University
Larry C. McCune, Monsanto
Allen C. Pauls, Monsanto
F. A. (Tony) Perris, ICI
G. V. Reklaitis, Purdue University
Royes Salmon, Oak Ridge National Laboratory
William E. Schiesser, Lehigh University
John J. Schorsch, Lummus
Stanley W. Wells, Phillips Petroleum
Arthur W. Westerberg, Carnegie-Mellon University
John M. Woods, Purdue University
Howard J. White, National Bureau of Standards

Software Evaluation

Jean P. Leinroth, Crawford and Russell (Chairman)
John W. Fish, Jr., Celanese Chemical
Richard R. Hughes, University of Wisconsin
Chester James, Chevron
R. L. Motard, University of Houston
Jeffrey N. Peterson, General Electric
Irven H. Rinard, Halcon
Fred S. Thatcher, Weyerhaeuser
Joseph E. Wolf, Amoco Oil

Benchmark Problems

J. D. (Bob) Seader, University of Utah (Chairman)
T. W. Clapper, Kerr McGee
Larry W. Kirsch, Argonne National Laboratory
Leonard M. Naphtali, Brookhaven National Laboratory
Lou Petrovic, Kennecott Copper
Allan Sass, Occidental Petroleum

Task Force Membership, continued

Advisory Committee Only (No Task Force)

Edward Abate, Sun Company
Robert Barneson, Fluor
William M. Hathaway, Fluor
E. B. Kretzmer, Exxon *
Kennard F. Stephenson, Jr., Allied Chemical
Matthew G. Zellner, Air Products and Chemicals

*Serving as liaison pending designation of a representative.

REPLY FORM

Preliminary Design Criteria for the ASPEN System

Name of person completing form _____

Company and Address _____

_____

_____

Telephone Number _____

Which activities related to process simulation have you been involved in within the past ten years? Comment on extent of your involvement, which simulator(s), etc.

☐ Used a Process Simulator _____

☐ Developed a Process Simulator _____

☐ Assisted Others to Use a Process Simulator _____

☐ Taught Courses on Process Simulation _____

☐ Conducted Research in Process Simulation _____

☐ Managed any of the above activities _____

Other activities may be described below:

Please answer the following questions to help resolve some specific issues. If a question is unclear or of no interest to you, leave it blank. Comments are welcome.

1. If ASPEN were available today and were installed in your company or organization, what is the most likely computer system that would be used?

Computer(s) (Make and Model)	Operating System and / or Comments	Maximum Allowable Core Region (if known)

2. Is it important that parts of ASPEN be usable on a small computer?

   Yes _____ No _____

   If so, what is the smallest computer you would envision using?

3. What language(s) [FORTRAN, PL/1, other] would you prefer or recommend (if any) for:

   (a) The executive program (preprocessor, command interpreter, etc.) _____

   (b) The building blocks (unit operations modules, property routines, etc.) _____

   (c) Report writing routines _____

4. What method(s) of input should be provided:

	not needed				essential
(a) Batch input by means of card reader	1	2	3	4	5
(b) Input by keyboard terminal	1	2	3	4	5

5. How important is it to provide:

	not needed				essential
(a) fixed-format fill-in-the-blanks input	1	2	3	4	5
(b) free-formal flexible input	1	2	3	4	5

6. What extent of interaction should be provided?

	not needed				essential
(a) Interactive entry and editing of input	1	2	3	4	5
(b) Prompted input	1	2	3	4	5
(c) Interactive input checking (for consistency, bounds, etc.)	1	2	3	4	5
(d) Display of intermediate results during execution	1	2	3	4	5
(e) Redirection of simulation during execution (e.g. for convergence)	1	2	3	4	5
(f) Interactive examination of selected output	1	2	3	4	5

7. Which of the following computational architectures should be implemented for solving the steady-state simulation problem?

	not needed				essential
(a) Sequential-modular (as in FLOWTRAN, DESIGN, SSI/100) where separate routines for each unit operation compute output stream variables as functions of input stream variables and unit parameters. Routines are called in sequence and convergence blocks force recycle convergence.	1	2	3	4	5

		not needed				essential
(b)	Simultaneous-modular where separate routines are provided as for sequential-modular, but they are called (in any order) to compute coefficients in linearized process model. Linear equations are solved and the process is repeated until convergence.	1	2	3	4	5
(c)	Equation-oriented (as in SPEED-UP and GENDER) where models of process units are in form of (nonlinear) equations. Complete set of equations is generated for the process and fed to general-purpose nonlinear equation solver with automatic partitioning and tearing.	1	2	3	4	5

8. For the sequential-modular approach, should the system determine the calculation order?

   ☐ definitely no

   ☐ leave as an option

   ☐ definitely yes

9. What features of simulators you have used have been particularly good or bad (indicate which).

A number of features proposed for ASPEN have been listed below in six categories relating to different functional criteria. For each feature or criteria, you are asked to indicate by circling a number whether it should have a high, average, or low priority. Even though some features are dictated by the needs of ERDA, we would like an indication of how important they are to you or your organization.

If a question is unclear or of no interest to you, leave it blank. Comments are especially welcome. Write them on the back of the sheet or on a separate page if you need additional space.

	PRIORITY low		average		high	COMMENTS
I. CRITERIA FOR CALCULATIONAL CAPABILITIES						
10. The System Must Be Able to Perform the Following Types of Flowsheet Analyses:						
(a) Steady-State Process Simulation	1	2	3	4	5	
(b) Equipment Sizing	1	2	3	4	5	
(c) Economic Evaluation	1	2	3	4	5	
11. The System Must Permit Analyses of Flowsheets with Different Types of Streams.						
(a) Conventional Vapor-Liquid Streams	1	2	3	4	5	
(b) Streams Containing Solids	1	2	3	4	5	
(c) Multi-Phase Vapor-Liquid Solid Streams	1	2	3	4	5	
(d) Energy Streams	1	2	3	4	5	
(e) Information Streams	1	2	3	4	5	
(f) User Defined Streams Containing Arbitrary Sets of Variables	1	2	3	4	5	
12. The System Should Estimate Physical Properties of:						
(a) Gases	1	2	3	4	5	
(b) Liquids	1	2	3	4	5	
(c) Solids	1	2	3	4	5	
(d) Multi-Phase Mixtures	1	2	3	4	5	
(e) Heterogeneous Materials	1	2	3	4	5	
(f) Complex Materials (Large Number of Chemical Components)	1	2	3	4	5	
(g) Coal-Derived Liquids	1	2	3	4	5	
(h) Shale-Derived Liquids	1	2	3	4	5	
(i) Other Fossil Fuel Intermediates	1	2	3	4	5	
13. The System Should Provide Automatic Regression (under user control) to Determine Model Parameters						
(a) Physical Property Coefficients Regressed from Experimental Data (such as VLE data)	1	2	3	4	5	
(b) Unit Parameters Regressed from Process Operating Data	1	2	3	4	5	
(c) Coefficients in Simplified Process Models (such as linear or polynomial approximations) Regressed from Results of Multiple Runs with More Rigorous Models	1	2	3	4	5	

	PRIORITY low		average		high	COMMENTS
II. CRITERIA FOR SYSTEM STRUCTURE						
14. It Should be Possible to Extend the System at a Later Date to Perform:						
(a) Transient process simulation	1	2	3	4	5	
(b) Balance on available energy around process unit	1	2	3	4	5	
(c) Energy integration (heat exchanger pairing, etc.)	1	2	3	4	5	
15. The System Must be Extendable and Modifiable						
(a) Easy to add new models	1	2	3	4	5	
(b) Easy to add new data	1	2	3	4	5	
(c) Easy to define new types of streams, components, etc.)	1	2	3	4	5	
(d) Easy (or at least possible) to develop new types of analysis	1	2	3	4	5	
16. The System Must be Adaptable to Different Computing Environments						
(a) Efficient on large, fast computer	1	2	3	4	5	
(b) Able to run on small computers	1	2	3	4	5	
(c) Readily transportable	1	2	3	4	5	
(d) Ability to use parts of the system with existing programs independently	1	2	3	4	5	
(e) Feasible to incorporate existing programs into the system						
17. The System Should be File-Oriented						
(a) The results of one analysis may serve as the input to the next	1	2	3	4	5	
(b) To permit retention of the current descriptive of an active problem	1	2	3	4	5	
III. CRITERIA FOR SYSTEM INPUT						
18. The same description of a flowsheet should serve all of the types of analyses for which that flowsheet description is applicable (steady state simulation, equipment sizing, or economic evaluation)	1	2	3	4	5	
19. The system should accept flowsheets at different levels of detail (simple block diagrams, more detailed diagrams, or very detailed flowsheets)	1	2	3	4	5	
20. It should be possible to manipulate descriptions of process flowsheets under control of a program (to permit implementation of synthesis strategies or to allow for automatic changing level of detail - from more to less)	1	2	3	4	5	

	PRIORITY low		average		high	COMMENTS
21. The user should communicate in a convenient form						
(a) Flexibility of engineering units for input data	1	2	3	4	5	
(b) A "fill-in-the-blanks" option for the problem-oriented language	1	2	3	4	5	
(c) Default values of input data should be available wherever possible	1	2	3	4	5	
22. The system should make it easy to determine parameters in simpler process model from multiple runs with more rigorous model	1	2	3	4	5	
IV. CRITERIA FOR SYSTEM OUTPUT						
23. It should be easy to interpret results						
(a) Output should be user-oriented	1	2	3	4	5	
(b) User should have flexibility regarding what, how, and when results are printed, and in what engineering units	1	2	3	4	5	
(c) A history of calculations should be provided at the option of the user	1	2	3	4	5	
(d) Diagnostics must be understandable	1	2	3	4	5	
24. It should be easy to make multiple parametric runs and save the results for sensitivity plots and special reports	1	2	3	4	5	
V. CRITERIA FOR SYSTEM QUALITY ASSURANCE						
25. Calculations must be trustworthy						
(a) Building blocks tested for correctness	1	2	3	4	5	
(b) Calculational methods clearly explained	1	2	3	4	5	
(c) Programs robust and dependable	1	2	3	4	5	
26. The assumptions employed in an analysis must be clear						
(a) Disclaimers printed with results at the option of the user	1	2	3	4	5	
(b) History of assumptions prepared for each analysis and available for selective printing at the option of the user	1	2	3	4	5	

	PRIORITY low		average		high	COMMENTS
VI. CRITERIA FOR USE/USER CHARACTERISTICS						
27. The system must be easy to learn to use						
(a) Well documented and designed so it is easy to learn to use	1	2	3	4	5	
(b) Capable of evolutionary learning — Get on system quickly and solve simple problems — Learn more complex features as you use them	1	2	3	4	5	
(c) Integrated — Learn each new convention and concept only once	1	2	3	4	5	
(d) The user should communicate in terms understandable to him	1	2	3	4	5	
(e) Good instructional material must be provided	1	2	3	4	5	
28. The system must be conveniently accessible to the user						
(a) On national network computer	1	2	3	4	5	
(b) On in-house computer	1	2	3	4	5	
29. The cost of use must be reasonable						
(a) No more expensive than present simulators such as FLOWTRAN for similar jobs	1	2	3	4	5	
(b) Installable on lowest-cost computer (dedicated mini or number-cruncher)	1	2	3	4	5	
(c) Efficient algorithms	1	2	3	4	5	
(d) Avoid large overhead for small problems	1	2	3	4	5	
30. The system will be designed to meet the specialized requirements of fossil energy processes						
(a) Extensive data base for coal, oil shale, and coal-derived liquids physical properties	1	2	3	4	5	
(b) Compatible with reactor conversion models currently available or being developed	1	2	3	4	5	
(c) Routines for solids handling	1	2	3	4	5	
(d) Routine for waste product recovery systems	1	2	3	4	5	

TASK 3: DEVELOPMENT OF PHYSICAL PROPERTY SUBSYSTEM AND DATA BANKS

During the past year, a preliminary version of the physical property subsystem was developed. In addition, methods of calculating multiphase equilibria were investigated under a subcontract with the University of Pennsylvania.

3.1 PRELIMINARY PHYSICAL PROPERTY SUBSYSTEM

The preliminary physical property subsystem is designed for PLEXSYS II, to be used in the simulations of three coal conversion processes. This prototype subsystem will assist in the design of the Physical Properties Subsystem for ASPEN.

Many of today's simulators have comprehensive physical property systems associated with them. Since most of these simulators are designed for vapor-liquid processes, the physical property subsystems also tend to be oriented towards vapor-liquid processes. Also the physical property subsystem is usually built into the simulator which makes it difficult to extract, modify and use parts of the system independently.

Two of the important criteria set forth for the design of a physical property system for ASPEN is modularity and ability to select the calculational route in the course of a simulation. Estimation of physical properties usually involves many subprograms and the best route depends upon the

degree of accuracy required, the components present and the process conditions. Some preliminary ideas on routing were discussed in a paper by Seider et al. (1976), which was included in the First Quarterly Progress Report.

Another important feature to be considered in the Physical Property System for ASPEN is the calculation of properties of homogeneous mixtures involving solids and heterogeneous materials such as coal. Since ASPEN is to be oriented toward energy conversion processes, it is important to include properties of coal and its associated data bank and to be able to calculate properties of coal-derived materials.

The PLEXSYS Physical Properties Subsystem (PPS) is designed to be used in a stand-alone mode. PPS is a preliminary version of the Physical Property subsystem to be incorporated in ASPEN. Modularity of the system results from the independence of each computational module from others. The building blocks of the system are the modules for calculating individual physical properties. The framework allows the addition of new data constants easily. The user can also store the same data constant from different sources. PPS will provide the framework for data banks and modules for calculating thermochemical, transport and equilibrium properties of gases, liquids and solids of pure substances and mixtures. Special attention will be given to the representation of coal and its properties.

3.1.1 Structure of the Physical Property Subsystem (PPS)

Figure 3.1 shows the schematic of the various sets of modules that constitute a PPS. Of the modules shown, we have implemented programs for calculating vapor - liquid properties and programs to estimate properties of coal. Other properties will be added as they are identified as required for simulating the three coal conversion processes.

The concepts of routing and modularity in physical property estimation systems introduced by Seider et al. (1976) have been extended to include multiple data banks.

Each module in the system consists of two types of subprograms: a Property submodule and a Method submodule.

Figure 3.2 shows the structure of a module to compute a physical property. The property module functions effectively as an 'OR' block that selects the appropriate method and calls upon it. The method modules are 'AND' blocks. They may call upon other property modules in the system.

Each property module must have supplied to it information telling which method to use to compute the property. This is contained in the route. Each property module will have associated with it documentation that explains the different methods available, the other properties required by these different methods, and the calculational parameters (if any) required for each method.

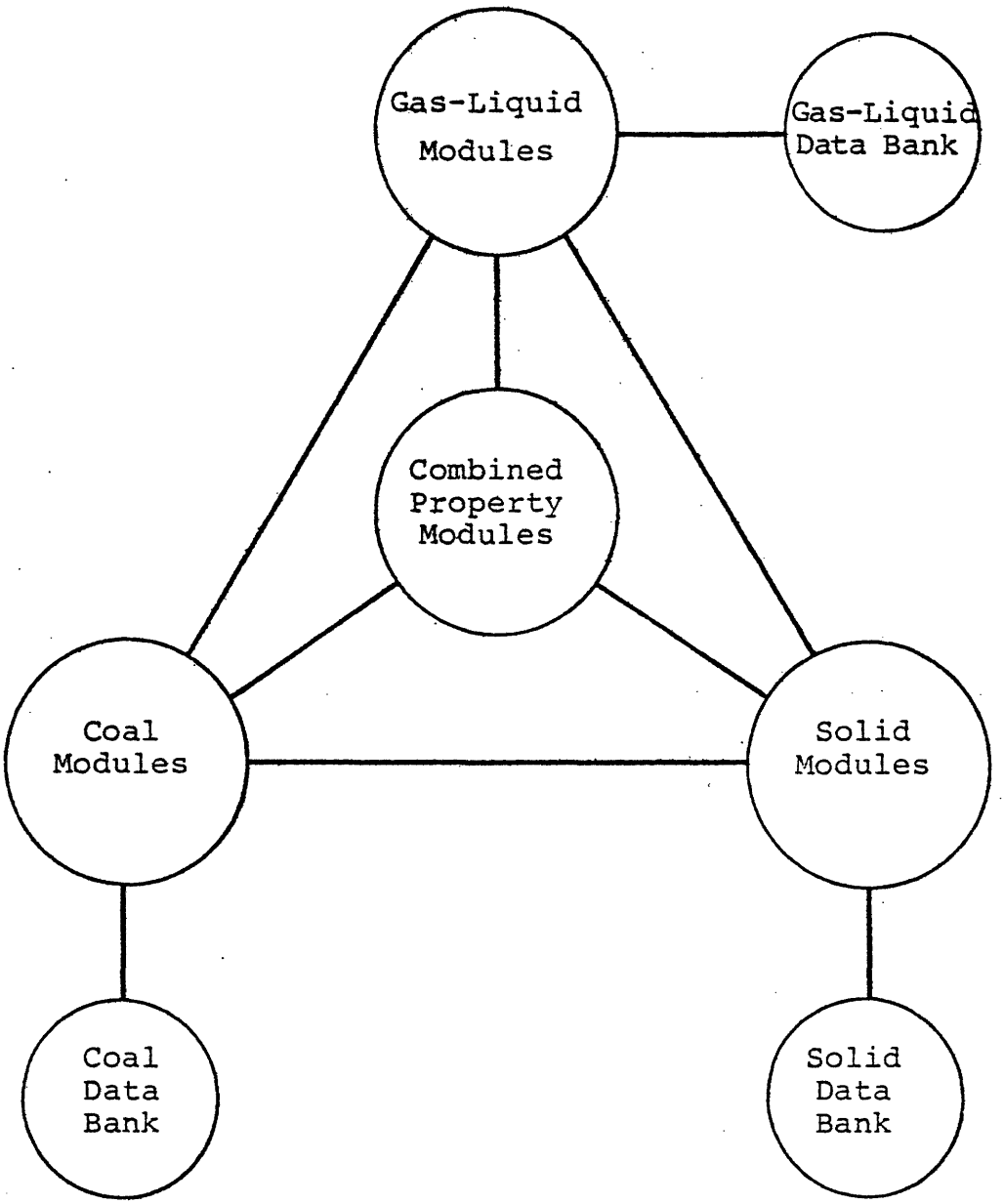


Figure 3.1 Schematic Diagram of Physical Property System for PLEXSYS II

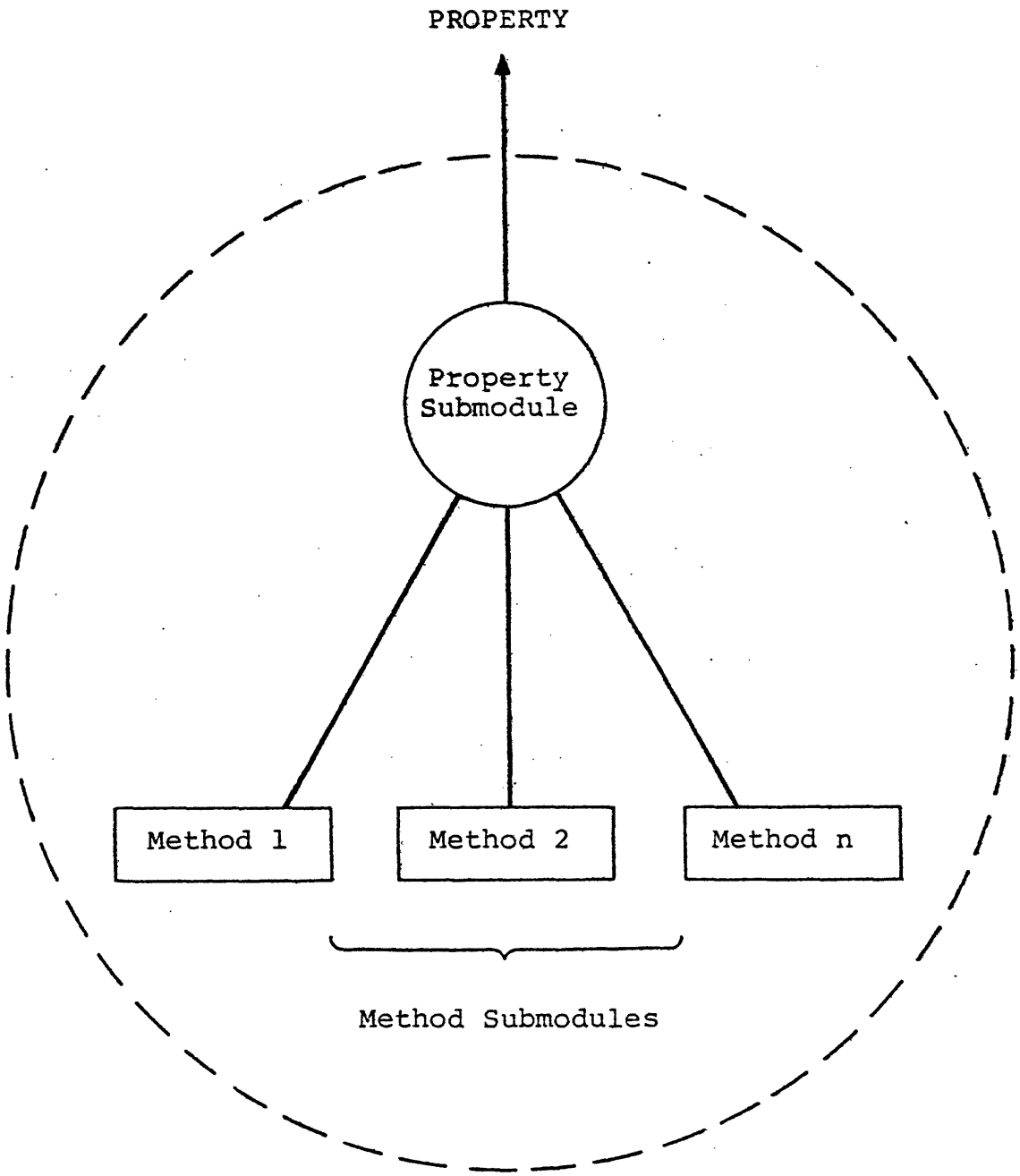


Figure 3.2 Structure of a Module for Computing a Physical Property

The method submodules can access constants from the data bank by calling on the appropriate data retrieval module with a route (if necessary) specifying the source of the data. Figure 3.3 shows a sequence of calls in a physical property estimation.

The Appendix A lists the modules that are incorporated in the preliminary PPS. The modules have been tested against published experimental data (where available) and the FLOWTRAN Physical Property System.

3.1.2 Coal Properties

A number of modules for estimating coal properties have been prepared. These modules are listed in the Appendix A.

Additional modules will be added as required by the three coal conversion processes being simulated. The properties of coal can be considered as the sum of the contributions from its constituents; such as moisture, fixed carbon, low boiling primary volatile matter and high boiling secondary volatile matter. The properties of these constituents are assumed to be semi-independent of the type of coal (IGT Report, May 1976). The properties of each constituent can be estimated from empirical correlations of experimental data (Kirov, 1976; Gomez, et al., 1965; Goodson, 1976).

Most of our information used in developing the set of coal property modules is from the IGT reports describing preparation of a Coal Conversion Systems Technical Data Book, November 1974 - April 1976. Programs to calculate heat capacity, enthalpy, true density, heat of combustion of char are included in the system.

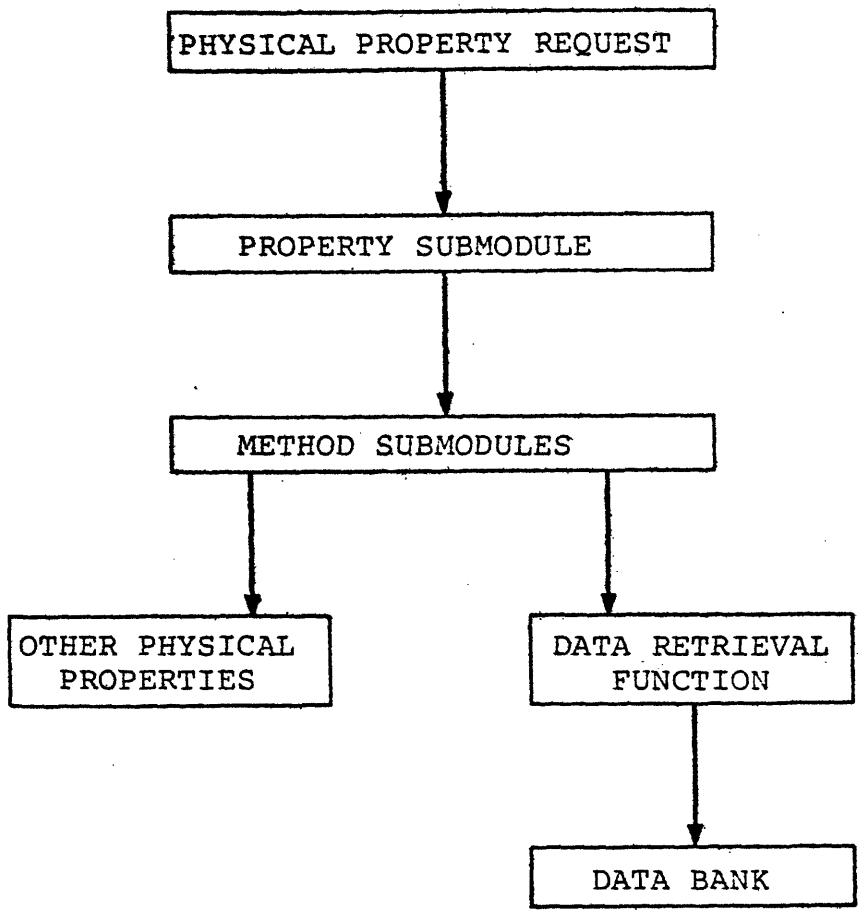


Figure 3.3 Sequence of Calls for Physical Property Estimation

Work is also being carried out on correlating the enthalpy of coal using an empirical model for mean heat-capacity as a function of temperature and original volatile matter content.

The model for $\bar{C}_p$ currently being tested is

$$\bar{C}_p(T,VM_o) = a+b*T+C*VM_o+d*VM_o*T+e*(T-f)^2*(VM_o-g) \qquad (3.2)$$

where a, b, c, d, e, f, and g are regression coefficients.

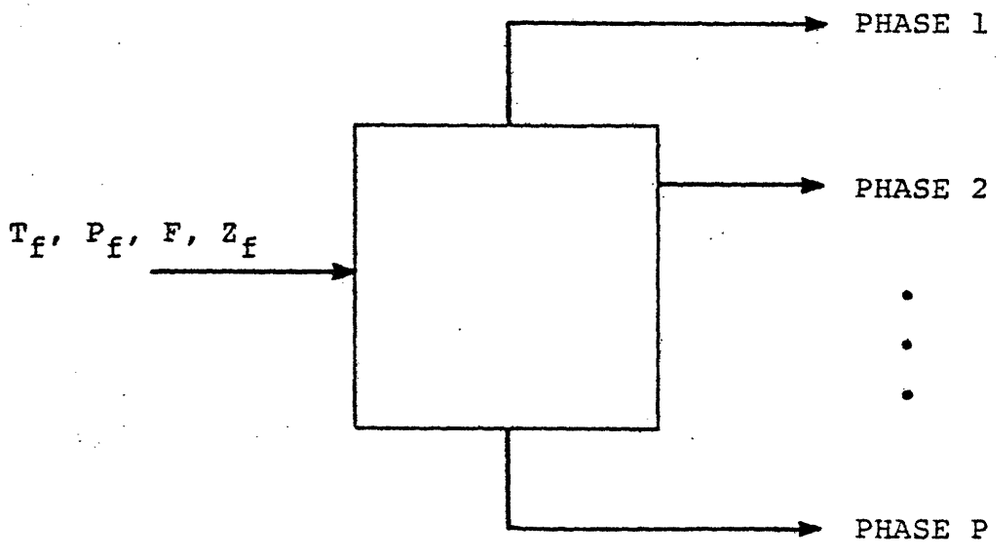
The preliminary PPS, although developed for PLEXSYS II, can be used independently without knowledge of the plex data structure. Detailed description on how to use the system will be available in the User's Manual currently being prepared.

3.2 DEVELOPMENT OF METHODS FOR MULTIPHASE CHEMICAL EQUILIBRIUM

Work is being carried out at the University of Pennsylvania under a subcontract to develop new methods for calculating phase and chemical equilibria that are applicable for use in simulators and for studying energy conversion processes. The methods should provide the proper blend of generality, reliability, and speed.

Figure 3.4 illustrates the physical situation in which a mixture of chemicals is allowed to reach equilibrium at T_f and P_f. The number of phases, P, and their compositions are unknown at equilibrium.

It is noteworthy that today's simulators permit calculation of phase equilibria for, at most, three phases (vapor-



Given T_f, P_f, F, and Z_f, compute flow rate and composition of each phase leaving in equilibrium

Figure 3.4 Physical Situation

liquid-liquid), involving no solids, and no chemical reaction.

Mathematically, the problem is to minimize the Gibbs free energy

$$G = \sum_{j=1}^{S} G^{oc} n_j^c + \sum_{j=S+1}^{C} \sum_{\ell=1}^{P} G_{j\ell} n_{j\ell} \qquad (3.3)$$

subject to atom balance constraints

$$b_k = \sum_{j=1}^{S} m_{jk} n_j^c + \sum_{j=S+1}^{C} \sum_{\ell=1}^{P} G_{j\ell} n_{j\ell} \qquad K = 1,2,... \qquad (3.4)$$

where C is the number of chemical species, P is the number of mixed phases (vapor, liquid, solid), S is the number of condensed species (appear in only one pure phase - normally solid - do not distribute amongst other phases), E is the number of elements, b_k is the number to gram-atoms of element k, m_{jk} is the number of atoms of element k in compound j, $n_{j\ell}$ is the number of moles of compound j in phase ℓ, $G_{j\ell}$ is the chemical potential of compound j in phase ℓ.

A search for the literature uncovered several methods to minimize the Gibbs free energy. Three of the best known methods are hereafter referred to as the Brinkley (1946, 1950), NASA (Gordon and McBride, 1971), and Rand (White, et al., 1958) methods. Though not immediately obvious, all three use Newton's method and are computationally similar. Hence, they encounter the same problems, which are:

(1) Inability to handle poor starting estimates of compositions and phases, and

(2) Slow convergence

This subtask of the project is devoted to finding better implementations of existing methods or a new method that is practical for determining multi-phase equilibria in energy conversion processes. For a particular system, it is usually possible to write a program to minimize computation time. However, for calculations involving a wide variety of chemicals, with broad ranges in independent parameters, it is desirable to have a general program with no restrictions on initial guesses, built-in safeguards to insure numerical convergence, and simplified input. The latter situation arises when algorithms for computation of equilibira are incorporated in a process simulator.

3.3 TESTING OF METHODS FOR MULTIPHASE CHEMICAL EQUILIBRIUM

A survey of existing methods was made during the past year and some new approaches were proposed to overcome their limitations. These are described below:

(1) Use of Newton's method for equilibrium calculations

An APL program called FREE was written to implement the Rand Method for calculation of equilibria in systems with multiple phases, with or without chemical reaction. FREE was developed as a prototype program to provide experience with various mixtures and to permit experimentation with new algorithms.

(2) Development of thermodynamic routines

To perform calculations in FREE and other programs to be developed, routines for calculation of fugacity coefficient, activity coefficient, vapor pressure and liquid fugacity are needed. Numerous equations exist for calculating these properties and the choice depends upon the particular system under study. Therefore, several options have been provided. In most cases, equations in the FLOWTRAN physical property system were chosen to permit use of the FLOWTRAN data bank and its programs to compute interaction coefficients for binary pairs given vapor-liquid and liquid-liquid equilibrium data.

A new method is planned involving a modified van der Waals' equation of state for calculation of fugacity coefficients and enthalpies in vapor-liquid and liquid-liquid mixtures. This method was presented by Wilson and Weiner (1977) and continues to be developed. It predicts equilibria for mixtures with large concentrations of polar substances at high temperatures, such as in coal gasification where CO_2, COS, H_2S and water occur at temperatures between 500°F to 3000°F and pressures between 1 atm to 100 atm.

(3) Experimentation with FREE

The program FREE is being used to calculate phase and chemical equilibria in a variety of systems taken from the literature which are summarized below. These systems were selected because they provide a good test of the methods.

(a) Cracking of ethane at 1000°K and 1 atm, (Balzhiser, et al., 1972)

This system is an ideal gas at 1000°K and 1 atm and involves chemical equilibra but not phase equilibria. Some problems were encountered in reaching equilibrium with trace components present. Although small quantities are present, their magnitude changes significantly with each iteration. Fortunately, these changes can be disregarded in tests for convergence, as they do not influence the composition at equilibrium.

(b) Carbon laydown in a blast furnace at 200°F and 1 atm, (Balzhiser, et al., 1972)

This system has pure condensed phases (C, Fe, FeO). The Rand Method does not converge when an incorrect number of solid phases is assumed. It computes negative mole numbers for solid species that are not present at equilibrium. Also, in the search direction, the minimum free energy occurs in the immediate proximity of the initial values. Hence, no change in composition occurs. To achieve convergence, it is necessary to remove solid species with negative mole numbers.

(c) BIGAS gasifier at 1700 - 3000°F and 100 - 1500 psia. (Hegarty and Moody, 1973)

Mixtures in the BIGAS gasifier involve a vapor phase which may be accompanied by char. Air Products, Inc., reported a design for the gasifier based upon pilot plant data in which the partial pressure of methane was measured and the water-gas shift reaction assumed to reach equilibrium.

FREE will be modified to permit modeling of reacting systems where some concentrations have been measured experimentally or predicted using kinetic models. The modified van der Waals' equation of state being developed by Weiner and Wilson (1977) will be used because this mixture consists of polar substances such as CO, CO_2, and H_2O.

(d) Sulfur plant simulation (James, 1975)

In simulation of a plant to recover sulfur from a feed containing H_2S and hydrocarbons, calculation of equilibria is required in the furnace and waste heat boiler, and sulfur condenser. We plan to test equilibria calculation in these units.

(e) Scrubbing of flue gas with alkali (Kerr, 1974)

Flue gases are often scrubbed with alkali solutions in gasification processes. In simulating absorbers, calculation of equilibria involving sodium sulfite, bisulfite, and sulfate, and their ions in aqueous solution is required. We plan to study this electrolyte system involving vapor-liquid and chemical equilibria.

(f) Nitroethane-Octane-1 Octene at 0°C and 1 atm. (Heidemann and Mandane, 1975)

This is a Type I system, as defined by Treybal (1963). This system will be studied because it involves equilibrium between two liquid phases.

3.4 WORK FORECAST

3.4.1 Prototype System

A report describing the preliminary version of the physical property system is being prepared. This will be delivered along with the programs to ERDA during the next quarter. Additional work is planned in the area of properties of coal, properties of homogeneous and heterogeneous solids and coal derived liquids.

3.4.2 Physical Property Requirements of ASPEN

Work has begun in outlining the physical property capabilities required in ASPEN. A list of modules and property estimation methods and a description of the data bank is being prepared. This will serve in identifying and evaluating the available systems which may be acquired to satisfy ASPEN requirements.

3.4.3 Development of Phase and Chemical Equilibrium Programs

(a) Heuristic Methods for Phase Equilibria

Algorithms have been developed to compute the phase distribution for systems involving a vapor and one liquid phase. These involve determination of bubble and dew point temperatures and, in the two phase region, solution of the flash equation.

For highly non-ideal systems that can form a second liquid phase, the problem is complicated and heuristic methods have been described by Henley and Rosen (1969). They recommend searching first for three phases. If not

found, two liquid phases are assumed in the absence of vapor and the equations for liquid-liquid equilibrium solved. If no solution is found, the bubble point is computed, and when the temperature exceeds the bubble point, the equations for vapor-liquid equilibrium are solved.

We plan to study the performance of this method for selected three phase systems in comparison with methods that minimize the Gibbs free energy objective function, such as the Rand method.

Furthermore, we will use heuristic methods to solve for phase equilibria in chemically reacting systems. This approach involves guessing extents of reaction, solving to determine the phase distribution, and checking whether chemical equilibrium are satisfied. If not, new extents of reaction are estimated and the procedure repeated.

Programs are being prepared to carry out these studies.

(b) Adaptive Random Search

Problems arise when the number of phases at equilibrium is incorrectly assumed. These include singularities in matrices to be inverted and the inability to reach a solution in a reasonable number of iterations.

The Adaptive Random Search method described by Gaines and Gaddy (1976) will be explored as a possibility for identifying a reasonable estimate for the phase distribution, prior to utilizing rigorous methods to calculate equilibria. A program named RANDMIN has been written that has been used to experiment with the method. Although slow to compute

accurate results, it shows promise for determining ball-park estimates in reasonable computing times.

(c) Hybrid Methods for Calculation of Chemical and Phase Equilibria

We recognize that often phase equilibria can be computed rapidly using heuristic methods, whereas chemical equilibria are more easily computed using methods that minimize Gibbs free energy. Hence, we plan to study use of the two approaches cooperatively. For example, one possibility is to perform one iteration of the Rand method followed by a few iterations of heuristic algorithms to approach phase equilibrium, given the distribution of chemicals computed by the Rand method. Such a procedure would be repeated until a solution to the phase and chemical equilibria is obtained. We plan to experiment with this and similar hybrid methods.

(d) Transient Methods for Phase Equilibrium

It may be possible to accelerate calculations to determine phase equilibria by preparing a hypothetical transient model that approaches the steady state more rapidly than conventional methods. Such an approach works successively in solution of many elliptic partial differential equations and may be applicable for calculations of equilibria. Transient models will be programmed and their results compared with the results using conventional methods.

(e) Effect of Equations for Activity Coefficients on Phase Equilibrium

Some equations for activity coefficients represent data for phase equilibrium better in particular regions of the phase diagram. The most popular equations will be studied and guidelines prepared for their usage.

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TASK 4: DEVELOPMENT OF UNIT OPERATIONS SUBSYSTEM

4.1 WORK ACCOMPLISHED

Work on this task is not scheduled to begin until July, 1977. During the past year, however, we have prepared a list of the unit operations modules that will be required in ASPEN. This list is presently being revised and more complete descriptions of the modules are being prepared. This will be submitted as a separate report to ERDA.

4.2 WORK FORECAST

During the next quarter, the list of unit operations modules required in ASPEN will be completed. This will be based on the ultimate use of ASPEN in simulating energy conversion processes. In addition to traditional unit operations such as stream addition, stream splitting, flash, distillation, extraction, pumps, compressors, heat exchangers, condensors, furnaces and reactors, ASPEN will have programs for unit operations involving solids such as fluidized bed reactors, dryers, crystallizers, screens, cyclone separators, crushers and grinders.

For each unit operation involved, the current availability of the program from external sources and the cost of developing the program in-house as opposed to buying it will be assessed.

TASK 5: DEVELOPMENT OF COST ESTIMATION SUBSYSTEM

5.1 WORK ACCOMPLISHED

The existing cost estimation and economic evaluation programs are being analyzed for possible acquisition and modification. The Task Force on Software Evaluation at its meeting in May, 1976 looked at this problem briefly while screening the programs for cost estimation. The subsystem should meet two requirements, namely:

(a) To generate preliminary cost estimates which can be incorporated into overall process optimization.

(b) To carry out project analysis (i.e., determine technical and economic feasibility of processes).

Using the output from the steady state simulator, the Cost Estimation Subsystem will carry out a comprehensive economic evaluation consisting of the following steps:

(a) Equipment sizing and costing of Main Plant Items

(b) Determination of operating requirements (labor, raw materials, utilities, etc.)

(c) Investment and operating cost estimation

(d) Sales volume and price forecasting

(e) Profitability computation

(f) Sensitivity analysis (to examine effect of changes in capacity, selling price and other economic parameters)

Preliminary evaluation of existing software for project analysis indicate that a modular approach, in which each of the

above steps is carried out in a stand alone module, would incorporate great flexibility into the Subsystem. A sketch of a possible organizational structure is as shown in Figure 5.1.

5.2 WORK FORECAST

Work on the design of the subsystem will begin as soon as the framework for ASPEN has been implemented. Meanwhile the existing cost estimation systems will be evaluated in greater detail to aid in designing the subsystem for ASPEN and also in deciding what portions of the subsystem can be acquired and what needs to be developed in house.

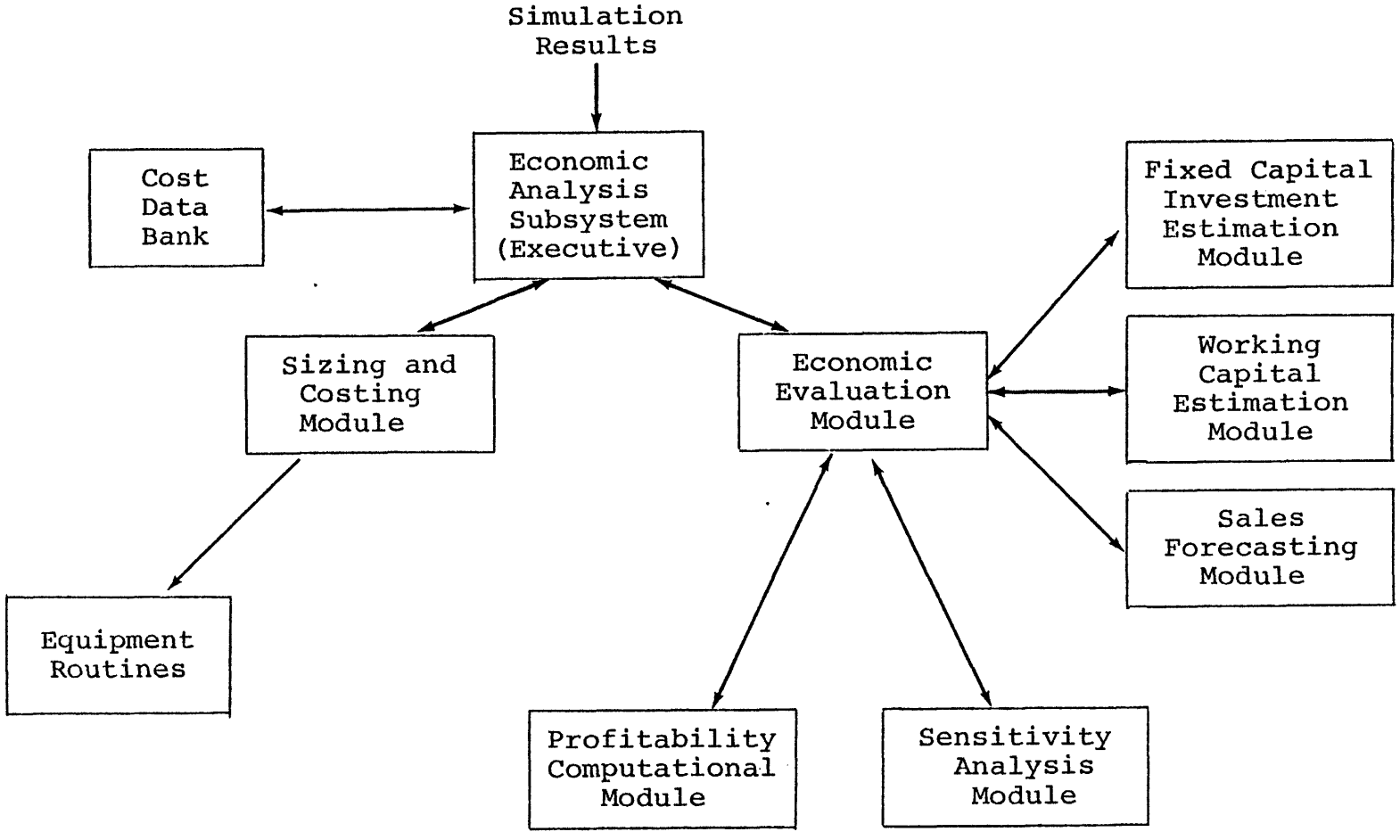

Figure 5.1 Structure of the Cost Estimation Subsystem

TASK 6: DEVELOPMENT OF DATA REGRESSION SUBSYSTEM

6.1 WORK ACCOMPLISHED

Work on this task is not scheduled to begin until late in the second year.

6.2 WORK FORECAST

Work will begin during the coming year to develop the data regression requirements for ASPEN. A primary use of this capability will be to correlate experimental data to fit physical property models.

The VLE (Vapor-Liquid Equilibrium) system of FLOWTRAN is an example of a subsystem to reduce experimental data as required for the simulator. Generally this involves non-linear regression of the data to fit equations. We are planning to study the methods used currently in reducing experimental data to define the requirements of ASPEN.

TASK 7: ACQUISITION OF PROPRIETARY SOFTWARE AND MODIFICATION FOR USE IN ASPEN

The objective of this task is to identify, evaluate, acquire, and modify software for inclusion in the ASPEN system. The software acquisition has been split into two parallel tasks. The first one was directed at the acquisition of a base simulator early in the project in order to assure that ASPEN will start with the current technology in process simulation. The second task concerned an extensive search in order to identify modules that may be incorporated into ASPEN.

The project staff has obtained the assistance and guidance of part of the Advisory Committee which is titled the Task Force on Software Evaluation. This group is comprised of individuals from various companies and universities who are familiar with different available computer programs.

7.1 ACQUISITION OF A BASE SIMULATOR

Since the acquisition of base simulator is scheduled for the early part of the project, considerable attention was paid to this task in the past year. Most of the simulators currently being used by the industry are proprietary in nature and considerable negotiations are required to reach an agreement on the acquisition of the simulator and its incorporation into ASPEN. The following simulators are examples of representative programs that could serve as a base simulator.

1. CAPES (Chiyoda, Japan)
2. CONCEPT (Computer-Aided-Design-Center)
3. DESIGN/DISTIL (Chemshare Inc.)
4. FLOWPACK II (ICI, London)
5. FLOWTRAN (Monsanto Company)
6. GPS II (Phillips Petroleum)
7. IPES (Union Carbide)
8. SSI/100 (Simulation Sciences Inc.)

Negotiations are underway with a company to purchase the base simulator and the details of a contract are being prepared. The Advisory Committee has proved to be a very effective mechanism in identifying and negotiating for proprietary software.

7.2 IDENTIFICATION OF EXISTING SOFTWARE

The base simulator will provide ASPEN with a minimal set of modules. There are still a large number of modules that are necessary to complete the system. The objective of this subtask is to identify if such modules already exist, and if so evaluate and acquire them if it is more expensive to develop them within the project.

The four phases of work required to acquire and install existing programs into ASPEN system are:

(1) Survey: Enough information must be obtained about each program to permit as complete and accurate an evaluation as possible.

(2) Evaluation: The evaluation phase should provide an objective review and comparison of the advantages and disadvantages of all programs being considered for acquisition.

(3) Procurement: Limited funds are available to assist in obtaining programs desired for use in ASPEN. These must be allocated in an optimal way so as to satisfy the requirements of ASPEN.

(4) Modification: All the programs purchased will require some modification. These modifications will have been identified before purchasing the programs. Since considerable effort is involved in Program Modification, the amount of modification required is an important criteria for selection of programs.

7.2.1 Types of Software

Four types of software have been identified, namely, commercial, university, proprietary, and specialty software.

Commercial software refers to programs developed by commercial systems houses and consulting companies. These companies are generally pleased to provide all the information needed to use their programs but they many be reluctant to sell their programs for use in ASPEN, because it would put these programs in the public domain.

University software is often typified by inadequate documentation and lack of programming standards. But it may also be the most innovative and contain many new ideas. Its cost is generally low.

Proprietary software included programs developed by companies in industry for their own in-house use. Getting information on these programs can be difficult and negotiating terms of a sale can be lengthy.

Specialty software of interest to ASPEN refers to program for modeling energy conversion processes, synthetic fuel research and development teams developed generally under ERDA contract. These may be available free of cost to ASPEN, if developed with government funds, or they may be considered as proprietary software, if developed with company funds.

7.2.2 The Survey

Each type of software identified above was surveyed in a different way. Surveys of commercial software were conducted by Chemical Engineering magazine in 1973 and 1975. It was felt that the best way to update this information was to repeat the Chemical Engineering survey using the same questionnaire. (A copy of the questionnaire was shown in the Second Quarterly Progress Report.) The information requested in this questionnaire is very similar to the information required for the ASPEN project.

The university software was surveyed through the CACHE (Computer Aids for Chemical Engineering Education) Committee which has nearly 150 representatives in universities throughout North America. Additional letters were sent to members of the American Institute of Chemical Engineers Machine Computation Committee.

Most of the large chemical process companies holding proprietary software had sent representatives to the Advisory Committee meeting of the ASPEN Project (December 13, 1976). A request was made during the meeting for information regarding proprietary software that might be made available to ASPEN.

A special form was developed for the survey of specialty software. These were sent out to all ERDA contractors who might be developing mathematical models or software for fossil energy processes. Copies of the letter and survey form were shown in the previous quarterly progress report.

Over 500 letters were sent out, mostly represented by sources for Chemical Engineering. The returns are immediately screened to eliminate irrelevant material and placed on file for further processing. About 210 returns have been processed so far. Over 440 commercial, university and proprietary programs have been identified. More returns are expected. The survey questionnaires will be sent out whenever new sources are identified.

7.2.3 Screening, Categorization and Evaluation of Programs

The steps in screening and categorizing have been divided as follows:

(1) First screening

(2) Categorization

(3) Second screening

(4) Preliminary evaluation

(5) Final evaluation

The purpose of the first screening was to ascertain if the program is relevant to ASPEN. This first screening was done using a staff familiar with the objectives of ASPEN and who had a working understanding of process simulation.

The purpose of the categorization phase was to identify the capabilities of each program on file. A software categorization form was prepared for this purpose. A computer program, Relational Data Management System (RDMS), was used to store and analyze the information gathered through these forms. Using RDMS it was possible to cross reference all programs on file by their capabilities.

A meeting of the Task Force on Software Evaluation was held on May 2 and 3, 1977 at MIT, Cambridge, Massachusetts to examine the programs obtained through the software survey and to screen out programs of inferior quality. The Task Force was supplied with abstracts of program modules ahead of time so that the screening procedure could be facilitated.

Two groups were formed to screen the programs. Dr. J. P. Leinroth chaired one group concerned with areas of heat exchangers, reactors and cost estimation. The other group, chaired by Prof. R. L. Motard, screened programs in areas of Separations and Physical Properties. By vastly reducing the number of programs to be evaluated further and by guiding the direction for evaluationg programs, the task force facilitated the software evaluation to be carried out by the staff in the future months. Minutes of the software evaluation task force meeting for second screening are available as an internal working report.

The preliminary evaluation of the programs picked by the Task Force is underway. This Phase will be to prepare reports on each of the areas of Physical Properties, Unit Operations and Cost Estimation. The purpose is to gather the facts required to complete the evaluation of the programs. It will also highlight the major features of each program and compare it with the requirements of ASPEN.

7.3 WORK FORECAST

Completion of reports for preliminary evaluation is scheduled for June, 1977. The next stage is final evaluation of these programs. The final evaluation will decide how to allocate the limited funds available for the purchase of programs in order to realize maximum benefit to ASPEN. The programs should be ranked in order of importance and

desirability to ASPEN. Negotiations with the vendors may begin at this stage to determine exact price and conditions of sale. Outside consultants may be engaged to make contributions to the final evaluation.

TASK 8: INTEGRATION, TESTING AND DOCUMENTATION OF ASPEN

8.1 WORK ACCOMPLISHED

No work on this task is scheduled until the third quarter of the second year. It is included, however, to provide a consistent means of reporting in the future.

8.2 WORK FORECAST

In the coming year benchmark problems will be defined that will be used eventually to test the system. The Task Force on Benchmark Problems of the Advisory Committee will assist us in developing the problems. The work on the prototype simulations of three fossil energy processes (see Task 1) will be extended to provide specifications for problems used to test ASPEN.

IV. CONCLUSIONS

TASK 1: DEVELOPMENT OF PROTOTYPE SIMULATOR AND SIMULATION OF SPECIFIC FOSSIL ENERGY PROCESS

The prototype simulator PLEXSYS II has shown the advantages and disadvantages of using a plex structure for process simulation. It is quite easy to represent the different types of streams and unit operations encountered in coal conversion processes using the plex structure. There is a modest increase, however, in execution time due to the extra data manipulation involved. The study using PLEXSYS II has identified a number of areas which are important in the design of ASPEN. There exists a need to have simple means of inputting information to the plex and modifying the plex. FORTRAN may not be the best medium to implement the plex and the use of other compilers should be studied with the objective of reducing the execution time. The implementation of the preliminary physical property subsystem was greatly simplified by the use of the plex data structure.

The three coal conversion processes have proved to be excellent benchmark problems to test the capabilities of Computer Simulation Methods. Study of these processes has exposed the areas in which current simulators are deficient.

TASK 2: DEVELOPMENT OF ASPEN SYSTEM STRUCTURE

The critical decisions to be made in setting the functional specifications of ASPEN have been identified. The feedback from the questionnaire on design criteria being circulated among the Advisory Committee will be used in setting up the functional specifications.

TASK 3: DEVELOPMENT OF PHYSICAL PROPERTY SUBSYSTEM AND DATA BANK

The preliminary physical property subsystem has shown that it is possible to implement the concepts of routing and modularity which were considered necessary for ASPEN. Using the plex data management system it is possible to set up a subsystem which can be expanded easily and taken apart if necessary for use on a stand alone basis. It is possible to use multiple sources of data and multiple choices of methods in the course of a simulation.

The implementation of coal property estimation methods has helped establish a data structure to store properties of coal. There exists a need to identify and develop methods to estimate properties of coal more accurately.

TASK 4: DEVELOPMENT OF UNIT OPERATIONS SUBSYSTEM

Many of the unit operation models needed for ASPEN are the same as those in existing simulators for vapor-liquid processes. A number of new routines will be needed, however, to model streams with solids. The specifications for these new models appear to be relatively straightforward and can be developed by analogy with models for vapor-liquid processes. Programs for these unit operations will probably have to be developed especially for ASPEN, either by the project staff or under subcontract.

TASK 5: DEVELOPMENT OF COST ESTIMATION AND ECONOMIC EVALUATION SUBSYSTEM

Cost estimation is a capability that is important for ERDA's use of ASPEN, but one in which there is a variety of methods and practices in use in industry. It will be important to get agreement, with the aid of the Advisory Committee and ERDA, on the methods to be implemented in ASPEN.

TASK 6: DEVELOPMENT OF DATA REGRESSION SUBSYSTEM

Work on this task has not yet begun and there are no important conclusions at this time.

TASK 7: ACQUISITION OF PROPRIETARY SOFTWARE AND MODIFICATION FOR USE IN ASPEN

The results of the software survey indicated that there are a large number of programs of potential interest to ASPEN. Since many of these programs have similar capabilities, it is necessary to carry out a detailed evaluation before deciding which of these programs should be acquired to be incorporated into ASPEN.

A number of companies have expressed a willingness to negotiate possible terms under which their proprietary software could be made available to the project. These include Union Carbide, Monsanto, ICI, Chiyoda and Simulation Sciences.

TASK 8: INTEGRATION, TESTING, AND DOCUMENTATION OF ASPEN

Work on this task has not yet begun and there are no important conclusions at this time.

APPENDIX A

Description of PLEXSYS II Physical Property System

1. Modules to Computer Properties of Gases and Liquids

The physical property system (PPS) for PLEXSYS II consists of a set of FORTRAN functions or subroutines that are called by statements of the form

RESULT = PROP (arguments)

where PROP is the name of the property module to compute the property. The arguments depend upon the type of property being computed. For gas and liquid properties they include some or all of the following:

T = temperature (Deg k)

P = pressure (atm)

NPC = pointer to data for a pure component (name and property constants)

NPM = pointer to the data for a mixture (mole fraction, name, and property constants for each component)

NRTE = pointer to the route specifying the method(s) to be used in computing the property

T and P are real variables, while NPC, NPM, and NRTE are pointer (or integer) variables.

The pointer NPC points to a plex data structure containing the data for a pure component. The form of this structure is shown in Figure 1. The data identification bead

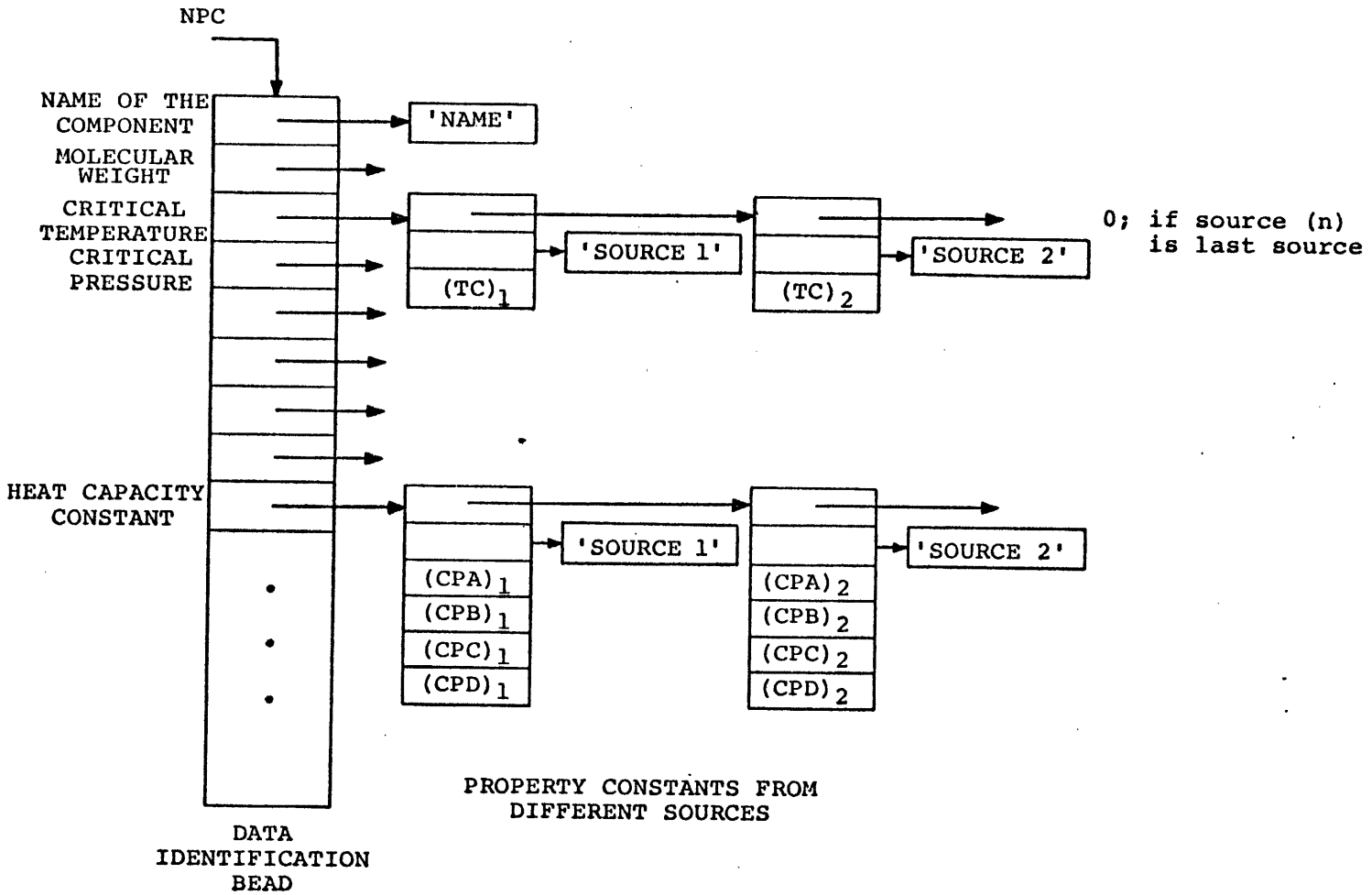

Figure 1. Structure Contains Data for a Pure Component

contains pointers to beads containing single constants characterizing the compound (critical temperature, pressure, etc.) and sets of constants (correlation constants for vapor pressure, ideal gas heat capacity, etc.). Data from more than one source for the same constant or set of constants may be included. This structure is expandable horizontally to include new sources of data and vertically to include additional property constants.

The pointer NPM points to a structure containing the data for a mixture. The form of the structure is shown in Figure 2.[illegible]. A header bead provides pointers to the mole fraction bead and the component identification bead.

The pointer NRTE points to the plex structure to define the route for computing the property. A route bead is shown in Figure 3.[illegible] The first entry in the route bead is a pointer to a character string (of exactly 16 characters including trailing blanks) giving the "calling code" designating the method to be used for computing the property. Succeeding entries in the bead are pointers to the route to be used in computing any other subordinate property modules called. The last entry in the route bead is a pointer to a character string (of 4, or a multiple of 4, characters) containing the name of the data source from which all property constants are to be obtained.

If NRTE = o, i.e., if no route argument is provided, the property module uses the default option for the method

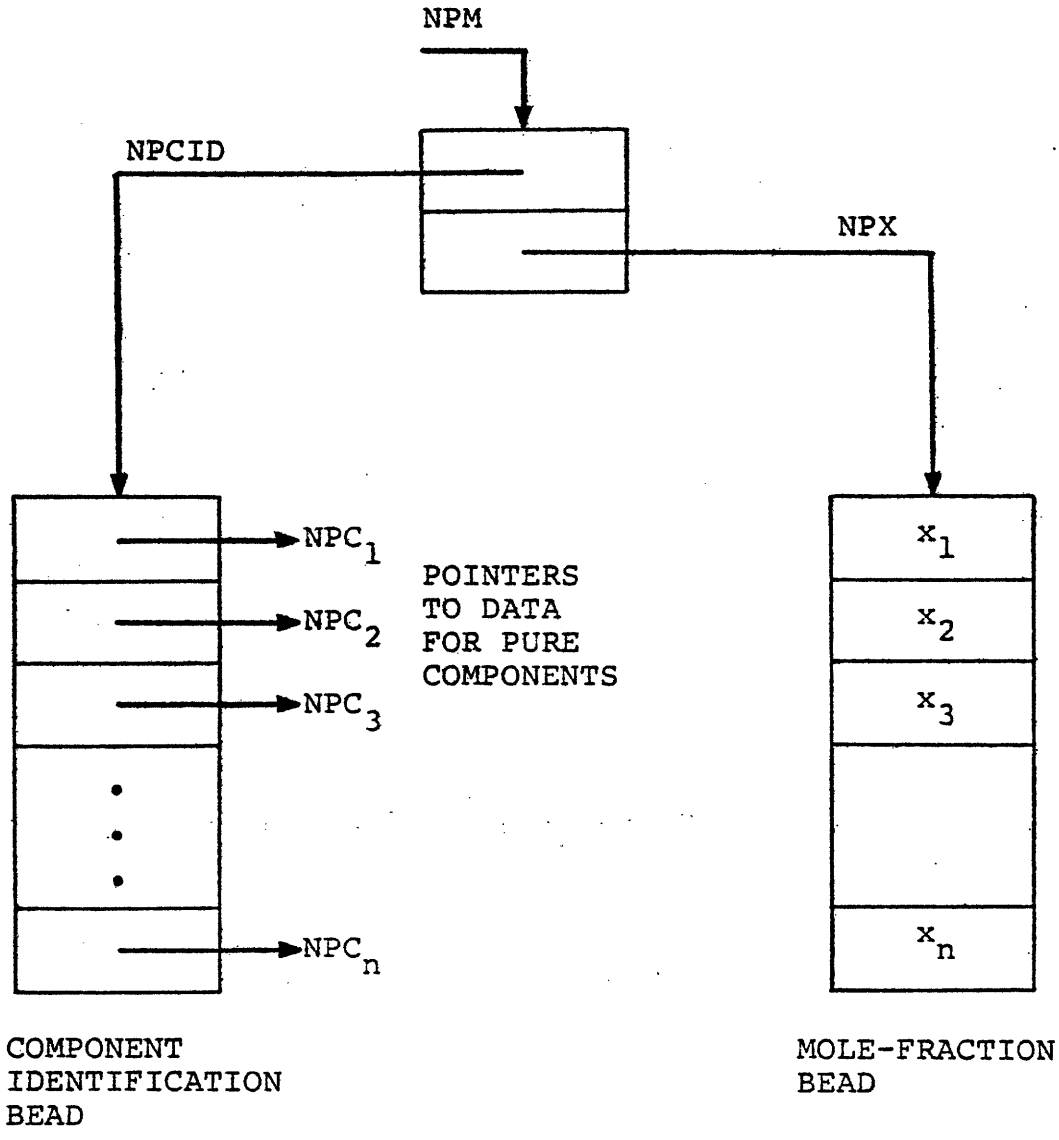

Figure 2. Data Structure for a Mixture

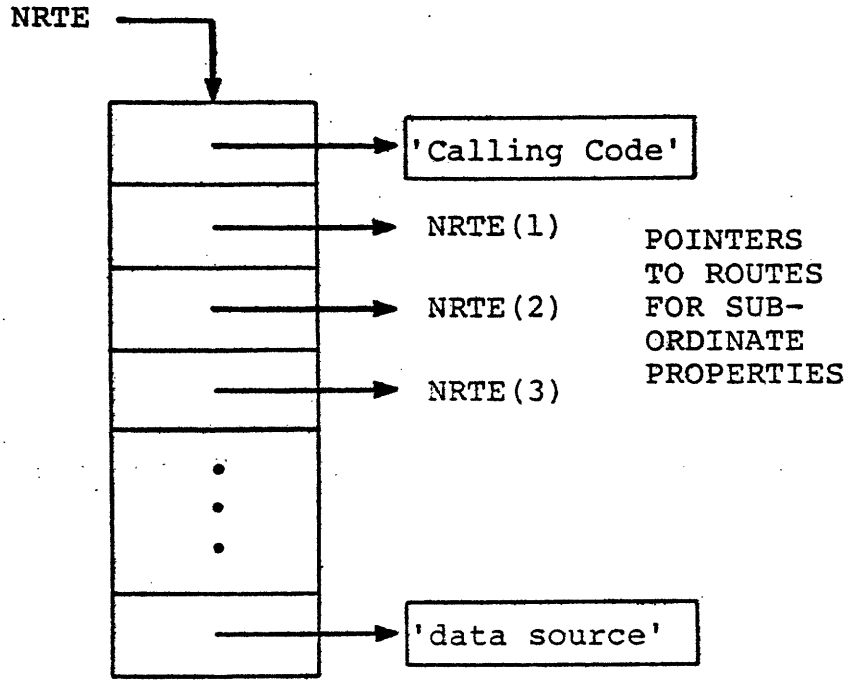

Figure 3. Route Bead

and it also specifies default options to be used by all subordinate property modules called and a default option for the data source.

Table 4.1 lists all of the vapor and liquid properties presently implemented in PPS. It gives under each property module the arguments of the call, the units of calculation, the methods available for computing the property, the calling code for each method, the subordinate property modules called by each method, and a short description of the property and the methods available. This table is necessary and sufficient to construct a route plex for property calculation. The calling code is, in effect, a password specifying the method to be used. The pointer to this password is placed in the first location of the route bead pointed to by NRTE. It should be noted that the calling code must be followed with blanks until 16 bytes are filled. The sequencing of pointers to the route beads of other property modules called is essential and should be followed as in the table. The pointer to the name of the source of the data bank wanted should be stored in the last location of the bead. If the pointer is zero, a default option will be used.

The parenthesis after the name of property modules called by each method is the recommended method to be used in those property calculations. Some methods call on other methods within the same module. In this case the Method

TABLE 1

Codes in the Arguments and Units column used in the following tables.

a = (T,P,NPC,NRTE)

b = (T,P,NPM,NRTE)

c = (T,P,NPM,NPC,NRTE)

d = (T,NPC,NRTE)

e = (H,P,NPM,NRTE)

f = (S,P,NPM,NRTE)

g = (S,T,NPM,NRTE)

h = (P,NPC,NRTE)

i = (P,NPM,NRTE)

j = (T,NPM,NRTE)

k = (NPM,NRTE)

1 = cal/gmole

2 = cal/gmole-°K

3 = gmole/cc

4 = atm

5 = °K

6 = cal/cm-sec°K

7 = centipoise

8 = cc/gmole

9 = g/gmole

10 = cm^2/sec

TABLE 1 continued

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
1	Enthalpy, Pure gases		HG			a,1	
		'IDEAL'	HG1	DHG	5		Assume ideal gas
		'NONIDEAL'	HG2	HG1 DHGR	1 6		Use nonideal gas departure function for nonideality
2	Enthalpy, gas mixtures		HGM			b,1	
		'IDEA1'	HGM1	DHGM	7		Assume ideal gas mixture
		'NONIDEAL'	HGM2	HGM1 DHGMR	2 8		Uses nonideal gas mixtures departure function term for nonideality
3	Enthalpy, Pure liquids		HL			a,1	
		'IDEAL'	HL1	HG HVV	1 42		Difference between gas enthalpy and heat of vaporization
		'HEAT CAPACITY'	HL2				Integrate the liquid heat capacity eq.
		'NONIDEAL'	HL3				Use the liquid-ideal gas departure function
4.	Enthalpy, Liquid Mixtures		HLM			b,1	
		'IDEA1 SOLUTION'	HLM1	HVV HGM	42 2		Assume ideal solution
		'NONIDEAL SOLUTION'	HLM2	PVAP HLM1 DHLM	29 4 10		Includes enthalpy of

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
		'AMAGAT'	HLM3	HL	3		Use Amagat's Law in Summation of enthalpy of each pure component
5	Enthalpy Deviation from standard state, ideal gases		DHG			a,1	
		'STANDARD CP'	DHG1	CPG	21		Assume ideal gases, standard state & constant cp.
		'INTEGRATED CP'	DHG2				Assume ideal gases, standard state and integrated cp. equation
6	Enthalpy departure from ideal gas, pure gases		DHGR			a,1	
		'REDLICH KWONG'	DHGR1				Uses Redlich Kwong equation of state
7	Enthalpy Deviation from standard state, ideal gas mixtures		DHGM			b,1	
		'AMAGAT'	DHGM1	DHG	5		Use Amagat's slow in summation of the enthalpy deviations of each component
8	Enthalpy departure from ideal gas mixtures, gas mixtures		DHGMR			b,k	
		'REDLICH KWONG'	DHGMR1				Uses Redlich-Kwong Equation of State

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
9	Enthalpy Deviation from liquids at standard temperature, Pure Liquids		DHL			a,1	
		'STERNLING BROWN'	DHL1	DHG	5		For pure Liquids, using the Sternling-Brown's heat capacity equation.
10	Enthalpy Deviation from liquid mixtures at standard temperature, Liquid Mixtures						
		'CHAO SEADER'	DHLM1	DGAM DFPL	35 33		For nonideal liquid mixtures, using 'Chao Seader' method.
11	Enthalpy Departure from ideal gas state, pure liquids		DHLG			a,1	
		'ERBAR SATURATED'	DHLG1				uses ERBAR, Persyn& method for saturated liq.
		'YEN SUBCOOLED'	DHLG2				Uses the Yen and Alexeander method for subcooled liquid

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
12.	Entropy, Pure gases		SG			a,2	
		'IDEAL'	SG1	DSG	16		Assume ideal gas
		'NONIDEAL'	SG2	SG1 DSGR	12 17		nonideal gas entropy departure function as a correction term for nonideality
13.	Entropy, gas mixtures		SGM			b,2	
		'IDEAL'	SGM1	SG	12		Assume ideal gas mixtures
		'NONIDEAL'	SGM2	SGM1 DSGHR	13 18		Using nonideal gas entropy departure from ideal gas mixtures as correction term for nonideality
14.	Entropy, Pure liquids		SL			a,2	
		'IDEAL '	SL1	SG DSL	12 19		Assume ideal liquid
15	Entropy, Liquid Mixtures		SLM			b,2	
		'IDEAL SOLUTION'	SLM1	SL	14		Assume ideal solution
		'NONIDEAL SOLUTION '	SLM2	SLM1 DSLMR	15 20		Uses the Hildebrand method as correction term for entropy of mixing

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
12.	Entropy, Pure gases		SG			a,2	
		'IDEAL'	SG1	DSG	16		Assume ideal gas
		'NONIDEAL'	SG2	SG1 DSGR	12 17		nonideal gas entropy departure function as a correction term for nonideality
13.	Entropy, gas mixtures		SGM			b,2	
		'IDEAL'	SGM1	SG	12		Assume ideal gas mixtures
		'NONIDEAL'	SGM2	SGM1 DSGHR	13 18		Using nonideal gas entropy departure from ideal gas mixtures as correction term for nonideality
14.	Entropy, Pure liquids		SL			a,2	
		'IDEAL'	SL1	SG DSL	12 19		Assume ideal liquid
15	Entropy, Liquid Mixtures		SLM			b,2	
		'IDEAL SOLUTION'	SLM1	SL	14		Assume ideal solution
		'NONIDEAL SOLUTION'	SLM2	SLM1 DSLMR	15 20		Uses the Hildebrand method as correction term for entropy of mixing

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
16	Entropy Deviation from the standard state, ideal gases		DSG			a,2	
		'HEAT CAPACITY'	DSG1	CPG	21		Assumes constant ideal gas heat capacity at standard state.
		'INTEGRATION'	DSG2				Integrates ideal gas heat capacity equation
17	Entropy departure from ideal gases, pure gases		DSGR			a,2	
		'S H F/P RELATION'	DSGR1	DHG FPG	5 30		Using entropy - Enthalpy-Fugacity coefficient Relation
		'REDLICH KWONG'	DSGR2				Using Redlich - Kwong Equation of state in nonideal gas entropy departure function
18	Entropy departure from ideal gas mixtures, gas mixtures		DSGMR			b,2	
		'S H F/P RELATION'	DSGMR1	FPGM DHGM	31 7		Using entropy, enthalpy and fugacity coefficient relation.
		'REDLICH KWONG'	DSGMR2				Using 'Redlich Kwong' Equation of state in nonideal gas mixtures entropy departure function

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
19	Entropy deviation from liquid at standard state, pure liquids		DSL			a,2	
		'STANDARD CPL'	DSL1	CPL	23		Assume constant liquid Heat capacity at standard state.
		'STERNLING BROWN'	DSL2				Integrating the Sternling Brown liquid heat capacity equation.
20	Entropy of mixing, liquid mixtures		DSLMR			b,2	
		'HILDEBRAND'	DSLMR1	GAMMAF FPL DFPL DGAM	34 32 33 35		Use the Hildebrand's method as described by Chao & Seader

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
21	Heat Capacity, pure gases		CPG			a,2	
		'IDEAL GAS AT SS'	CPG1				for ideal gas at standard state
		'IDEAL GAS AT T'	CPG2				For ideal gas at T
22	Heat Capacity, gas mixtures		CPGM			b,2	
		'AMAGAT'	CPGM1	CPG	21		using AMAGAT's LAW in Summation of each component's gas heat capacity
23	Heat Capacity, Pure Liquids		CPL			a,2	
		'DELTA H'	CPL1	HL	3		Difference of liquid enthalpy.
		'STERNLING BROWN'	CPL2	CPG	21		Using Sternling Brown Equation for liquid heat capacity
24	Heat capacity, Liquid Mixture		CPLM			b,2	
		'AMAGAT'	CPLM1	CPL	23		Using AMAGAT's LAW in summation of each component's liquid heat capacity.

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
25	Density, pure gases		RHOG			a,3	
		'IDEAL GAS'	RHOG1				Assume ideal gas
		'REDLICH KWONG'	RHOG2				Using Redlich - Kwong's Equation of state in calculating compressibility
26	Density, gas mixtures		RHOGM			b,3	
		'IDEAL GAS'	RHOGM1				Assume ideal gas mixtures
		'REDLICH KWONG'	RHOGM2				Using Redlich - Kwong's Equation of state in calculating the mixtures compressibility.
27	Density, Pure Liquids		RHOL			a,3	
		'GOLDHAMMER'	RHOL1	RHOG	25		Gold Hammer's correlation
		'YEN AND WOODS SATURATED'	RHOL2				Assumes saturated liquid, using Yen and WOODS Method
		'YEN AND WOODS COMPRESSED'	RHOL3	PVAP RHOL2	29 27		Assumes compressed liquid using YEN and WOODS method.

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
28	Density, liquid mixtures		RHOLM			b,3	
		'IDEAL SOLUTION'	RHOLM1	RHOL	27		Assume ideal solution using Amagat's Law in summation of each component's liquid density.
		'YEN AND WOODS COMPRESSED'	RHOLM2	TCC PCC ZCC VCC	60 61 63 62		Using Yen and Woods Method for compressed liquid mixtures

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
29	Vapor Pressure pure component		PVAP			d,4	
		'ANTOINE'	PVAP1				Using ANTOINE's vapor-pressure equation.
		'HARLACHER'	PVAP2	Tolerance Iteration			Using Harlacher's correlation
30	Fugacity Coefficient, pure gases		FPG			a	
		'IDEAL'	FPG1				Assume ideal gas
		'REDLICH KWONG'	FPG2				Using Redlich-Kwong's Equation of state
31	Fugacity Coefficient, Ith component in gas mixtures		FPGM			c	
		'IDEAL'	FPGM1				Assume ideal gases
		'REDLICH KWONG'	FPGM2				Using Redlich-Kwong's Equation of State
32	Fugacity Coefficient, pure liquids at reference state		FPL			a	
		'IDEAL SOLUTION'	FPL1	PVAP	29		Assume ideal solution
		'CHAO SEADER'	FPL2				Using Chao Seader method for general compounds except H_2, N_2, CO, and CH_4
		'CH4 CHAO SEADER'	FPL3				Using Chao Seader method for CH_4
		'CO CHAO SEADER'	FPL4				Use Chao Seader method for CO

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
		'H CHAO SEADER'	FPL5				Use Chao Seader Method for H_2
		'N CHAO SEADER'	FPL6				Use Chao Seader Method for N_2
33	Derivative of the ln of the liquid fugacity coefficient with respect to temperature		DFPL			a	
		'CHAO SEADER'	DPFL1				Using Chao Seader's Method
34	Activity Coefficient, component in liquid mixtures		GAMMAF			c	
		'IDEAL SOLUTION'	GAMMA1				Assume ideal solution
		'CHAO SEADER'	GAMMA2	RHOL	27		Using Chao Seader's Method
35	Derivative of the ln of the activity coefficients with respect to temperature		DGAM			c	
		'INTERPOLATE'	DGAM1	GAMMAF	34		By interpolating the activity coefficients between 10°K interval
36	Phase Equilibrium constant, of component in mixture		EQKGL			c	
		'IDEAL'	EQKGL1	PVAP	29		Assume ideal behavior
		'NONIDEAL'	EQKGL2	FPL GAMMAF FPGM	32 34 31		Use the thermodynamic relation between fugacity and activity coefficients

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
37	Heat of vaporization, pure liquid		HVV			a,1	
		'STANDARD'	HVV1				Standard state heat of vaporization
		'WATSON'	HVV2				Using Watson's Method
38	Boiling temperature		TBB			h,5	
		'ANTOINE'	TBB1				Using Antoine's vapor-pressure Equation
39	Bubble point, temperature		TBBL			i,5	
		'HALF'	TBBL1	TBB EQKGL TOLERANCE	37 36		Using subroutine HALF to find root of $f(TBBL) = (1 - \sum_{i=1}^{W} x_i * EQKGL_i) = 0$
40	Bubble point, pressure		PBBL			j,4	
		'HALF'	PBBL1	PVAP EQKGL TOLERANCE	29 36		Using subroutine HALF to find root of $f.(PBBL) = (1 - \sum_{i=1}^{W} x_i * EQKGL_i) = 0$
41	Dew Point, Temperature		TDEW			i,5	
		'HALF'	TDEW1	TBB EQKGL TOLERANCE	37 36		Using subroutine HALF to find root of $f(TDEW) = (1 - \sum_{i=1}^{W} x_i / EQKGL_i) = 0$

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
42	Dew Point, Pressure		PDEW			j,4	
		'HALF'	PDEW1	PVAP EQKGL TOLERANCE	29 36		Using subroutine HALF to find root of f(PDEW) = $(1 - \sum_{i=1}^{W} x_i / EQKGL_i) = 0$

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
43	Temperature of gas mixture (given enthalpy)		THGM			e,5	
		'STANDARD'	THGM1	CPGM	22		Assumes constant standard state gas mixtures heat capacity
		'NEWTON'	THGM2	HGM CPGM	2 22		Iteration using Newton-Ralphson Method
44	Temperature of liquid mixture (given enthalpy)		THLM			e,5	
		'STANDARD'	THLM1	CPLM	24		Assumes constant standard state liquid mixture heat capacity
		'NEWTON'	THLM2	HLM CPLM	4 24		Iteration using Newton-Ralphson Method
45	Temperature of gas mixture (given enthalpy)		TSGM			f,5	
		'STANDARD'	TSGM1	CPGM	22		Assume constant standard state gas mixture heat capacity
		'NEWTON	TSGM2	SGM CPGM	13 22		Iteration using Newton-Ralphson Method
46	Pressure of gas mixture (given entropy)		PSGM			g,4	
		'STANDARD'	PSGM1	SGM	13		Assumes ideal gas mixture pressure deviation

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
47	Temperature of liquid mixture (given entropy)		TSLM			f,5	
		'STANDARD'	TSLM1	CPG HVV CPLM	21 42 24		Assumes constant standard state heat capacity of gas and liquid mixtures, and heat of vaporization
		'NEWTON'	TSLM2	SLM CPLM	15 24		Iteration using Newton Ralphson Method

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
48	Viscosity, pure gas		VISG			a,7	
		'HIRSCHFELDER'	VISG1				Using Hirschfelder, Bird, and Spotz's Equation.
		'NON-POLAR'	VISG2				For low pressure, non-polar gases, using Stiel and Thodos' Method
		'POLAR NO H BONDS'	VISG3				For low pressure gases, polar, no hydrogen bonding. Stiel & Thodos' Method
		'POLAR H BONDS'	VISG4				Polar gases with hydrogen bonding. Stiel & Thodos' Method
49	Viscosity, gas mixtures		VISGM			b,7	
		'LOW PRESSURE'	VISGM1	VISG	48		For low pressure gas mixtures, using Wilke Estimation Method
		'HIGH PRESSURE'	VISGM2	TCC PCC VCC RHOGM VISGM1	60 61 62 26 49		For non-polar gas mixtures at high-pressure. Using Dean & Stiel's Method

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
50	Viscosity, pure liquid		VISL			a,7	
		'VAN VELZEN'	VISL1				Using Van Velzen, Cardozo, and Langenkamp's Method
51	Viscosity, liquid mixtures		VISLM			b,7	
		'AMAGAT'	VISLM1	VISL	50		Using Amagat's Law to sum the function of VISL; funct. = ln (VISL)

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
52	Thermal conductivity of pure gas		TKG			a,6	
		'EUCKEN'	TKG1	VISG CPG	48 21		Uses Eucken correlation
		'MISIC-THODOS HC'	TKG2	CPG	21		Misic-Thodos correlation for hydrocarbons
		'MISIC-THODOS NONHC'	TKG3	CPG	21		Misic-Thodos correlation for non-hydrocarbons
		'STIEL-THODOS'	TKG4	RHOG TKG1	25 52		Stiel-Thodos pressure correction correlation
53	Thermal conductivity of gas mixture		TKGM			b,6	
		'MASON SAXENA'	TKGM1	VISG TKG	48 52		Mason-Saxena modification of Wassiljewa equation
		'LINDSAY NONPOLAR'	TKGM2	VISG TKG	48 52		Lindsay-Bromley modification for nonpolar gas mixture
		'LINDSAY POLAR'	TKGM3	VISG TKG	48 52		Lindsay-Bromley modification for mixtures of gases with polar components
		'STIEL-THODOS'	TKGM4	RHOGM TKGM1	26 53		Stiel-Thodos pressure correction correlation

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
54	Thermal conductivity of pure liquid		TKL			a,6	
		'SATO-RIEDEL'	TKL1				Sato-Riedel correlation
55	Thermal conductivity of liquid mixture		TKLM			b,6	
		'AMAGAT'	TKLM1	TKL	54		Uses Amagat's rule of mixing

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
56	Diffusion coefficient, self diffusivity, pure gases		DIFG			a,9	
		'IDEAL'	DIFG1				Assume ideal gas law in Chapman and Enskog Equation
57	Diffusion coefficient, component in gas mixtures		DIFGM			c,9	
		'BLANC'	DIFGM1				Apply to a trace of a component in a homogeneous gas mixture, using Blanc's law
58	Diffusion coefficient, self diffusivity of liquid		DIFL			a,9	
		'SCHEIBEL'	DIFL1	VISL RHOL	50 27		Using Schiebel, Wilke, Chang modified equation
59	Diffusion coefficient, component in liquid mixture		DIFLM				
		'PERKINS'	DIFLM1	RHOL VISL VISLM	27 50 51		For dilute solution using Perkins and Geankoplis Equation

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
60	Pseudocritical temperature of a mixture		TCC			k,5	
		'KAY'	TCC1				Uses Kay method
		'JOFFE S B V'	TCC2				Uses Joffe-Stewart-Burkhardt-Voo rule
61	Pseudocritical pressure of a mixture		PCC			k,4	
		'KAY'	PCC1				Uses Kay Method
		'PRAUSNITZ GUNN'	PCC2				Uses method of Prausnitz and Gunn
		'JOFFE S B V'	PCC3				Uses Joffe-Stewart-Burkhardt-Voo rule
62	Pseudocritical volume of a mixture		VCC			k,8	
		'KAY'	VCC1				Uses Kay Method
		'EQUATION OF STATE'	VCC2	ZCC TCC PCC	63 60 61		Uses equation of state V = ZRT/P
63	Psuedocritical compressibility of a mixture		ZCC			k	
		'KAY'	ZCC1				Uses Kay Method
		'JOFFE S B V'	ZCC2				Uses Joffe-Stewart-Burkhardt-Voo rule
64	Pseudocritical Pitzers accentric factor of a mixture		OMM			k	
		'KAY'	OMM1				Uses Kay Method

MODULE #	PROPERTY MODULE	CODES FOR METHODS	FUNCTIONAL NAME	SUBORDINATE PROPERTIES NEEDED & ITS MODULE #		ARGUMENT & UNITS	DESCRIPTION
65	Average molecular weight of a mixture		AMWT			k,9	
		'AVERAGE'	AMWT1				Calculates weighted average of molecular weight of mixtures

Submodule calls on the other method directly since FORTRAN does not allow it to call the operation subroutine of the same module. Therefore we made an exception that a Method Submodule may call directly on another Method Submodule within the same module.

2. Modules to Compute Properties of Coal

The approach in developing the coal property modules is analogous to that used for properties of gases and liquids. Coal is treated as a heterogeneous mixture of constituents such as ash, primary and secondary volatile matter, fixed carbon, nitrogen and sulfur.

To calculate a property of coal, one uses a statement of the form

RESULT = PROP (T, P, NPCL, NRTE)

where T and P are the temperature and pressure and NRTE is the pointer to the route; these are the same as their counterparts for properties of gases and liquids.

NPCL is a pointer to the coal data plex. Its structure is shown in Figure 4. The Coal Analysis Bead contains the percent composition and other data, e.g., the proximate and ultimate analyses, which is unique for each coal. This is similar to the Mole Fraction Bead for gas-liquid Property Coal. The Data Identification Bead is also similar to its counterpart in the plex. Each location of this bead contains a pointer to a bead containing the correlation coefficients and specific data constants for the constituents of coal (e.g., ash, primary and secondary volatile matter, fixed carbon and coal as a whole). The user has the flexibility of choosing the source of these constants. Entries in the Coal Analysis Bead and the Coal Data Identification Bead

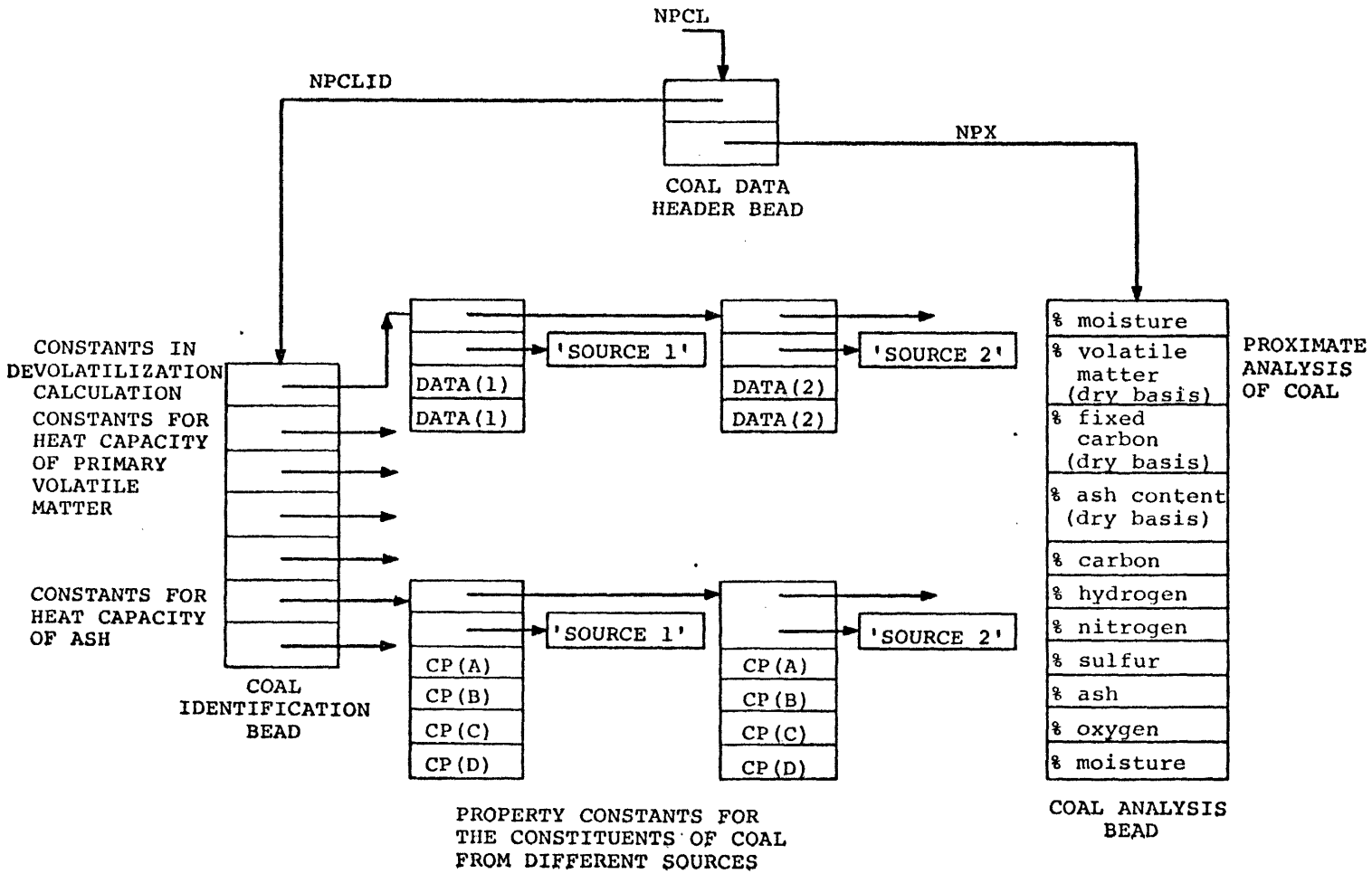

Figure 4. Coal Data Plex

are referred to by name, therefore the length of these two beads are not fixed.

With this data structure, we start organizing the property modules for heat capacity. There is a distinction between specific heat capacity at temperature T and mean heat capacity between temperatures T (reference) and T. To estimate a property based on original analysis, we have to take into account the effect of devolatilization. There are correlations for estimating the amount of volatile matter (VM) present in coal as a function of T. We have used a function similar to the Gregory and Littljohn correlation presented in the IGT report (May, 1976).

The heat capacity of coal can be calculated by summing the contribution from ash, fixed-carbon (FC) and volatile matter (VM), or by direct correlation. We do not include moisture in the calculation, i.e., the property estimations are on a dry basis. The properties of each component in coal (ash, FC, VM) can be estimated by the correlation constants in the Coal Data Identification Bead. This means that the property of each component is independent of the type of coal. But since we provide the flexibility of choosing the source, the user can indicate the source applicable to any specific coal for estimation of each component's property if those data are available (either proprietary or public). Different models for the process of devolatilization can also be added to each module.

Table 2 lists the coal property modules in the PLEXSYS system.

Property Module	Method Submodule Available or (Arguments)	Calling Code or (Units)	Other Property Module Called	Description of Module or Method Used
CPASH	(T,P,NPC,NRTE)	(Cal/g K)		Heat capacity of ash
	CPASH1	'SPECIFIC'		Specific heat capacity of T°C by polynomial equation.
	CPASH2	'MEAN'		Mean heat capacity between 0 and T°C by polynomical equation
CPFC	(T,P,NPC,NRTE)	(Cal/g K)		Heat capacity of fixed carbon
	CPFC1	'SPECIFIC'		
	CPFC2	'MEAN'		
CPVM	(T,P,NPC,NRTE)	(Cal/g K)		Heat capacity of volatile matter
	CPVM1	'SPECIFIC'	VMT	
	CPVM2	'MEAN	VMT	
	CPVM4	'GREGORY'		Mean heat, capacity between 0 and T°C using Gregory and Littlejohn percent volatile matter correlation
	CPVM3	'MEAN NODEVOLAT IL'		Mean heat capacity between 0 and T°C assuming no devolatilization
CPCOAL	(T,P,NPC,NRTE)	(Cal/g K)		Heat capacity of coal
	CPCOL1	'SPECIFIC'		
	CPCOL2	'MEAN'		
	CPCOL3	'SUMMATION'	CPASH CPFC CPVM VMT	Summation of CP for all components.

TABLE B.2 List of Coal Property Modules

Property Module	Method Submodule Available or (Arguments)	Calling Code or (Units)	Other Property Module Called	Description of Module or Method Used
TVM	(P,NPC,NRTE)	(K)		Temperature which devolitilization commences
	TVM1	'GREGORY'		Use Gregory and Littlejohn correlation
	TVM2	'ARBITRARY'		Arbitrary function to indicate no devolatilization
VMT	(T,NPC,NRTE)			Minimum percent volatile matter presence in coal at T
	VMT1	'GREGORY'		Use Gregory and Littlejohn correlation
	VMT2	'ARBITRARY'		Arbitrary function to indicate no devolatilization.

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