U.S. Energy Research & Development Administration

Materials—Process—Product Model Analysis of Coal Processing Technology

Phase I Final Report

MASTER

February 1976

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Materials—Process—Product Analysis of Coal Process Technology

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FINAL REPORT FOR PROJECT PHASE I

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GLOSSARY

Functional Module -

An operation on a raw material or an intermediate material that transforms it into an end product or another intermediate material.

Unit-Process Route -

A series of functional modules that form a path leading from a marketable raw material to a marketable product. (There are a multitude of unit processes for each unit-process route, each corresponding to a specific set of competing configurations of the functional modules.)

Road Map -

The fold-out at the rear of this report that shows functional modules and unit-process routes from coal to salable products.

Competing Configuration or Configuration -

A collection of equipment that is capable of performing a Functional Module operation.

Economic Unit Process or Unit Process -

A series of configurations which inputs a marketable raw material and outputs a marketable product. Each configuration is taken from a succeeding functional module along a unit process route. The unit process is the smallest manufacturing entity for which economic records are normally kept, i.e. records of investment cost, operating costs, raw material cost, sale prices of products, and profits.

Process Chain -

A series connection of two or more economic unit processes. For example, one unit process would convert coal to a clean solid fuel, and a second would convert this solid fuel to electrical energy. The series connection of the two unit processes is a process chain for converting coal to electrical energy.

Linking Model (LM) -

The algorithmic structure that assembles feasible unit processes from competing configurations within a unit process route.

Process Chain Evaluation Model (PCEM) -

The algorithmic structure that evaluates the costs and process residuals of unit processes

Industry Development Model (IDM) -

The algorithmic structure that evaluates cumulative effects of industry development scenarios and strategies.

EXECUTIVE SUMMARY

1. BACKGROUND

The purpose of materials-process-product analysis is systematic evaluation of alternative manufacturing processes--in this case processes for converting coal into energy and material products that can supplement or replace petroleum based products in current use. The methodological steps in the analysis include

- definition of functional operations that enter into coal conversion processes, and modeling of alternative, competing methods to accomplish these functions.
- compilation of all the feasible conversion processes that can be assembled from combinations of competing methods for the functional operations.
- systematic, iterative evaluation of all feasible conversion processes under a variety of economic situations, environmental constraints, and projected technological advances.
- aggregative assessments (economic and environmental) of various industrial development scenarios.

The materials-process-product methodology was previously developed by IR&T under an NSF grant, and applied to a segment of the chemical industry. An integral part of the present project is additional development of the existing computer model, the Materials-Process-Product Model (MPPM), to include

- a data base for coal-related materials and coal conversion processes.
- an algorithmic structure that facilitates the iterative, systematic evaluations in response to exogenously specified variables, such as tax policy, environmental limitations, and changes in process technology and costs.

As an analytical tool, the MPPM is intended to satisfy the needs of an analyst working at the process selection level of detail. At this level engineering design and costing models are too detailed and time consuming, while large scale energy/economic models do not reveal the nature of the process-related tradeoffs. In the case of coal process technology, many processes of interest are in embryo, pre-commercialization stages of development. The interests of the Fossil Energy Branch, ERDA, the sponsor of this contract, center on allocation of RD&D funds to competing technologies. Construction of an MPPM attuned to the specific interests of the sponsor is the goal of this contract.

The MPPM establishes comparative valuations for each of the processes it considers. Since the economic data on competing configurations is continually evolving, relative comparisons of processes must be considered in terms of broad bands of uncertainty. Nevertheless, the more promising possibilities can be identified and subjected to more detailed appraisal. Such comparative evaluations, on a consistent basis, form an essential input to assessing the economic implications of coal RD&D strategies.

The project has been designed to proceed in three phases. In the first phase, just completed, work has centered on bounding the areas of technology to be modeled, defining the specific level of detail appropriate to analyses that will aid the sponsor in the allocation of RD&D funds, and indicating the feasibility of adapting the materials-process-product analytical method to the new and evolving technology of coal conversion. In Phase I we accomplished these tasks and defined a Phase II program that provides for delivery of an operational, validated MPPM to the sponsor. The development sequence will be to first establish a prototype Model A version of the MPPM that is operational but limited in scope. Model A will be followed by a broadening and deepening of the data base until all important (as presently perceived) technologies are included. Phase III of the project will establish the necessary interrelationships for cooperative use of the MPPM with the large energy/economic computer models now extant.

2. PROGRAM OBJECTIVES

Six specific objectives have been defined to implement the overall goal of constructing an MPPM as a useful tool in the analysis and evaluation of coal process technologies. These are

- (1) Extend the existing Materials-Process-Product Model to accomodate coal-process technology at an appropriate level of detail, i.e., at the "functional module" level.*
- (2) Assemble a data-base on coal-process technology in a format compatible with the MPPM.
- (3) Utilize the MPPM to construct a library of feasible "economic-unit processes" from the collections of "competing configurations" filed under each "functional module"
- (4) Use the MPPM to evaluate the "economic-unit processes" in the context of an exogenously specified economic and regulatory environment.
- (5) Conduct sensitivity analyses of these evaluations for perturbations in the exogenously specified variables, and for uncertainties in process data.
- (6) Conduct policy scenario evaluations within an enlarged energy/economic context using both the MPPM and other large scale computer models such as the ESNS** and BESOM*** models of the Brookhaven National Laboratory or the SEAS+ model developed by the Environmental Protection Agency.

* We use a specific terminology in materials-product-process analysis that includes some terms not used in conventional engineering or economic literature. These are defined in the glossary and discussed in Section 1.3. of the report. These terms are shown in quotes above.

** ESNS = Energy System Network Simulator

*** BESOM = Brookhaven Energy System Optimization Model

+ SEAS = Strategic Environmental Assessment System

The first of these objectives is clearly the critical step to the success of the project, since all succeeding objectives depend upon it. A major part of the effort in Phase I has been to discover the appropriate level of detail, to enumerate and specify a set of desired end-products, to define the necessary extensions to the MPPM, and to construct the critical "Linking Model" algorithm that connects functional module configurations together to form feasible economic unit processes.

The second objective, collection of an appropriate data base, is not so straightforward as it might appear. A considerable effort will be required to insure that engineering and cost data derived from a wide range of sources are compatible. This includes recognition, by engineering analysis, of the significant external parameters that determine the cost of a configuration, and use of a reasonably uniform costing methodology. To demonstrate the feasibility of assembling data in the required form, some example cases of configuration data files were assembled in Phase I.

The other objectives relate to the use of the MPPM. Clearly a certain minimum level of development is required before they can be addressed. The MPPM will be tested against each of these objectives as soon as algorithmic development and data collection warrant.

3. METHODOLOGY AND PHASE I RESULTS

● Bounding the Problem

In accord with the sponsor's needs, this project encompasses the full range of processes for converting coal into useful products. To select processes, one must first define the products desired. A set of coal-derived products has been identified. These products are listed in Table 1,* within three categories--energy products, material products, and byproducts. The materials products are probably of greatest interest at the moment, because they offer to offset the anticipated shortfall

*Tables are placed at the end of the Executive Summary.

in meeting our requirements for gaseous and liquid fuels and petrochemical feedstocks. A significant advance in technology for coal gasification and liquefactions is required, however, before the promise of large quantities of such gaseous and liquid products can be fulfilled. The need for monitoring the evolution of this process technology is great. Hence the emphasis at the beginning of Phase II will be on the material products. The data base for processes leading to energy products will be developed after the data base for material products is established.

As part of the Phase I effort, a set of "Proposed Product Specifications" were developed for seven of the material products considered of greatest interest. The products are SNG, Medium-BTU gas, low-BTU gas, clean liquid boiler fuel, clean solid boiler fuel, low molecular weight gaseous hydrocarbon mixtures, and middle distillate oil. Their specifications are given in Appendix A. They are written in a form that facilitates their use in MPPM evaluations. Product specifications will be developed for other materials during Phase II as the need arises. Likewise, as new technology develops, new coal-derived products of importance may appear. The MPPM should not be regarded as a fixed structure with respect to either products or processes. The MPPM must be continually evolving in both structure and richness of data in response to an ever changing perception of where coal process technology is heading.

It is necessary at this point to consider several aspects of MPPM terminology. The evaluations to be made by the MPPM will be at what is termed the economic unit process (or unit process) level. *Unit processes* are defined to be the smallest sets of equipment that start with marketable commodities as raw materials and end with marketable products. For example, coal to SNG is a unit process, while coal drying is not. Each unit process consists of a number of discrete steps, such as shift conversion, methanation, etc. The equipment involved in accomplishing each step is said to compose a *functional module*. There are usually a number of different ways, or *competing configurations*, for

performing the functional step. The general path along functional modules from raw materials to product is termed a *unit process route*. In this context, each *unit process* represents a specific set of competing configurations along the unit process route.

The totality of equipment possibilities now being used, or being conceived for use, in coal conversion processes is enormous. Process equipment have been selected for inclusion within the MPPM data base using three criteria: (1) those for which ERDA is providing the development funds, (2) those that seem to be attracting serious financial support from commercial sources, and (3) those that are already contributing to the conversion of coal into marketable energy products. A systematic review of coal processes using these criteria led to the identification of 42 functional modules. These are identified, within the context of their participation in unit process routes, in a separate "Road Map" foldout contained in the pocket at the back of this report. This Road Map consolidates the flow scheme for all reviewed coal processes into the MPPM format. It is estimated that more than one-half million unit process possibilities are represented on the Road Map. The function of the MPPM is to identify which of these potential unit processes are physically feasible, and to evaluate their comparative economics so that the most promising opportunities can be discerned.

Several hundred competing configurations were identified as participants within the 42 coal-based functional modules. These competing configurations are listed within module groups in Appendix B. One hundred twelve of the most interesting configurations were selected for inclusion within the MPPM data base. These are listed in Table 2 within two classes--first generation and advanced. First generation processes are those that have either become state-of-the-art or have reached the pilot plant demonstration phase with promising results. Configurations marked by a * will be included within a prototype Model A version of the MPPM to be developed and tested during the first nine months of Phase II. This model will act as a large-scale feasibility demonstration for the MPPM approach to analysis of coal processes.

- Data Base Requirements

A performance data set is required for each competing configuration associated with a functional module. The data set requirements are:

- Input-output materials balance relationships and restrictions
- Net utility requirements (electricity, fuel, steam, and cooling water)
- Capital cost data
- Operating cost data

The data must be expressed in a form that permits computation of configuration costs, utility requirements, and material balance as a function of throughput (amount of primary product made by the configuration per unit time) and other pertinent parameters, such as the pressure and composition of input gases, etc. The standard format file will consist of: descriptive title, description of the primary input and output materials, list of process parameter values for a nominal design with scaling factors that enable cost computations for other throughput and design parameter values, and list of materials and utility inputs and outputs at the nominal design conditions. Materials are classified into eight categories on the basis of their role--primary raw materials, liquid wastes, etc. A separate file of materials data is maintained that includes numerical designation, descriptive name, chemical name, chemical and physical properties, and market values.

An important aspect of data base construction is consistency. Design data from different organizations must be checked as to their cost basis. Surprisingly large variations can be found in the costs assigned to rather common items of equipment, such as compressors and pressure vessels. These hidden cost variations could, if not recognized and corrected, undercut attempts to fairly compare competing unit processes. The ability of the MPPM to use a carefully prepared data base to provide consistent process comparisons is a great asset.

The development of a competing configuration description was demonstrated during Phase I by the establishment of such a description for three of the five apparently viable alternative methanator configurations. Overall configuration costs were determined as a function of throughput, input gas pressure, and input material composition. A complete discussion of the methanator configuration descriptions development is provided in Section 3.1.3. of the main body of this report.

- Linking Model

The Linking Model (LM) is the first of three major components within the MPPM. The LM identifies which of the multitude of combinationally possible unit processes that could be formed from the competing configurations are physically feasible. It does this by working backward from the designated product, such as SNG, through the functional modules along the unit process routes shown on the Road Map until the basic input material, coal, is reached. At each step, each of the potential competing configurations is assessed. Acceptability depends upon the output of that configuration being able to satisfy the input requirements of the already specified downstream configuration. In this way, all configurations that might participate in unit processes are evaluated in turn. A complexity in these evaluations is that frequently the output characteristics of a configuration may depend upon the nature of preceding (or upstream) configurations that have yet to be assessed. In such a case, the configuration's characteristics are left unspecified until the upstream configuration is reached, then the entire sequence to that point is jointly assessed.

- Process Chain Evaluation Model

The Linking Model identifies the feasible unit processes and stores them in a library file. It does not attempt to establish their value. Valuation is the role of the second major component of the MPPM-- the Process Chain Evaluation Model (PCEM). The PCEM itself consists of

a set of four components--Sizer, Gross Coster, Residuals Evaluator, and Net Coster. The Sizer establishes the quantitative matching between the unit process' participating configurations so that internally consistent overall material balance and utility requirements can be determined. The Gross Coster establishes the value added for the unit process by annualizing investment and operating costs. The unit process costs are obtained using the cost scaling parameters of each configuration, and summing over all configurations included in the unit process. The Residuals Evaluator calculates aggregate unit process waste releases and waste treatment costs. The Net Coster computes realistic product sales prices. It does this by applying to the Gross Coster results exogenous charges, such as corporate income taxes, investment tax credit, value added taxes, effluent charges, efficiency surcharges, and payroll taxes.

Through its four subprograms the PCEM establishes comparative valuations for each of the unit processes. Since the quantities of residual environmental pollutants are determined for each process, environmental effects can be appraised and incorporated into the process evaluations.

- Industry Development Model

The Industry Development Model (IDM) is the third and final major component of the MPPM. The IDM keeps track of the cumulative implications in bringing coal conversion capacity onstream. Process selection criteria are applied to the PCEM-evaluated unit processes, the processes are chosen on the basis of their timing for commercial availability, and the best set of processes is designated to accomplish an exogenously specified development schedule. The IDM compiles the composite industry product spectrum--SNG, coal liquids, electricity, wastes, etc.--for its chosen set of processes and compiles the related requirements for capital, labor, and raw materials. In effect, the IDM performs a bookkeeping role in aggregating into an overall result the individual requirements and contributions from a selected set of individual unit processes.

● Policy Analysis

Development and utilization considerations are inseparably intertwined for any technology. This is particularly true for coal processes since they are expected to replace existing energy processes in a timely and compatible fashion. To the extent that they do not, economic dislocations will occur among the end user community. Participation of the government in deciding which aspects of coal process technology to emphasize is therefore extremely significant and will be subject to continuing review. Assessment of coal process R&D alternatives must be conducted in the presence of uncertainties as to the timing, level of demand, and product composition for coal-derived products. In addition, the technology of the processes themselves is continually changing, and alternative approaches are being simultaneously pursued. The goal of the coal-based MPPM is to organize the data for the coal processes so that it includes latest technological developments and it can be easily assessed in a form compatible with policy analyses. The MPPM system will be a comprehensive model of RD&D alternatives which can be sorted and selected in terms of policy criteria. In Phase III, the MPPM will be utilized in this way in conjunction with selected economic and energy computer models to evaluate coal process RD&D alternatives within the context of the nation's overall energy development path. For this purpose, a comprehensive review of other economic/energy models was conducted during Phase I, and their potential for joint evaluations with the MPPM identified. The role of these computational models in energy supply and demand assessments is schematically shown in a foldout contained at the back of this report. A narrative description of the models and their use with the MPPM is provided in Chapter 5. The Brookhaven Energy System being developed within ERDA provides the most likely path for relating MPPM results to general economic/energy models. These economic models provide projections for future economic sector energy demands.

The MPPM provides two types of coal process RD&D policy evaluations: aggregative assessments and sensitivity analyses. An example of an aggregative assessment is: "What are the aggregate

investment requirements, using the best available process, to produce middle distillate oil from coal by the amount required to meet 25% of 1990 U.S. residential heating demand?" An example of sensitivity analysis evaluations is: "What is the potential payoff in capital and operating cost benefits of a breakthrough in magneto-hydrodynamic technology?" The MPPM by itself can answer such questions.

Use of MPPM in conjunction with other energy/economic models enables an appraisal of broader policy problems. For instance, the scheduling of capital investments in coal liquefaction process plants will need to be assessed not only in terms of projected process availabilities and costs, but also in terms of the anticipated supply of domestic and imported petroleum, and oil derived from shale oil. Domestic energy demand projections as influenced by government policies toward conservation, mass transit, and taxes will also need to be included in overall assessments.

4. PLANS FOR PHASE II AND PHASE III

During the first nine months of Phase II a prototype version of MPPM will be developed that will include the Linking Model (LM) and the Process Chain Evaluation Model (PCEM) algorithmic structures as operating programs together with a data base of limited scope. The purpose of this initial effort is to bring a coal-based working model of the MPPM on line for experimentation. We call this prototype our "Model A". The product categories for the Model A prototype will be limited to the gaseous fuels derivable from coal (Low-BTU, Medium-BTU, and Substitute Natural Gas) plus on-site electric and mechanical energy, and appropriate by-products. A data base limited to fifteen (out of forty-two) functional modules and twenty-six competing configurations will be developed for Model A. The development of the algorithmic structure and production of working programs will be the major part of the Model A effort. MPPM capabilities using the Model A data base will be tested as development of the algorithmic structure allows, culminating in a "feasibility demonstration" six to eight months after the start of Phase II.

During the remainder of Phase II, the data base will be expanded to include all forty-two functional modules with over a hundred competing configurations. This data base will be sufficient to encompass all important (as presently perceived) conversion technologies. The full gamut of major products derivable from coal will be included from electric energy to the liquid hydrocarbons substitutable for petroleum products. For planning purposes a "Model B" of the MPPM, which will include about 75% of the ultimate Phase II data base and a working version of the Industry Development Model (IDM), is scheduled for completion and demonstration by the fourteenth month of Phase II. Of course, the MPPM data base should never be expected to be "complete". It will require continuous updating and revision as more methods of accomplishing functional operations are discovered and presently conceived methods are improved and brought closer to commercial application.

During the last six months of Phase II a computer support group will be brought into the project to help with final packaging of the MPPM into a maximally efficient computer program. This will include programming of data file maintenance routines (including programs for maintaining historical records), input-output routines with maximum operational flexibility, writing of user's manuals, and other documentation. This work will also include considerations of compatibility with other energy/economic models with which MPPM may be interfaced. At the end of Phase II, a completed model will be available to facilitate the computational work of Phase III.

Phase III of the project, scheduled to last for twelve months, is primarily concerned with the sixth objective listed in Section 2, namely use of the MPPM, alone and with other energy/economic models, to aid in policy analysis. The computer support group will play a major role during this phase in effecting the interface programming and inter-model data transfer procedures. A user's guide to integrated model use will be developed and a training program for ERDA personnel will be conducted. IR&T will work closely with ERDA to develop test scenarios, conduct tests of the model, and continue the work of keeping the MPPM data base up to date.

TABLE 1
PRODUCTS OF COAL PROCESSING TECHNOLOGY

A. ENERGY PRODUCTS

- o High Temperature Thermal Energy ($T \geq 400^\circ\text{F}$)
- o Low Temperature Thermal Energy ($T < 400^\circ\text{F}$)
- o Base/Intermediate Load Electric Energy
- o Peak Load Electric Energy
- o On-Site Electric (Mechanical) Energy

B. MATERIALS PRODUCTS

- o Low-BTU Gas*
- o Medium-BTU Gas*
- o Substitute Natural Gas (SNG)*
- o Anhydrous Ammonia
- o Methanol
- o Oxygenated Hydrocarbon Mixtures
- o Low Molecular Weight Gaseous Hydrocarbon Mixtures*
- o Aromatic Mixtures
- o Low Molecular Weight Liquid Hydrocarbon Mixtures
- o Middle Distillate Oils (Low Sulfur No. 2 Distillate Fuel Oil Equivalent)*
- o Clean Liquid Boiler Fuel (Low Sulfur Residual Oil Equivalent)*
- o Clean Solid Boiler Fuel*

C. BY-PRODUCTS

- o Sulfur/Sulfur Compounds
- o Ammonia/Ammonia Compounds
- o Aggregates
- o Gypsum
- o Argon
- o Nitrogen
- o Carbon Dioxide

*"Proposed Product Specifications" (PPS) for these materials products are given in Appendix A.

TABLE 2

First Generation and Advanced Configurations
to be Included in the MPPM Data Base

<u>Functional Module</u>	<u>First Generation</u>	<u>Advanced</u>
1. Low BTU Gasifier	1,A,1 Lurgi * 1,B,1 Winkler 1,C,1 Koppers Totzek	1,B,2 Westinghouse 1,B,3 BCR 1,B,4 IGT* 1,D,1 Atomics Int.
2. Medium BTU Gasifier- Internal Heat Type	2,A,1 Lurgi* 2,B,1 Winkler	2,B,3 Synthane* 2,B,4 Single-vessel HYGAS 2,C,2 Bi-Gas
3. Medium BTU Gasifier External Heat or Circulating Heat		3,A,1 CO ₂ Acceptor* 3,A,3 Ash-Agglomerating
4. Gaseous-Phase Coal Hydrogenators		4,A,2 Hydrane 4,A,3 COED
5. Liquid-Phase Coal Hydrogenators		5,A,1 H-Coal 5,A,2 Synthoil
6. Solvent Extractors		6,A,1 SRC
7. Chemical Extractors		7,A,1 Battelle
8. Coal Pyrolyzers		8,A,2 TOSCOAL
9. Methane Synthesizers	9,B,1 Multiple-Fixed-Bed*	9,A,1 Tubewall with PGR* 9,A,2 Tubewall without PGR* 9,D,1 Chem Systems
10. Methanol Synthesizers	10,A,1 High Pressure Catalytic	
11. Fischer-Tropsch Synthesizers	11,A,1 Kellogg 11,B,1 Ruhrchemie-Lurgi	
12. Ammonia Synthesizers	12,A,6 Haber Bosch 12,A,7 American (Large)	

TABLE 2 (Continued)

<u>Functional Module</u>	<u>First Generation</u>	<u>Advanced</u>
13. Shift/Reverse Shift Synthesizers	13,A,1 Chromium Promoted Iron* 13,B,1 Cobalt-Moly 13,D,1 Reverse Shift	
14. Gas Phase Separators/Purifiers	14,C,4 Benfield* 14,E,1 Rectisol 14,F,2 Selexol	
15. Hydrogen Purifiers	15,C,4 Benfield 15,E,1 Rectisol 15,F,2 Selexol 15,H,1 Methanator 15,J,2 Linde	
16. Coal Preparation	16,A,3 Roll Crusher* 16,B,2 Ball-Race Pulverizer 16,B,4 Ball-Mill Pulverizer*	
17. Mineral Preparation	17,A,2 Roll Crusher 17,B,1 Hammer Mill* 17,B,4 Ball Mill* 17,G,1 Thickener 17,I,1 Dissolver 17,N,1 Centrifuge	
18. Oxygen Producers	18,A,1 Liquid Air Distillation*	
19. Liquids/Suspensions Separators/Purifiers	19,B,1 Pressure Filter 19,C,1 Vacuum Filter 19,D,1 Classifier 19,E,2 Dorr Thickener 19,H,2 Centrifuge 19,J,1 Distillation 19,L,1 Decanter	
20. Hydrotreaters		20,A,1 COED 20,C,1 SRC
21. Liquids/Gases Separators/Purifiers	21,B,1 Condenser 21,D,2 Cyclone 21,F,1 Flash Distillation 21,G,s Distillation	

TABLE 2 (Continued)

<u>Functional Module</u>	<u>First Generation</u>	<u>Advanced</u>
22. Hot Gas Cleaning	22,A,1 Cyclone*	22,B,1 High Temp Electrostatic Precipitator 22,D,1 Expanded Bed Filters
23. Oxidation-Reduction Hydrogen Producers		23,A,1 IGT Steam-Iron
24. Conventional (Furnace/Boiler)	24,A,1 Gas Furnace 24,A,2 Oil Furnace 24,C,1 Pulverized Coal Furnace	
25. Fluidized Bed (Furnace/Boiler)		25,A,1 Westinghouse 25,B,1 Pope, Evans, and Robbins
26. Cyclone Furnace	26,A,1 Cyclone Furnace	
27. High Pressure Burners/Furnaces		27,C,1 Solid Fuel Fired
28. Hot Gas Pyrolyzer		28,A,1 MHD Exhaust Suspension Gasifier
29. Direct Coal Burning MHD		29,A,1 Single Stage MHD
30. High Temp Thermo/Turbo-Electric Converters	30,B,1 Gas Turbine	30,A,1 MHD
31. Flue-Gas Clean-Up Processes	31,B,2 Cyclone 31,D,1 Electrostatic Precipitator 31,F,1 Limestone Scrubber 31,G,1 Envirotech 31,I,1 Chemico 31,J,1 Wellman-Lord 31,M,1 Citrate 31,N,1 TVA-EPA	31,R,1 Consolidation Coal
32. Flue-Gas Thermal Energy Recovery	32,A,1 Tubular Feed-Air Heater	31,B,1 Steam Boiler for MHD Exhaust
33. Low-BTU Gas Clean-Up	33,A,1 Cyclone* 33,B,1 Scrubber* 33,E,1 Electrostatic Precipitator	

TABLE 2 (Continued)

<u>Functional Module</u>	<u>First Generation</u>	<u>Advanced</u>
34. Mineral Recovery & Waste Treatment	34,D,1 Ammonia Stripping* 34,F,2 Liquid/Liquid Extraction 34,G,1 Evaporation Pond 34,CC,1 Claus Plant* 34,FF,1 Stretford 34,GG,1 Chance*	
35. Turbo-Electric Power Converters	35,B,1 Reaction Turbine	
36. Outlet Cooling	36,D,3 Hyperbolic Cooling Tower	36,F,1 Dry Cooling Tower
37. Gas Turbine/Electric Power Generators	37,A,1 Basic Gas Turbine* 37,A,2 Gas Turbine with Regeneration	
38. Waste Disposal	38,I,2 Landfill* 38,K,1 Stack* 38,L,1 Lagoon*	
39. Demethanators	39,A,1 Methane Reformer	
40. Coal/Chemical Slurry Separators	40,A,1 Centrifugal Filter 40,A,2 Filter Press	
41. Char Preparation	41,A,1 Ball-Mill Pulverizer*	
42. Nuclear Disassociation of Water	42,A,1 Thermal Disassociation	

1. PROJECT OVERVIEW

The fundamental goal of this project is to develop a computer model that facilitates the systematic analysis of coal-process RD&D policy options. International Research and Technology Corporation has developed a model of this type for use in the chemical industry. The approach to be followed will be to extend the chemical industry-based model, termed the Materials-Process-Product Model (MPPM), in such a way as to facilitate its use in analysis of coal processes.

This chapter begins by discussing why a coal-based MPPM is needed. It then describes the specific objectives, scope, organization, and anticipated difficulties of the present project. It discusses the basic approach to materials-process-product (mpp) analysis,* and describes the principal attributes of the Materials-Process-Product Model as they are being established for analysis of coal processes. Finally, it outlines the organization of the material presented in the remainder of this report.

1.1. NEED FOR A COAL-BASED MATERIALS-PROCESS-PRODUCT MODEL

The developmental and utilization aspects of any technology are inseparably intertwined. This is particularly true in the case of coal process technology. New coal conversion processes are being counted on to smoothly replace existing oil and gas processes in the provision of various forms of energy, the quintessential ingredient of the U.S. economy.

There are many directions in which the development of coal conversion processes can proceed. Potential coal-derived products span the range from gaseous, liquid, or solid fuels to thermal, mechanical, or electrical energy. Each of these products has an existing level of demand now being satisfied primarily by petroleum fuels.

* In this report, the term materials-process-product (mpp) analysis denotes the general analytic technique (as described in Section 1.3.), while Materials-Process-Product Model denotes the computer model developed by IR&T for conduct of mpp evaluations.

It is an open question whether the two major developing energy sources--coal and nuclear--can be expected to meet existing patterns of energy demand. To the extent that they do not, economic dislocations may occur as petroleum supplies are depleted. The participation of the government in deciding which aspects of coal process technology to emphasize is therefore extremely significant and will be subject to continuing review.

The assessment of coal process RD&D alternatives must be carried out in light of uncertainties as to the anticipated participation of other energy sources. Conduct of this assessment will be further hampered by the fact that the technology of the coal processes themselves is continually evolving. Many alternative approaches are being simultaneously pursued. There is diversity both in the types of products and in the approach to be taken toward specific products. The demand for various product types can be expected to fluctuate in time. For example, an accelerating decline in apparent natural gas reserves may inspire expanded demand, and willingness to pay, for gaseous products. At the same time, advances in technology may also promote shifts in the pattern of demands. For example, an advance in the environmental control aspects of direct combustion may cause downstream users to orient toward increased reliance on direct combustion of coal for the generation of thermal, mechanical, and electric power. There is a tendency toward self-fulfillment in such cases. A technology perceived to be most promising by the user community may thereby gain greater financial support. The counter example is obvious.

Evaluation of competing sets of coal process alternatives, when considered by themselves, is usually straightforward. Complexity arises when the fullness of alternatives and the changing economic context is considered. Uncertainties in demand--with respect to both the type of product and the quantity--, as well as in the capabilities of the developing processes, have already been noted. The 1973 oil embargo furnishes a graphic example of the complex nature of the tradeoffs to be encountered. During the embargo, the Federal Energy Administration allocated energy

products among the various users. The difficulties inherent in the allocation process quickly became apparent. For example, the allocation process raised the question whether it is more important, economically, to use energy materials in the production of chemicals or in the manufacture of steel. The old adage about the squeaky wheel was frequently observed. There are many intangibles in such an assessment under any circumstances. In fact, however, there was at that time insufficient knowledge regarding the way energy is employed in the various industries to support informed judgements. The situation has improved considerably since then. Nevertheless, the development of analytical techniques suitable for such tradeoff decisions continues to be urgently needed. The Materials-Process-Product Model is an important step in this direction.

Utilization of domestic coal resources represents one of an increasing number of areas in which governmental decisions have a direct and pervasive influence on the development of private industry. The magnitude of the effort and its importance to the nation have necessitated governmental participation. The direction taken by governmental RD&D programs for coal process development will have, in many cases, an immense impact. We refer not only to the obvious effect upon those industrial concerns sponsoring coal process technologies, but also to the resultant impact on the downstream user. Should emphasis be given to those developing processes whose principal products are in the form of gases, liquids, or solids--or in the form of some particular combination of these? There are user industries favoring each of these alternatives. How much investment is required to establish a network of low BTU gas facilities? The promise of such a network would have a direct effect on the regional development plans of industry. Can the potential chemical industry demand for synthesis gas be easily satisfied? If useful answers to such varied questions are to be obtained, the questions must be systematically posed within the economic and technological context to be encountered by the developing coal processes.

The materials-process-product approach to process assessment is specifically tailored to help answer questions of the type just described.

Briefly stated, materials-process-product (mpp) analysis identifies the fundamental component parts of the processes leading from given raw materials to desired products, determines feasible alternative configurations of these component parts, and systematically evaluates each of the alternatives under a variety of economic situations and advances in the technology of the component parts. The various aspects of mpp analysis are discussed in Section 1.3.

A particularly important consideration is the selection of level of detail to be addressed by the analysis. The focus must be sharp enough to reveal the nature of the technological tradeoffs, but not so narrow as to obscure the overall economic context. The implications of this requirement are discussed in the following sections.

1.2. PROJECT DESCRIPTION

This section provides a descriptive summary of the present project. Some readers may prefer to advance to Sections 1.3. and 1.4. in order to gain first an understanding of materials-process-product analysis.

1.2.1. Objectives

The fundamental goal of the project, as stated on page 1, is the development of a computer model to facilitate assessment of coal-process RD&D options. This goal will be achieved via six specific objectives:

- (1) Extend the Materials-Process-Product Model (MPPM) in those ways necessary for the analysis of coal process technology.
- (2) Assemble a coal process data base in a format compatible with MPPM analysis.
- (3) Utilize the MPPM to generate a library of economic unit processes.*

*The terminology employed in materials-process-product analysis is discussed in Section 1.3. and summarized in the glossary at the beginning of this report.

- (4) Evaluate the unit processes within the context of coal RD&D policy scenarios
- (5) Conduct sensitivity analysis of the scenario results, including an evaluation of the significance of data uncertainties.
- (6) Establish compatibility with other energy/economic computer models, then conduct coal policy scenario evaluations within an enlarged energy/economic context as provided by these other models.

Objective 1: Extend the Materials-Process-Product Model

The first two objectives represent the most difficult aspects of the project. Consider Objective (1). The ways in which the MPPM must be extended are discussed in greater detail in Section 1.3. and 1.4. and Chapter 3. As described in 1.3., the existing MPPM utilizes economic unit processes (see glossary) as its basic units. This level of detail is sufficient for analysis of alternative chemical industry process configurations. In dealing with coal processes, however, it is necessary to proceed to an additional level of detail. Functional modules (see glossary) have been defined. As discussed in Chapter 3, the functional modules that compose a unit process route act together. The operations that define individual module configurations are both equalities and limitations. For example, the shift converter employed in coal-to-SNG unit processes can accept entering streams containing variable quantities of hydrogen and carbon monoxide. The shift converter adjusts the hydrogen and carbon monoxide quantities so that they bear a specified relationship to each other, e.g., slightly greater than 3:1 H_2CO for methanation. The converter does not produce a set amount of either material. Thus, the hydrogen, carbon monoxide, and other stream materials cannot be precisely specified. These modifications to the MPPM lie within the province of what is termed the Linking Model. The Linking Model identifies and characterizes all feasible unit processes leading from coal to a desired product, like SNG, clean boiler fuel, etc.

A second case requiring MPPM extension is the formulation of an Industry Development Model (IDM). This model acts as an intermediary between the investigator wishing to assess alternative coal policy options and the comparative process evaluations established by the Process Chain Evaluation Model (PCEM). In effect, the IDM accepts formatted statements by the investigator, including specification of necessary exogenous data, then selects from among the processes evaluated by the PCEM, and then determines the composite effect of the selected processes. In one possible role, the IDM might accept as inputs a year-by-year schedule of regional expenditures for a particular coal process route, e.g., coal to SNG, and the specification of regional coal availability by type. The IDM then selects from the PCEM data base the best unit process* for each region (coal type) by year, and generates a computer printout specifying the selected processes and identifying factors of interest (by region), such as growth in installed capacity by year, coal consumption by year, effluents generated by year, etc. The IDM will also act as the interface between the MPPM and other energy/economic models in achieving Objective (6).

Objective 2: Assemble Coal Process Data Base

The second objective is difficult because it requires a review of the large quantities of data now being generated for alternative coal processes by the ERDA Research Centers, other governmental agencies, and private firms. An important aspect of this project will be the utilization of the best available process data. The manner in which such data can be assembled into a functional module description is presented in Section 3.1.3. The process for developing a systematic data base composed of numerous such module descriptions will be demonstrated in arriving at Model A during the first nine months of Phase II (See Section 1.2.3.).

* Usually, the best unit process will be that producing the desired product at minimum production cost while complying with designated environmental requirements. There will frequently be a number of roughly equivalent processes, with the best process acting as a representative of this group rather than as a uniquely determined optimal process.

Objectives 3 & 4: Generate Unit Process Library and Evaluate Unit Processes in the Context of Coal RD&D Policy Scenarios

Objectives (3) and (4) pertain to the application of the MPPM to an evaluation of coal policy options, once the data base has been assembled and the MPPM generalized to the functional module level. Generation of a library of unit processes is the basic function of the Linking Model (Section 3.2.2.). Evaluation of the unit processes within the context of coal policy scenarios is the basic function of the Process Chain Evaluation Model. These two objectives are, in effect, a *demonstration* of the achievement of the basic goal of the project--to develop a computer model for materials-process-product analysis of coal process technology.

Objective 5: Conduct Sensitivity Analysis

It is in the nature of materials-process-product (mpp) analysis that the computational results are indicative, rather than exact. The reasons for this are discussed in Section 1.3. One capability of mpp analysis is to identify areas that should be explored in greater depth using more detailed computational models. The focus is upon the interrelationships among the functional alternatives, rather than on one alternative in particular. For example, the MPPM may determine that the economics of some processes benefit more substantially from a breakthrough in methanator technology than do others. Objective (5) represents an exploration of the sensitivity of unit processes to such variations in process technology and in economic context. The effect of data uncertainties will be evaluated in the same matter.

Objective 6: Employ MPPM in Conjunction With Other Models For More General Coal Policy Evaluations

This represents the last step in achieving the fundamental goal set for the project. The MPPM is intended to be used in conjunction with other models. As discussed in Section 1.1., there are uncertainties both in demand--with respect to the type and quantity of product--and in the

capabilities of the developing coal technology. The MPPM assists in resolving the latter by organizing the data for the evolving technology in such a way as to facilitate evaluation within a variety of economic contexts. The demand estimates can be best provided by other models. MPPM evaluations made in Phase II will utilize scenario evaluations based on exogenous economic inputs. In achieving Objective (6), the necessary computer compatibilities will be established so that joint model evaluations can be made with larger scale economic/energy models, such as the Brookhaven BSNS and BESOM, the EPA SEAS, and other models of interest to ERDA.

1.2.2. Scope

The study will focus upon coal conversion and utilization processes. Transport and mining steps will not be included, although their influence may be directly assessed through joint studies with other models in Phase III.* The four major coal process areas will be examined: (a) gasification, (b) liquefaction, (c) conversion to clean solid product, and (d) direct combustion. First generation and advanced processes will be included. For example, direct combustion processes range from conventional furnaces to fluidized bed furnaces to MHD power generation. Regional considerations will be taken into account by identifying the effect of different types of coal upon the characteristics of each process. The four general categories of coal--lignite, sub bituminous, bituminous, and anthracite--will be matched against the relevant processes.

Consistent with the materials-process-product approach, the functional modules participating in each of the major coal-to-product unit process routes were identified during Phase I of this study. The products considered are listed in Table 2.1. within three categories--energy products, material products, and byproducts. The functional modules and their participation within unit process routes (see glossary) are shown in the "Road Map" Foldout enclosed at the back of this report.**

* Separation of the project into distinct phases is described in Section 1.2.3.

** Since this "Road Map" will be frequently referred to, it has been placed in the back of the report along with one other particularly important diagram (to be discussed later), to facilitate utilization by the reader.

Forty-two functional modules were identified. Each of the paths leading from coal through a set of functional modules to an end product is termed a unit process route. The assembly of functional modules and unit process routes is represented by the "Road Map" for mpp analysis of coal processing technology, described earlier.

A number of competing configurations exist for each functional module. For example, Module 2--Medium BTU Gasifiers of the Internal Heating Type--includes fixed bed, fluidized bed, entrained flow, and molten bath bed alternatives. Examples of the fixed bed variety include the Lurgi, Wellman-Galusha, USBM Stirred Bed, GE Gas, and Thyssen-Galosz Gasifiers. Each competing configuration is part of a set of alternative ways of following the functional module path corresponding to a single unit process route. Each alternative is denoted as a unit process associated with that unit process route. As discussed in Section 1.3.2., the combinatorial number of unit processes depicted in the Road Map is over one-half million. Not all of these unit processes are physically meaningful, and the majority are not of economic interest. Nevertheless, the number of feasible unit processes on the Road Map that are of potential interest is quite large--in the thousands. An important function of the Materials-Process-Product Model is to screen the feasible unit processes within the specified context in order to identify those processes of greatest interest. For example, an investigator might request a listing of the top ten or top one hundred unit processes, e.g., coal to SNG, that satisfy specified criteria, such as thermal efficiency and cost constraints.

The scope of the present study will be restricted through the numbers of competing configurations included for each functional module. At least one configuration will be defined for each module. The planned distribution of configurations by module is shown in Table 2.2. of Chapter 2. The configurations are allocated between Model A and the final version MPPM, and the state of technology is indicated as first generation or advanced. From Table 2.2., it is seen that Model A focuses mainly upon those

modules participating in the coal gasification unit process routes. The 26 configurations for Model A could lead to a theoretical maximum of 576 unit processes. At the end of Phase II, the MPPM will include 112 configurations that could potentially lead to more than 500,000 unit processes. There are, of course, physical constraints imposed by the MPPM in identifying feasible unit processes. As a result, the number of unit processes to be included in the MPPM unit process library at the end of Phase II is likely to be on the order of 10,000.

1.2.3. Organization

The project is being carried out within three sequential phases. This report is the final step of Phase I. In this phase, the following objectives were accomplished:

- (1) The level of detail appropriate for mpp analysis of coal processes was identified
- (2) A Road Map was established relating coal processes to the mpp format
- (3) An illustrative functional module data file was developed to demonstrate the procedural approach. Aspects of the Linking Model algorithm for assembling unit processes from functional module competing configurations were developed.
- (4) Other energy and economic models were reviewed to identify potential joint model configurations for Phase III evaluations.
- (5) The Phase I report was written to clearly identify what will be accomplished in the project, and the specific work plan to be followed.

Selection of the best level of detail represents an extremely critical decision for the project. An extensive review of the literature on coal processes was conducted. As will be discussed in Section 1.3.2., functional modules were identified as the basic computational units. Experience

of other investigators has shown that the use of greater detail than that represented by the functional module overwhelms a permutational approach such as that employed by the MPPM (see discussion in Section 1.3.3.). On the other hand, the use of less detail does not permit analysis of the type of developmental tradeoffs that must be made.

Establishment of the Road Map described in Section 1.2.2. (see the foldout in the back of the report) was an early highlight of Phase I. This diagram provides a graphic illustration of the kinds of insight which can be achieved by viewing coal processes from the mpp perspective. As noted above, the number of possible ways to traverse this map from coal at the left to the spectrum of products at the right is enormous--even when the various physical limitations and economic constraints are taken into account. The Materials-Process-Product Model provides a computational device for systematically evaluating the many process alternatives and selecting the best from those found to be feasible under specified conditions.

In Section 3.1.3., a functional module description is developed for the methanation step in substitute natural gas (SNG) production. Methanation synthesis is the functional module (No. 9 on the Road Map), and the description subsumes models of three alternative competing configurations (see glossary) for that functional module. These configuration descriptions were developed to illustrate the type of data employed, the techniques used to assemble the configuration data file, and the characteristics that the configuration description must have to permit its use in the MPPM assessments. In most instances, engineering development programs will have developed data that facilitates preparation of a configuration description. The emphasis in Phase II will be placed upon working with those organizations developing the coal process hardware systems so that the best data is utilized. It is the function of this project to provide an information handling system, not improved data on coal processes. Linking of competing configurations to form different unit processes will provide additional insights regarding possible alternative methods for converting coal to useful energy products.

The review of other energy and economic models is fully discussed in Chapter 5. Each model was assessed as to its strengths and weaknesses, and as to how it could productively be employed in joint evaluations with the coal-based MPPM. The way in which the models interact to illuminate the national or regional energy supply and demand systems is shown in the second of the two diagrams (the first being the Road Map) enclosed at the back of the report. This diagram displays potential interactions of the MPPM with larger scale energy/economic models. Three specific computational system possibilities are identified and appraised in Section 5.2.3. The compatibility conditions will be established and joint evaluations conducted using one of these configurations during Phase III.

As stated, this report concludes Phase I. A work plan for Phases II and III is provided in Chapter 6. The following paragraphs briefly summarize what is to be accomplished.

Phase II will itself be conducted via three sequential steps. The first step, nine months in duration, will demonstrate the *feasibility* of the mpp approach to coal process analysis through development of a prototype *Model A* of the MPPM. This model will contain 26 competing configurations for 15 functional modules participating in 10 unit process routes that could potentially lead to 576 unit processes from coal to SNG, medium BTU gas, low BTU gas, and on-site electrical/mechanical energy. The second step, six months in duration, will enlarge the *usefulness* of the mpp approach by greatly expanding the number of competing configurations, to about 90, while establishing *Model B*. This model will include the development and first use of the Industry Development Model (see Section 3.2.5.). Step three, accomplished during the final three months of the 18 month Phase II, will expand the MPPM data base to about 112 competing configurations, and will be concluded with the Phase II final report.*

*The number of competing configurations for the 15 functional modules of Model A will be doubled in the final MPPM. This increases the number of associated unit processes to 109,188. Systematic evaluation of process alternatives is clearly essential.

During the last five months, the Control Data Corporation (see Section 3.3.) is expected to work with IR&T in making an efficient computational package from the developmental Model B of the MPPM.

The 12 month Phase III effort will be devoted to the accomplishment of Objective (6)--the conduct of joint economic/energy evaluations with other computational models. As already indicated, one of the strengths of the MPPM is that it organizes the coal process data in such a way that it can be accessed for general policy evaluations. The need for such evaluations was described in Section 1.1. The focus of the MPPM is upon the coal processes. The economic context within which the coal processes must be evaluated can be best provided by computational models such as those described in Chapter 5.

1.2.4. Difficulties

Development of a coal-based MPPM is a challenging project. The accomplishments of Phase I serve to indicate that the goal can be achieved. Nevertheless, a number of obstacles remain. They are clustered primarily within three of the six objectives, i.e., Objectives (1), (2), and (6). These are, respectively: extending the MPPM to the functional module level, establishing the coal process data base, and developing compatibility with other computational models.

The necessity to extend the MPPM to the functional module level in analyzing RD&D options for coal process development is discussed in Sections 1.3.2. and 1.3.3. As stated in the latter section, synthesis models involving greater detail have yet to succeed*, while those involving less detail are not sufficiently sensitive to the ways in which advances in coal technology will be made. To illustrate, technical advances in the conversion of coal to SNG are likely to be made at the functional levels of gasification, shift conversion, or methanation, rather than simultaneously along the entire process sequence. In fact, the advances are sometimes made at the still more detailed level of the unit operation, such as flow

* As discussed in Section 1.3.3., process synthesis models have been attempted at the unit operations level. So far, the large number of potential combinations and the feedback loops between units have precluded successful process synthesis at this level of detail.

distribution within a gas absorption column or development of a catalyst with an extended life. The functional module is an effective point for tying such advances together, since it is the function that must be achieved. Frequently an entirely different approach to the functional operation proves more advantageous than a number of incremental improvements within the original unit operation.

Although proceeding at the functional module level is necessary, it is an added complexity beyond that involved in the chemical-industry-based MPPM (see discussion in Section 1.3.2.). Characterization of a module configuration is frequently not unique. For example, a pump at the end of a series of unit operations might be included within either that functional module or the succeeding one. Some ground rules of this type were established during Phase I. Others will be established during the development of prototype Model A. The overriding ground rule is to define module boundaries so that *feedback loops between modules are avoided*. Otherwise, it would not be acceptable to treat such modules as separable entities.

It is important to remember that the MPPM does not act as an engineering design program. Rather, it assembles functional components into various unit processes, as might an experienced engineer. That is, a process engineer can usually develop a good estimate of the general characteristics for a suggested new process within a day or so. He does this by using approximate functional descriptions for the process components and taking estimated performance limits into account. The resulting process description usually comes within 30% or so of the values later established via a detailed engineering evaluation.* The MPPM systematically establishes such estimates for alternative unit processes. As discussed in Chapter 3, some configuration descriptions for the functional modules will be obtained by disaggregating process designs,

* Lack of experience regarding some of the innovative aspects of the process will, of course, tend to degrade the quality of the estimate.

such as the design for conversion of Montana Sub-bituminous Coal into SNG, using a version of the IGT HYGAS gasifier as reported in Reference 7 of Chapter 3. One of the unit processes formed by the Linking Model will be similar to the complete process designs from which the data for the competing configurations was obtained. Thus, independent unit process evaluations will be available for comparison with MPPM evaluations.

The difficulties involved in establishing a coal process data base in mpp format pertain directly to the amount of material that must be reviewed. The procedure was illustrated in developing the methanator configuration description in Section 3.1.3. As is obvious from this example, a knowledgeable engineer is needed to perform the analysis and synthesis steps involved in assembling such a configuration description. Many processes must be reviewed in this manner in order to establish the desired MPPM data base. An added difficulty is that the process information will not always be easily obtained, being considered proprietary in some instances and being insufficiently documented in others. The approach to be taken will be to utilize data developed under ERDA-sponsorship as much as possible, and to establish cordial relationships with private firms and industrial consortiums so that providing the necessary information is rightly perceived as in their best interest. That is, these groups must sense that the information will be used in an appropriate manner.

Establishing the necessary compatibilities for conducting joint evaluations with the MPPM and other large computer models will not be an overly complex undertaking, but will require extreme care and attention to detail. Twelve months is allocated to accomplish this objective during Phase III, and the assistance of the Control Data Corporation will probably be employed (see Section 5.3.).

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1.3. MATERIALS-PROCESS-PRODUCT ANALYSIS

1.3.1. Motivation

Materials-process-product analysis is an approach to the evaluation of industrial process technology that emphasizes the *interrelatedness among the processes, the available raw materials, and the products desired*. The premise is that processes can only be meaningfully assessed within their materials-product context. From this viewpoint, present industrial technology is the result of process decisions made within a past materials-product context. Similarly, process decisions made at present must consider the manner in which the materials-product context will change in the future. International Research and Technology Corp. has developed a computer model based upon the activity analysis concepts of Prof. T. C. Koopmans that facilitates materials-process-product evaluations. This model is called the Materials-Process-Product Model (MPPM).

There are many ways in which analysis of the materials-process-product linkage can lend insight into the options available to industry and government in dealing with specific problems of process economics, resource availability, etc. For example, several possible responses may be made to an oncoming shortage in a basic raw material, such as natural gas or crude oil. An equivalent raw material may be employed that necessitates few changes in downstream process technology. The provision of substitute natural gas (SNG) is, from the user's standpoint, an example of this approach. Alternatively, another raw material may be utilized that requires changes in process technology and may or may not lead to a somewhat different product. An example of this second possibility is the development of coal liquefaction processes that lead via syncrude to refined petroleum products having a larger aromatic fraction. Another example of material shifts is the displacement of natural gas and fuel oil by coal in some boiler fuel applications. The existing process must be modified to accommodate the physical and combustion characteristics of coal, as well as the different residuals generated.

Development of coproduct markets is an aspect of the inter-relationship between process and products that plays an important role in process economics. Sometimes, the emphasis among multiple products from a single process may change such that an initially undesired or unimportant product achieves equal, or greater, stature relative to the other products. Consider the case of chlorine manufacture. Caustic soda (NaOH), produced as a coproduct in greater quantity than the chlorine, represented a disposal problem for many years. Over the last decade, however, development of additional applications for caustic soda has strengthened its market structure. Now it is occasionally in even greater demand than the chlorine. As a result, consideration of the caustic soda market is integral to an evaluation of chlorine process economics. The refining of crude oil is another example. In Europe, the climate necessitates an emphasis on provision of fuel oil. A large quantity of coproduct naphtha is produced that until recently was priced rather low. The European organic chemical industry utilizes the naphtha as its principal feedstock. Crude oil refining in the United States, on the other hand, has focused upon the production of gasoline, with less naphtha produced as coproduct. At the same time, there have been until recently abundant domestic supplies of natural gas liquids (NGL) and liquified petroleum gases (LPG). For these reasons, the United States organic chemical industry has been based upon the lower molecular weight hydrocarbons, primarily ethane and propane. A final example of the significance of coproducts to process economics is the combustion of high sulfur coal. There are a number of methods for control of the sulfur oxides produced during combustion. One method generates sulfuric acid and sludge, while another generates a calcium sulfate sludge. The extent to which markets can be developed for the components of these sludges is an important factor in the viability of this approach to SO_x control, and in comparing direct coal combustion with other processes for providing electrical energy.

A few concluding examples serve to underscore the economic importance of the materials-process-product linkage. To some extent, advances in process technology occur on a predictable basis. For example, for most new processes there is a learning curve that reflects process debottlenecking and the fabrication of larger and more efficient equipment. An estimate of the learning curve for a particular process can be inferred from prior experience with similar types of processes. The effect on process economics is significant. Similar estimates can be made for the impacts of technological advances in older processes, since the principal characteristics of these advances are generally recognized within the research community five years or more preceeding commercial introduction. This information, for both new and established processes, permits a projection of future production cost behavior. The future relative economic viability of competing products can be estimated in this way.

1.3.2. Basic Approach

Materials-process-product analysis of alternative process technologies emphasizes consideration of the materials-product context. The entire sequence of processing steps leading from basic raw materials to desired final product is appraised. This is done by breaking the sequence up into discrete components. The components are then reassembled into *permuted combinations* that represent all physically realistic component linkage patterns. This procedure is at the heart of the materials-process-product analysis approach. Its feasibility has been demonstrated by the chemical industry case study of Reference 2. The approach to be employed in dealing with coal processes is discussed in Chapter 3 of this report. The algorithms for joining components into physically realistic--and excluding nonrealistic--combinations compose the *Linking Model* portion of the Materials-Process-Product Model.

In the chemical industry model the basic components were termed *economic unit processes*. These unit processes transform purchasable raw materials into one or more salable products. The economic unit processes have a unique economic identity in the sense that the material inputs and outputs have market value, such that separate accounts can be kept for the facility. No smaller subset of processing steps have this unique identity. The process sequences formed by linking unit processes together are termed *process chains*.

The participation of chemical unit processes in process chains, and some insights to be gained by materials-process-product analysis, are illustrated by Figure 1.1.* Here, two different final unit processes in the process chains leading to vinyl chloride monomer (VCM) are depicted--pyrolysis of ethylene dichloride (EDC) and direct chlorination of ethane. Present industrial practice is dominated by EDC pyrolysis, with the two precursor ethylene chlorination processes usually operated in parallel to utilize the waste hydrogen chloride produced by ethylene dichloride pyrolysis. However, the other, new process, termed "Transcat" by its developer (Lummus Co.), makes possible the direct conversion of ethane without going through the ethylene stage. Although no domestic Transcat plants have yet been built, the general nature of this technology is known, so that its effect upon VCM economics can be evaluated. One important aspect of the process is its ability to accept chlorinated hydrocarbon wastes as part of its feed, and to produce essentially no pollutants. Not surprisingly, the elimination of two process steps by the Transcat process (and its inherent waste control) enable it to gain significant economies relative to the ethylene-based processes. As a result, the future economics of VCM production may be relatively little affected by improvements in the ethylene process, although other products derived from ethylene will benefit.**

** The two chlorine processes represent another example of process competition that affects the economics of the entire process chain. Recent environmental considerations have led to the resurgence of the diaphragm cell process that had been being displaced by its mercury cell counterpart.

* Figures and tables are placed at the end of each chapter.

It is the function of materials-process-product analysis to comparatively evaluate *all* process chains leading to the desired product. Of course, the necessary unit process data must be included in the model's data base. In Figure 1.1 there are nine unit processes (listed) participating in five process chains leading to VCM. For example, one chain is $\begin{pmatrix} 1 \\ 3-5 \end{pmatrix} \rightarrow 6-8$ and another is $\begin{pmatrix} 1 \\ 3 \end{pmatrix} \rightarrow 9$. In a study of 26 processes participating in VCM manufacture, 399 process chains resulted. All chains were physically realistic, but many were not economically competitive under present conditions.

This observation leads us to another emphasis of materials-process-product analysis--the evaluation of process chains under alternative economic circumstances. The potential rearrangement of processes under different circumstances is illustrated in Figure 1-2. Here, the VCM process chains have been compared (1) on a venture cost of sales basis for standard U.S. industry (in 1972), (2) for several types of developing countries, and (3) in the presence of an energy use tax. Considerable rearrangement in the process rankings is seen. This, of course, is merely a type of *sensitivity analysis*. A similar sort of analysis can be used to examine the significance of data uncertainties for developing processes.

The discussion to this point has utilized the chemical industry to illustrate the nature of materials-process-product analysis. In Phase I of the present study, a set of unit process routes leading from coal to its many derivative products has been identified. The full set of unit process routes is depicted in the Road Map at the back of this report. In considering coal processes, it has been necessary to include a greater level of process detail than in the chemical industry model. This is done to facilitate the study of process tradeoffs at the level at which investment decisions will be made.* In the chemical industry, established unit processes exist for which the technology is relatively fixed. As a result, investment decisions usually involve tradeoffs

* The considerations leading to identification of the coal unit process routes are presented in Chapter 2.

between unit processes. In coal process technology; however, the basic unit processes have yet to be established. The development and investment decisions are focused upon subprocess steps, such as gasifiers, shift converters, methanators, etc. We designate these steps as *functional modules* in that they each embody one principal function--chemical conversion, coal preparation, gas cleanup, waste treatment, etc. A linked set of functional modules constitutes a complete, coal-based unit process route.

Forty-two functional modules have been identified as participating in coal processing. These are displayed and their linkages depicted in the Road Map. For example, the unit process route for producing pipeline quality substitute natural gas (SNG) consists of the functional module sequence 16-2/3-14-13-14-9. There are a number of alternative ways or *configurations* for accomplishing each of the functional module operations. For example, some work is underway on over 24 gasifier approaches. A rough estimate of the number of alternatives being pursued for each of the other modules in the SNG process is: coal preparation, 5; shift conversion, 4; gas cleanup, 14; and methanation, 5. These alternatives are designated "competing configurations." While these alternatives are not all interchangeable, there is considerable flexibility in terms of physical compatibility. To furnish some idea of the complexity involved, if the alternatives for each module were fully interchangeable,* the number of possible ways of accomplishing this conversion of coal to SNG would be 33,600. As noted in section 1.2.2., when all processes shown in the Road Map are considered, the possible combinations exceed one-half million.

Clearly, it is imperative that a consistent method be used in evaluating such a multitude of unit process alternatives (see footnote).

*The alternatives are, of course, not all interchangeable. The Linking Model part of the MPPM identifies which combinations represent physically realistic alternatives. The Process Chain Evaluation Model then applies economic criteria to reduce the number of alternatives to manageable proportions. It is estimated, however, that the number of unit processes of potential interest is of the order of 10,000.

It must be borne in mind that the economic context will be changing, and process data--with incumbent uncertainties--will evolve as process development continues. Hence, the process evaluations will need to be repeated periodically. Such systematic comparative process evaluations are a principal attribute of materials-process-product analysis.

1.3.3. Comparison with Other Computational Approaches

There are numerous alternative approaches to process evaluation and process-related policy analysis. These can be loosely grouped into two categories relative to material-process-product analysis--those embodying less and those embodying more detail. So far as we know, no other calculational approach utilizes the permutation method and operates at the level of detail associated with materials-process-product analysis. Obviously, the differences between calculational methods relate directly to the specific motives underlying a particular evaluation.

Methods employing less detail range from the production function of microeconomic theory to parametric process descriptions, such as those employed in the Brookhaven Energy Model discussed in Section 5.1.5. Production functions portray the output response of a production system to changes in variable inputs, i.e., capital or labor. The focus of such functions is the *empirical matching* of observed production behavior to aid in optimizing resource allocation. They do not in themselves embody sufficient detail to project the characteristics of a developing technology, e.g., that of coal processes. Instead, they can be used to analytically express the resource tradeoff results from a more detailed model.

The Brookhaven Energy System Optimization Model (BESOM) is a linear programming model for determining the optimum national mix of energy processing and transport systems. BESOM identifies alternative paths from raw materials--coal, crude oil, nuclear fuel, etc.--to demand categories--iron and steel production, petrochemicals, automobiles, etc. The paths between the raw materials and demand categories are

composed of processing and transport steps. The approach is somewhat akin to materials-process-product (mpp) analysis, but at a higher level of aggregation.* BESOM considers each coal process as a single entity, whereas the mpp approach deals with coal processes as a set of functional modules. In fact, the difference is greater than this because BESOM acts upon a nationally aggregated single coal process for each product, such as SNG. A subprogram could be written for BESOM to assemble the aggregate process description from estimates of individual process participation. This subprogram would not be altogether simple in that it must accomodate not only the diversity of processes but also their different characteristics when handling different types of coal. Such a subprogram would move BESOM in the direction of mpp analysis. However, the advantages to be gained from the permutation analysis would still not be achieved.

In BESOM, processes are described in terms of 41 parameters-- 12 efficiencies, 12 water residuals, 8 air residuals, 2 solid waste variables, 4 human health factors, and 3 annual costs.** The difference between BESOM and materials-process-product analysis is reflected in the choice of parameters, and relates directly to the purpose of the analysis. As stated, the focus of BESOM is upon determining the role aggregated coal processes should play in the overall energy picture. The focus of mpp analysis is upon identification of the characteristics of

* As discussed in Chapter 5, the Materials-Process-Product Model (MPPM) and BESOM can be used in interactive calculations. In such calculations, the MPPM will upgrade the fidelity of the coal process descriptions and the BESOM will identify the values to be placed on alternative coal-derived products, such as synthetic natural gas (SNG), synthesis gas, clean liquid boiler fuel, etc.

** There are four additional parameters for nuclear processes.

the coal processes themselves, and organization of the data for these processes so that they can be used in a BESOM-type evaluation.*

The differences between BESOM and MPPM are illustrated by the financial parameters. BESOM utilizes three: fixed cost, operating cost, and total annual cost. The MPPM includes considerably greater detail. Fixed costs are broken into fixed capital, auxiliary capital, and working capital. Scale parameters are included for each so that the capital requirements of different size facilities can be estimated. Operating cost parameters include labor manhours (and scale factor), wage rate, overhead multiplier, process materials requirements (from the material/energy balance), materials prices, maintenance and insurance cost factors, and equipment lifetime estimates. This level of detail is necessary to assess individual facilities in particular regional sites, including the significance of different regional taxing procedures. In summary, the MPPM is designed to comparatively evaluate individual process facilities in specific regional locations utilizing specific coal inputs, and to identify all feasible alternative processes for manufacturing the desired product at that site. BESOM is not intended to, and cannot, accomplish such an evaluation.

Computational approaches involving more detail than mpp analysis may be generally classed as *engineering models*. We have identified four different types of engineering models: determination of physical/chemical properties, process design, process simulation, and process costing.

* It is important to bear in mind that the MPPM is, in effect, a materials/energy accounting device designed to evaluate the implications of alternative sequential patterns. The materials/energy balance information must be provided in the form of functional module descriptions. At present, the coal processes themselves are in their initial stages of development. Accordingly, the materials/energy balance information for these processes is incomplete. The results to be achieved with the MPPM will directly reflect such limitations in the data base, as will all other calculations made at this time. As the data base improves, the MPPM results will improve correspondingly.

The material property models act in a support role for the process design and simulation models. Estimates are made for material properties such as viscosity, density, vapor pressure, etc. Most systems can deal with both pure substances and mixtures. Usually, several alternative methods are available for estimating each property.

Process design models are, as the name suggests, employed during the design and development phase of a project. Using material property data and algorithms for equipment performance, design models establish the detailed material and energy balance for the process. They also establish the required equipment sizes and performance criteria. The focus of design models is upon the interrelated behavior of the chemical engineering *unit operations* composing the process. This is a level of detail significantly finer than that of mpp analysis. Typical unit operations are distillation columns, filter presses, centrifugal separators, gas absorption columns, pumps, etc. The functional module employed in mpp analysis encompasses a single functional step, such as gas clean-up, that usually involves several unit operations. This is a critical difference, in that the number of permutations arising at the unit operation level is immense--far beyond that at the functional module level.

Process simulation models are highly refined versions of the process design type of model, and are intended for use as proxies of the actual process. Simulation models are employed to evaluate alternative modes of process operation, to determine optimal process control under unsteady state conditions, and to support open- or closed-loop computerized process control systems. The basic entities in the simulation model, as in the design model, are the unit operations and their control devices.

The process costing model requires as input a process flowsheet description, such as that furnished by the design model. It then determines in great detail the construction costs, construction timeline, capital requirements, and operating costs. For example, the construction

costs usually include a breakout of labor costs (on a regional basis) into skilled and unskilled labor, supervision, and G&A related expenses. The labor costs are further specified as to aspect of the construction process--electrical, civil, etc.

The use of engineering models is well established. Process design, simulation, and costing, and property evaluation, are a large part of the practice of chemical engineering. Some of the major design and simulation models have by themselves accounted for hundreds of man-years in development and utilization. There has even been a concerted attempt, mainly since 1968, to develop algorithms for computerized process synthesis* at the unit operations level.³ However, while there has been a great deal of creative work in this area, it has been possible to solve only parts of the problem. The large number of possible combinations among unit operations, and the feedback loops between them, have proven too complex for systematic analysis. Most productive have been the programs, such as AIDES, that emphasize man/computer interactive procedures.

Discussion of process synthesis has served to highlight a critical element of the mpp approach--*proper selection of level of detail*. Synthesis among unit operations has proven too complex, in spite of the best efforts of a number of highly skilled investigators. The process level of detail does not reflect the tradeoffs being made during the developmental program, e.g., between alternative methanator configurations, etc. Functional modules, on the other hand, provide significant insight into the intra-process flexibilities while avoiding most of the complexity associated with unit operations process synthesis.

*Process synthesis is roughly analogous to mpp analysis at the unit operations level. One prime example is the AIDES program developed at the University of Wisconsin. In the words of the developer--"The differences in the design of chemical processes arise quite naturally from the statement of design problems. One state is the final product stream or streams. The other is the state of the possible raw material inputs. The problem is to transform the inputs into the desired output in an efficient manner, when there are many ways to make this transformation."⁴

In particular, functional modules are defined in such a way as to circumvent feedback loops and their attendant difficulties.

Having identified the differences between process design/simulation models and mpp analysis, it is important to point out that the two approaches are complementary rather than competitive. The objective of mpp analysis is to systematically evaluate alternative coal unit processes. The data describing the functional modules must come from process design analysis. All of the more interesting unit processes determined by mpp analysis should be subsequently evaluated in detail by process design models. Mpp analysis enables a rapid, first cut, systematic appraisal of the effect of developmental breakthroughs and/or changes in the overall economic situation upon the relative economics of competing coal unit processes. Its focus is upon all the coal processes, rather than on any one in particular.

1.4. MATERIALS-PROCESS-PRODUCT MODEL (MPPM)

Description of the MPPM is limited here to a brief synopsis, since detailed discussion of all model elements is presented in subsequent chapters of this report. Chapter 2 describes how coal processes can be arranged into a format compatible with materials-process-product analysis; Chapter 3 discusses the functions and structure of the MPP; and Chapter 4 describes the utilization of the MPP in the analysis of coal RD&D policy evaluations.

1.4.1. Structure

The MPPM is composed of three submodels: the Linking Model (LM), the Process Chain Evaluation Model (PCEM), and the Industry Development Model (IDM). A schematic representation of the interaction among the three submodels is given in Figure 3.1. of Chapter 3.

1.4.1.1. Linking Model

The Linking Model assembles a library of feasible unit processes. It does this by utilizing algorithmic rules to identify acceptable linkages between the competing configurations occurring along each unit process route (see Glossary or Section 1.3.2. for discussion of terminology). For example, one present groundrule is that synthesis gas entering the methanator functional module in the SNG unit process route must have a hydrogen sulfide concentration less than one ppm for those configurations employing nickel catalyst. The upstream configurations that produce more than one ppm of hydrogen sulfide are not joined with the "nickel catalyst" configurations. Thus, the input requirements of a configuration will determine the upstream configurations that can be linked with it in the formation of a unit process.

Development of a configuration description is illustrated for the case of the methanator functional module in Section 3.1.3. Each configuration description contains: the materials balance, utilities

requirements (electricity, steam, etc.), and capital and labor requirements. The configuration by itself represents only one part of the unit process. Thus, it is selected for its characteristics by the other configurations participating in that unit process. Configuration materials, utilities, capital, and labor requirements are expressed in equation form for each unit process formed by the linking model. These aspects of the configuration description are illustrated for the methanator functional module in Tables 3.4. to 3.11. in Chapter 3.

In addition to its algorithmic structure and configuration descriptions, the Linking Model has access to three data files: raw material specifications, product specifications, and environmental constraints. The raw material specifications designate for each participating material: molecular weight; heat of formation; number of carbon, hydrogen, and oxygen atoms; and the process categories within which this material participates, e.g., raw material, main product, air-borne waste, etc. Other material specifications can be added as needed. Illustrative product specifications are given in Appendix A. The specifications are usually expressed in the form of limits. For example, SNG must contain less than 0.015% H₂O by volume to satisfy present pipeline requirements. Environmental constraints act as product specifications for those process streams entering the environment. For example, threshold limits may be specified for air-borne metallic trace contaminants. The Linking Model utilizes its algorithmic structure, configuration descriptions, and data files to compile a library of feasible unit processes.

1.4.1.2. Process Chain Evaluation Model (PCEM)

The PCEM employs five subprograms and three data files to evaluate the unit processes assembled by the Linking Model. The subprograms are: Sizer, Gross Coster, Net Coster, Taxer, and Residuals Evaluator. The three data files are: environmental constraints, materials costs, and financial groundrules.

The Sizer identifies the proper size of each configuration within the unit process based on the user's specification of desired product output level. Environmental constraints are employed in sizing the waste treatment configurations. The sizer establishes the materials balance, utilities requirements, and capital and labor requirements for the unit process at the designated level of output.

Determination of process costs is accomplished by means of the Gross Coster, Taxer, and Net Coster. The Gross Coster combines the process descriptions developed by the Sizer with the data files for materials costs and financial groundrules to determine the value added and gross product sales price of the product generated by each unit process. The gross sales price is that which would be demanded in the absence of taxes or market competition. If desired, venture profit may be specified for inclusion within the value added determination. The Taxer parametrically specifies several kinds of charges, taxes, and incentives. Examples of possible Taxer-imposed levies include: corporate income tax, investment tax credit, value-added tax, waste energy charge, and payroll taxes. The Net Coster determines realistic sales prices for the product, based upon adjustment of the Gross Coster results under the Taxer-imposed external burden.

The Residuals Evaluator is the fifth PCEM subprogram. This subprogram keeps track of the costs of residuals treatment prior to discharge, and nets total effluent production for the entire process. Charges for disposal which may also be incurred, such as for waste disposal, are included in unit process costs by the Gross Coster.

1.4.1.3. Industry Development Model (IDM)

The IDM organizes and interprets the process evaluation data developed by the PCEM where an aggregative assessment is required. The PCEM is, in effect, a single-point-in-time comparative evaluation of coal processes. For example, the conditions for one PCEM evaluation might be those projected for 1985. Since coal process technology will

be continuously evolving, it is necessary to make a series of such PCEM evaluations--for 1980, 1985, 1990, etc. The overall effect of a coal policy will be that achieved over a period of years. The IDM performs the necessary integrative role in the coal policy evaluations. It monitors which unit processes are used where (regionally) and when, and their characteristics based on PCEM assessments. The IDM then combines these results to provide a composite result. For example, one question requiring IDM use would be, "What are the aggregate investment requirements, assuming that the best available process is used, to incrementally increase syncrude capacity by 350,000 bbl/d in each of three years--1985, 1987, 1989?"

The IDM also will serve as the interface between the MPPM and other computational models during Phase III joint-model evaluations. The characteristics of the IDM necessary to perform this role will be identified at the onset of Phase III.

1.4.2. Utilization

1.4.2.1. Process Evaluation

A major function of the MPPM is to provide comparative process evaluations on a consistent basis. The perturbation approach employed by the Linking Model insures that all pertinent unit processes are being considered. As discussed in Section 1.4.1.2., the PCEM evaluates each unit process within the same financial, taxing, materials costs, and environmental constraints context. The process evaluations obtained by this approach provide a fair comparison of the different processes. Present approaches to process evaluation usually highlight the benefits associated with the subject process or set of processes. A substantial effort would be required to reconcile the many diverse process evaluations already conducted. Frequently, it is impossible to discern important underlying assumptions.

Model A of the MPPM will illustrate MPPM use in process evaluation. Four products are involved: on-site electric/mechanical energy, low-BTU gas, medium-BTU gas, and substitute natural gas (SNG). Fifteen functional modules participate in ten unit process routes leading to these four products. There are a total of 26 competing configurations for the functional modules. This leads combinatorially to 576 possible unit processes: 180 for on-site electric/mechanical energy, 108 for low-BTU gas, 72 for medium-BTU gas, and 216 for SNG. For each product, Model A will: (1) identify the feasible unit processes; (2) assemble these feasible unit processes into library storage for evaluation by the PCEM; (3) evaluate the unit processes under financial, taxing, materials costs, and environmental constraints specified by the user; and (4) print out a comparative listing of processes as requested by the user--top ten, bottom 50, entire list, etc. with product cost comparisons.

1.4.2.2. Policy Evaluation

The coal-based MPPM can assist in coal-process RD&D decisions. The two principal types of policy evaluations are sensitivity analysis and aggregative assessment. Use of the MPPM in both of these areas of policy analysis is illustrated in Chapter 4.

One use of MPPM for sensitivity analysis is exemplified by the question, "What Changes would occur within the top 25 unit processes for SNG upon successful development of a liquid-phase combined shift-conversion/methanation functional module?" A second use is exemplified by the question, "How do the data uncertainties of the configuration descriptions affect the comparative rankings among the top ten low-BTU-gas unit processes?"

Application of the MPPM to aggregative assessment is exemplified by the question, "How would the installed capacity for coal-derived methanol production increase over time, assuming a specified capital investment schedule?" This assessment requires that the unit processes

leading to methanol be identified. These unit processes themselves change over time. That is, an improved configuration for achieving the methanol synthesis step may be anticipated circa 1990. Similarly, a medium-BTU gasifier brought on stream in 1985 may be expected to achieve economies of scale by 1990. Such changes will tend to establish a different set of "best" unit processes in 1990 than in 1985, thereby leading to a change in the economics of the 1985 processes. The effect of inflation must be taken into account, perhaps by expressing the investment schedule in constant dollars. Another, related investment question is "What investment schedule is necessary to achieve a desired capacity for coal-derived methanol production?" Regional evaluations must take into account the types of coal to be employed.

1.5. REPORT ORGANIZATION

The report contains six chapters. Three appendices are included in a separately bound volume.*

Chapter 2 discusses the organization of coal-process technology data within the MPPM format. Based on our survey of the applicable literature during Phase I, we define a set of products and a set of 42 functional modules for deriving them from coal. "Unit process routes" through these functional modules have been organized into a "Road Map" of coal process technology, separately placed as a foldout contained at the back of this report.

Chapter 3 provides a detailed description of the MPPM as it is being developed for use in coal process analysis. A synopsis of this material was presented in Section 1.4. The manner in which the Linking Model identifies feasible unit processes is illustrated in Chapter 3. The methodology for developing competing configuration descriptions is also illustrated, for the case of the methanator functional module.

Chapter 4 discusses the need for coal process RD&D policy evaluation, and discusses the use of the MPPM for this purpose. Two illustrative cases are considered. The types of exogenous data, performance of the MPPM, and outputs provided are described for each example.

Chapter 5 assesses the use of the MPPM with other computational models. Seven of the principal models that could participate in a computer system for energy supply analysis are assessed. A diagram of the potential interaction among these models is also attached separately (along with the Road Map) at the back of this report. The strengths and weaknesses of each model are appraised in Chapter 5. Three potential sets of economic models are identified for joint computations with the MPPM. The attributes of each configuration are described and evaluated.

*The appendices contain product specifications, a catalogue of competing configurations, and detailed cost calculations for the methanator module.

Chapter 6 describes the project timeline and staffing. A detailed work plan is provided for Project Phases II and III. Project staffing is organized within the context of the project tasks. This report represents the final task in Phase I. The remainder of the project is 30 months in duration.

FIGURE 1.1

CHEMICAL PROCESS CHAINS LEADING TO VINYL CHLORIDE MONOMER
(Partial Representation for Illustration)

PROCESSES

- (1) Chlorine via diaphragm cell electrolysis, with coproduct caustic soda
- (2) Chlorine via mercury cell electrolysis, with coproduct caustic soda
- (3) Ethane via natural gas stripping, with coproduct propane
- (4) Oxygen via air separation, with coproduct nitrogen
- (5) Ethylene via fired tube pyrolysis of ethane (or propane)
- (6) Ethylene dichloride via direct chlorination of ethylene
- (7) Ethylene dichloride via oxychlorination of ethylene
- (8) Vinyl chloride monomer via ethylene dichloride pyrolysis
- (9) Vinyl chloride monomer via direct chlorination of ethane
("Transcat" process)

FIGURE 1-2

RESULTS OF A SENSITIVITY ANALYSIS AMONG VCM PROCESS CHAINS
(Chains Ranked on the Basis of Venture Cost of Sales)

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4. Powers, G. J., and Rudd, Dale F., "Heuristic Synthesis in Process Development," presented at the 71st National ALCHE Meeting, Dallas, Texas, February 20-23, 1972.

2. COAL PROCESS TECHNOLOGY

2.1. SCOPE OF COAL PROCESS TECHNOLOGY TO BE MODELED

The first chapter dealt with the objectives and organization of this project and gave some background on the techniques which we call materials-product-process analysis. This chapter will bound and particularize the manufacturing processes--coal processing technology--for which a new version of the Materials-Product-Process Model (MPPM) is being developed.

2.1.1. Products and Raw Materials

In accordance with the interests of the sponsor, the technological bounds of this project encompass the full range of means by which coal can be converted to useful energy products. However, to identify processes one must define products. A list of *every* marketed energy product would be unmanageable, and instead we have developed a list which encompasses products of major significance for production from coal, some of which can be competitors in established markets, and some of which are new products for which new markets must be identified. The list is shown in Table 2.1.

In Table 2.1. we classify products into three categories: energy products, material products, and by-products. Electric energy is classified into peak load (load factor of 0.2 or less with daily cycling of load) and base/intermediate load, because the types of equipment and fuel used to service these demands are likely to be quite different. A more detailed breakdown may prove to be desirable eventually. Thermal energy and on-site electric or mechanical energy is not presently thought of as a marketable commodity but we include them because they may prove to be attractive alternatives for the use of coal to replace other fossil fuels. For instance a large coal fired central plant to produce industrial process energy, which could be distributed within a local industrial complex as a heated working fluid (e.g., steam).

could prove more attractive than a multiplicity of small coal, oil, or synthetic liquid fuel fired furnaces distributed throughout the complex. The industrial user who now purchases fuel to make process heat, should be just as willing to buy thermal energy directly if the price is competitive.

The materials products are probably the focus of most intensive short-term interest, since they hold promise for the direct replacement of hydrocarbon products derived from petroleum and natural gas. During Phase II of this project, primary emphasis will be placed on building a data base for the evaluation of unit processes which lead to materials products.

As part of the Phase I effort we have developed a set of "Proposed Product Specifications" (PPS) for seven of the materials products with most immediate interest. These are marked in Table 2.1. with asterisks. The specifications are written so as to facilitate their use in the MPPM. Thus Substitute Natural Gas (SNG) is specified in terms of certain limits on its composition (principally methane content), rather than in terms of BTU content, although a gas which meets the composition requirements will have a BTU content which is comparable to that of natural gas (at least 910 gross BTU/SCF). Product specifications will be developed for other materials products during Phase II of this project, as the need arises and general agreement on requirements can be established. Thus a realistic product specification on Methanol will require that automotive transport manufacturers and/or gas turbine manufacturers establish standards for methanol use in their products. In the absence of industry guidelines we will develop "strawman" specifications for MPPM use.

The list of products in Table 2.1. should not be regarded as fixed or complete. As new technology is developed, new product forms derivable from coal will appear with the potential to compete with established products, perhaps in novel ways. The MPPM should not be regarded as a fixed structure with respect to products, any more than it should be regarded as finalized in its data base.

The input end of the coal-process technology is, of course, the raw material, coal. In itself, it is a diverse product, classified in numerous ways, e.g., by "rank", by sulfur content, by coking properties, by ash content, by heating value. The importance of each of these properties varies by type of conversion intended. Thus, certain gasifiers require non-coking coal and some can accommodate any type of coal. Sulfur content, in certain coal refining processes, must be specified as organic or inorganic.

Rather than make a list of "standard" coal types, we prefer to reference coal type to the initial conversion configuration, since this is the point of maximum sensitivity to variation in coal composition and properties. Thus the material balance relationships for a particular gasifier configuration as well as cost parameters will be particular to each type of coal; in effect each initial conversion configuration will have a set of variants which are differentiated by the type of coal being used as a raw material. Some configurations may be able to accommodate only a limited number of coals; others may be relatively insensitive to coal type. The data base for each configuration will be structured to reflect this diversity and to operate compatibly with the Linking Model.

The reason for handling the diversity of coal types in this manner is a pragmatic one; we expect that the developers of the various initial conversion configurations will have data on material balances and equipment costs by the types of coal they expect to be used with their conversion configuration. For example, the CO₂ Acceptor Gasification Process being developed by the Consolidation Coal Company is thought to be best suited to low-rank Western coals. We expect that the developer could supply data on the material balance and costs of this process for the low rank coals he would be able to mine on his western properties, but would have virtually no data on the use of this process with a high-rank Eastern coal.

2.1.2. Processes

The totality of all equipment configurations that are now being used, or have been conceived for use in converting coal to the products listed in Table 2.1. is, of course, enormous. The selection of equipment configurations to include in the MPPM data can only be an incomplete list, almost by definition. Manufacturers and researchers are each advocates of their own variants, and a certain amount of judgement is required to apportion the evaluative effort available in this project over a practical set of all possibilities. The immediate goal is to include, first, those conversion configurations for which the sponsor, ERDA, is providing development funds, second, those that seem to be attracting serious financial support from commercial sources, and third, those which are presently major factors in converting coal to marketable energy products. As noted in Chapter 1, the number of equipment configurations within these limited bounds is enormous, but it must be emphasized that omniscience is not an attribute of MPPM; it must be constantly evolving in both structure and richness of data in response to an ever changing perception of where coal-processing technology is proceeding.

Before defining an initial subset of processes to be modeled, it is necessary to define some terminology. In common usage a "process" is usually identified with a particular developer or manufacturer, and is more or less what the manufacturer defines it to be. Thus the "Lurgi Process", as it is usually thought of,* combines a certain design of a pressurized, fixed bed, reaction chamber where coal is partially oxidized with steam and oxygen to produce a gas which can subsequently be "shifted", "purified", and "methanated" to make SNG. The Lurgi company has designs for some very definite equipment configurations for accomplishing each step, but it is clear the Lurgi reaction chamber (i.e. "gasifier") could be followed by a number of variants in the operations subsequent to the gasifier. Similarly, a different gasifier (such as the synthane reaction chamber) could be combined with the Lurgi-advocated "Rectisol" purification step.

*The "Lurgi Process" is the SNG production method being marketed by Lurgi Gesellschaft für Mineralöltechnik, West Germany

The evaluations to be made by the MPPM are to be made at the level of "Economic-Unit Processes" (or Unit Processes), which are defined to be sequences of sets of equipment which start with marketable commodities as raw materials, and end with marketable products.* These sets of equipment accomplish identifiable functions such as gasification, purification, separation, methane synthesis, and ammonia synthesis. Each of these identifiable functions defines a "Functional Module", and each Functional Module represents a number of different possible (i.e., competing) sets of equipment. Each of these sets of equipment is called a "configuration." A complete Unit Process will be made up of a selection of one competing configuration from each Functional Module required for the desired operation. A "Unit-Process Route" is a certain sequence of Functional Modules, while a Unit Process is a particular selection of a competing configuration from each module along a unit process route. Thus the functional components of what is commonly known as the "Lurgi Process" are entered into the MPPM data base as particular competing configurations in a series of Functional Modules. When MPPM assembles a library of Economic Unit Processes, one entry will be the "Lurgi Process"; but many other entries will contain one or more functional components from the "Lurgi Process".

As part of the Phase I effort we have examined many sources of information on processes for transforming coal to other energy products, and from these we have assembled a catalogue of competing configurations which we have organized into forty-two Functional Modules. Our method of identifying Functional Modules, Unit-Process Routes, and Competing Configurations is discussed in the next section.

* The glossary contains definitions of terms which have specific meanings for materials-product-process analysis.

2.2. IDENTIFICATION OF COAL PROCESS TECHNOLOGY MODULES

2.2.1. Module Definition and Boundary Choices

A Functional Module is a defined operation, i.e. it accomplishes a task that can be quantified in terms of an input and an output. We allow the quantification to be parametric if necessary; an example of a parametric input/output relationship is that of a shift converter (discussed in Chapter 3 under the operation of the Linking Model), where the amount of H_2 to be made from CO and H_2O by the so-called shift reaction

is governed by requirements of other module configurations which precede and follow it in any particular Unit Process.

All competing configurations listed under a given Functional Module accomplish the same quantified task. Thus the output of the Functional Module we call "Methane Synthesizers" is defined to be "Substitute Natural Gas" delivered at standard, pressure, temperature, and moisture content, such that it is acceptable as an input to a natural gas pipeline. All competing configurations in this module must deliver this defined product.

Engineering "process flowsheets" are usually the best source of information for defining functional groupings of equipment. Examples of two such flowsheets are shown in Figures 2.1. and 2.2. We have marked on these diagrams the boundaries of some candidate configurations for various Functional Modules, e.g. Gasification, Shift Conversion, Gas Purification, Methane Synthesis. (During the course of Phase I we have examined several hundred flowsheets that depict "processes" in varying levels of equipment detail. These were collected together in a special report to the contract sponsor.*) Obviously there is a good deal of judgement involved

* IRT-405-R "Flow Diagrams and Process Modules for MPPM Analysis of Coal Utilization Processes", October 1975.

in deciding where to place the boundaries between modules. For example, the char towers in Figure 2.1. could have been included in the Gas Purification block. However, the function of these char towers is to remove the last trace amounts of sulfurous gasses in the input to the methanator, due to the sensitivity of the methanator catalyst to these impurities. For this reason, the char towers do not represent a general requirement for all module configurations that could use the output of the Gas Purification Module as an input.

Comparing Figure 2.1. and Figure 2.2. we also see that the Methane Synthesis Module configuration in the latter includes a drying tower for the product gas while the configuration in the former does not. In fact, the product gas of the system shown in Figure 2.1. would not meet the defined moisture content standard for SNG. The methane synthesis configuration in Figure 2.1. would not be acceptable as shown; a drying tower or other dehydration device would have to be added, and the cost parameters of the configuration adjusted. Standardized methane synthesis configurations are discussed in detail in Chapter 3.

Another anomaly appears in Figure 2.2. in the form of the coal slurry preheater in the methane synthesis block. This is an energy recovery strategy dictated by the peculiarities of the particular process integration employed. In MPPM models, energy recovery is always assumed to be through a utility module which nets fuel, steam, cooling water, and electric energy requirements of an entire Unit Process. Thus the configuration for methane synthesis shown in Figure 2.2. would be modified for the MPPM by using steam generation as the thermal energy recovery device. The gasification configuration would be modified to include a steam input to provide coal-slurry preheating. Cost parameters would be adjusted to account for these changes. For any Unit Process, the relative cost inequities due to such adjustments should be well below the accuracy threshold of the available cost data.

The selection of a proper level of detail for disaggregation of process flow diagrams into module configurations is an extremely important aspect of the application of the MPPM to analysis of coal-

processing technology. The level of detail must be sufficient to reflect important parametric variations yet it is essential to avoid unnecessary detail that can lead to increased computational load while adding little to the ultimate result. The MPPM is intended to work in conjunction with detailed engineering designs, not to replace them.* The MPPM seeks to deal with functional units rather than to focus on an individual unit operation--such as the absorber columns used within the gas purification section. Engineering calculations are made at the unit operation level, and then are aggregated into functional unit operating characteristics and costs. The input needed by the MPPM is functional unit data.

2.2.2. Module Interconnections

We have discussed the Unit Process Routes (sequences of Functional Modules) in terms of the raw materials and products of interest. One of the two diagrams in the back cover pocket of this report is the "road map" of these routes. The products listed in Table 2.1. are shown on the right side of the diagram, raw materials on the left. The forty-two numbered squares represent Functional Modules; the circles represent materials or energy forms.

Waste and by-product streams and modules for processing these materials are included on the road map. These form branches off the main flow of raw materials to products, but should be considered as integral parts of complete Unit Process Routes. All inputs and outputs are accounted for in the MPPM, at least to the extent that data is, or becomes, available. Thus, Module #38 ("Waste Disposal") includes stacks for release of cleaned gaseous effluents, lagoons for storage and

* The relationship between the MPPM and conventional engineering computational models is discussed in Section 2.3. In brief, the MPPM organizes the results from detailed engineering studies into a form that allows wide-spectrum comparative analysis of Unit Processes and develops the results into suitable input for generalized energy and economic models.

evaporation of liquid wastes, and land-fills for disposal of solid wastes. Costs of these disposal operations, as well as for all required waste treatment operations, are included in the evaluation of Unit Processes.

Some "feedback" routes exist on the road map, such as recovery of various minerals and chemicals for reuse. "Seed" recovery (usually potassium carbonate) from MHD (Magneto-Hydro-Dynamic) electric power generation flue gases is an example of mineral recovery. Interesting feedback paths occur with so-called "char" (unreacted carbonaceous wastes), which results from many gasifier configurations. Char is a suitable input to many types of gasifiers. Thus char from a Module No. 4 ("Gaseous Phase Coal Hydrogenation") configuration can be the input to one of several medium BTU gasifier configurations (Modules 2 and 3), with the product gas used to produce part or all of the hydrogen required as input to the Module No. 4 configuration. This is precisely the mode of operation for some variants of the IGT "HYGAS" process.

An implied example of a process chain also occurs in the road map. The "Clean Solid Fuel" and "Clean Liquid Fuel" circles on the upper lefthand edge of the road map are products that appear on the lower right edge. Thus some Unit Process Routes lead from coal to clean solid fuel, and others from clean solid fuel to electric energy. The series combination of Unit Processes from these routes is a Process Chain leading from coal to electric energy.

2.2.3. Catalogue of Competing Configurations

Several hundred Competing Configurations have been identified within the forty-two modules shown on the "road map". These are listed in Appendix B in module groups, each with an assigned module, sub group, and sequential number. To illustrate, in module group no. 14 ("Gas Purification"), subgroup "C" comprises those configurations where acid gases are absorbed in an alkaline salt solution. The Benfield gas purification method, which uses a hot potassium carbonate solution, is assigned sequential number "4" and is thus designated configuration 14,C,4.

Other entries in the tables in Appendix B indicate whether a flow chart and/or an equipment schematic is available for the configuration, and our classification of the configuration as "advanced", state-of-the-art" or "out-of-date" technology.

Building a data file for each of the configurations listed in Appendix B would be beyond the resources available to this project. Therefore, we have compiled a reduced list of 112 of what presently appear to be the most interesting configurations. This list is given in Table 2.2., classified into two groups called "First Generation" and "Advanced". The "First Generation" appellation is given to those configurations which are commercially available or which appear to be very close to commercial application, i.e. which have either become the "state-of-the-art" or have reached the pilot-plant demonstration phase with promising results.

The initial effort in Phase II of the project will be concerned with executing a feasibility demonstration version of the coal-processing technology MPPM, our so-called Model A. This will be done using a restricted subset of products, a delimited set of Functional Modules and routes from the "road map", and a limited number of configurations for each selected module. The products will be

- Low-BTU Gas
- Medium-BTU Gas
- Substitute Natural Gas
- On-Site Electric (Mechanical) Energy
- Appropriate By-Products

The extracted "road-map" for these products is shown in Figure 2.3. The competing configurations to be modeled are marked by asterisks in Table 2.2.

After the initial data base of files for the asterisked configurations has been completed and used with the algorithmic structure of MPPM to demonstrate the feasibility of the approach, modeling of the remaining configurations in Table 2.2. will proceed. Products and Modules will be added until the complete road-map structure is in place.

The order in which configurations will be added will be decided pragmatically, as the sponsor expresses particular interests and as data becomes available. The list in Table 2.2. should not be regarded as immutable; additions and subtractions will undoubtedly be made as new insights are gained in the progress of coal-processing technology. However, the list does represent an order-of-magnitude estimate of the expected size of the MPPM data base at the conclusion of Phase III of the present project.

2.3. COLLECTION OF COAL PROCESS DATA

2.3.1. Content of the MPPM Data Base

In the MPPM data base, engineering and cost data for the competing configurations are organized into individual files for each configuration. Typical complete files are developed in Chapter 3 for three configurations under the Methane Synthesis Functional Module (No. 9). Configuration data files include material and energy input/output data, and cost data at a nominal design point, together with scaling parameters that allow computation of equivalent values at other design points. External variables that control scaling include, besides the obvious one of configuration throughput,* such input/output descriptors as gas pressure, composition of liquids and gases, and physical form of materials.

The MPPM data base also includes a Utilities and Materials data file which is a tabulation of all materials and energy forms that appear as an input or an output to any configuration in the data base. For each entry, the file stores, as may be appropriate:

- a numerical code
- chemical properties (formula composition, heats of combustion, chemical oxygen demand, biological oxygen demand, etc.)
- physical properties (density, freezing and boiling temperatures, etc.)
- value or price

2.3.2. Data Sources

With the many diverse alternatives for coal utilization currently being developed, and the large amounts of government funds being channeled through ERDA and other agencies for RD&D work, the advocates of each competing method have a vested interest in maintaining government attention to--

* "Throughput" is defined as the amount of main product manufactured per unit time.

and confidence in--their approaches. Therefore, it is to their advantage to supply the best possible information on their processes to an evaluative program like MPPM, provided that they have confidence in its fairness and objectivity. With commercial developers, the desire to retain the privacy of advantageous proprietary information will be a countervailing influence. The availability of data from developing organizations will probably vary greatly, and the active support of ERDA personnel will be critical to the success of the MPPM data gathering effort.

While MPPM is basically interested in externalities (i.e., in a "black box" view of configurations), sufficient insight into the internal design is required to assure consistency of cost data, and compatibility with a standard analytical method of accounting for utility requirements. Surprisingly diverse estimates of costs for similar items, such as compressors and pressure vessels, can be quoted by different engineers, depending on assumptions about materials, safety margins, design details, and cost escalation allowances. While it is reasonable to expect some of this divergence to "average-out" when large numbers of individual component-cost estimates enter into the final total cost, part of the data gathering effort will require some probing into design methods and assumptions.

A logical sequence for gathering data on particular configurations would be to start with published descriptions and data, identifying, if possible, the critical external variables that will influence costs, and finally consulting with the developing organization (or the manufacturer, for units using state-of-the-art technology) for firm design data. In Chapter 3 and Appendix C we develop the data files for three "Methane Synthesis" configurations, as an example to show the feasibility of MPPM modeling. Because of limited time and funds during Phase I, we were able to effect only limited contact with the groups doing the research and development on the configuration. Instead we adapted standardized configuration designs from published reports and derived costing equations, using vendor data for component costs, to produce the required design

data. This data is in the form of costs, input/output material balances, and utility requirements as a function of throughput and certain other external parameters. The exercise of developing the methanator module configuration data files was instructive in providing insight into the problems of obtaining the type of data required for MPPM. The amount of work required is not trivial, and may be more than some developing organizations can afford to provide. Our approach will be to work with ERDA personnel, ERDA contractors, and independent experts to develop configuration data files from available designs, and to extend this data, by joint effort, where necessary.

Other possible sources of assistance in developing parametric design data (if additional funding is provided by ERDA) would be engineering computational models. (MPPM is, in fact, intended to form the necessary bridge between detailed engineering models and more general systems-analytic, or policy-analytic, models.) These engineering models involve three levels of computation: determination of physical/chemical properties, such as viscosity, van Laar coefficients, etc.; evaluation of equipment performance, such as the composition of streams flowing into and out of a distillation column with accompanying column diameters, number of plates, heat balance, etc.; and costing of equipment, including capital requirements and operating costs, such as raw materials, labor, electric power, etc.

The APPES (A.I.Ch.E. Physical Property Estimation System) program developed by Arthur D. Little under the sponsorship of the A.I.Ch.E. is representative of the physical property estimation programs. This system can estimate properties of both pure substances and mixtures. In the original formulation, 122 estimation methods were provided. Usually, several alternative methods are available for estimating each property.

There are a number of commercially available programs that focus primarily upon equipment performance. Usually these programs also estimate equipment costs, but most of the computational effort is devoted to the performance evaluation. Two program packages are representative of the type of computational programs available. PACER^R, an acronym for

Process Assembly Case Evaluation Routine, is marketed by Digital Systems Corporation, Hanover, New Hampshire.

FLOWTRAN_{TM}, short for Flowsheet Translator, was originally developed by Monsanto for in-house use, but several years ago was offered commercially. Both models incorporate detailed property data for many materials, and engineering and economic descriptions in parametric terms for most types of chemical process equipment. The user must provide a flow sheet description of the configuration, plus property data and equipment models not furnished with the program. The user must also specify the states of the entering raw materials and desired product. The computer program employs the necessary subroutines to provide a steady-state flow pattern for plant operation, and to determine the associated equipment and operating costs. PACER and FLOWTRAN offer several levels of computational complexity. The range is from approximate economic evaluations to specification of the exact operating conditions for plant equipment, and in the case of PACER an optimum can be established.

ICARUS Corporation has developed a computational program--called CØST--that focuses upon providing detailed cost data. In one mode of operation, the user provides the equipment specifications; then CØST designs each piece of equipment, prices it, and determines installation costs by calculating the required direct labor and bulk materials, such as steel, cement piping, etc. Indirect costs and contingency and fee percentages are also estimated. EPA has used this system to cost water treatment facilities, and ERDA has used it to evaluate a number of coal processes.

In general, these engineering programs offer reliable, flexible, and rapid means for obtaining configuration models. The costs of program use are very high, however, when placed in the context of a study program such as the present one--although not when compared to other costs encountered during an RD&D program. The present project will seek to use estimates from the various development programs, rather than directly funding detailed engineering computations. ERDA may, however, continue to fund such engineering computations, in which case the information will be available for use in the MPPM analysis.

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FIGURE 2.2.

FLWSHEET FOR SNG PRODUCTION USING THE
IGT "HYGAS"-(SINGLE VESSEL) GASIFIER

TABLE 2.1
PRODUCTS OF COAL PROCESSING TECHNOLOGY

A. ENERGY PRODUCTS

- o High Temperature Thermal Energy ($T \geq 400^\circ\text{F}$)
- o Low Temperature Thermal Energy ($T < 400^\circ\text{F}$)
- o Base/Intermediate Load Electric Energy
- o Peak Load Electric Energy
- o On-Site Electric (Mechanical) Energy

B. MATERIALS PRODUCTS

- o Low-BTU Gas*
- o Medium-BTU Gas*
- o Substitute Natural Gas (SNG)*
- o Anhydrous Ammonia
- o Methanol
- o Oxygenated Hydrocarbon Mixtures
- o Low Molecular Weight Gaseous Hydrocarbon Mixtures*
- o Aromatic Mixtures
- o Low Molecular Weight Liquid Hydrocarbon Mixtures
- o Middle Distillate Oils (Low Sulfur No. 2 Distillate Fuel Oil Equivalent)*
- o Clean Liquid Boiler Fuel (Low Sulfur Residual Oil Equivalent)*
- o Clean Solid Boiler Fuel*

C. BY-PRODUCTS

- o Sulfur/Sulfur Compounds
- o Ammonia/Ammonia Compounds
- o Aggregates
- o Gypsum
- o Argon
- o Nitrogen
- o Carbon Dioxide

*"Proposed Product Specifications" (PPS) for these materials products are given in Appendix A.

TABLE 2.2

First Generation and Advanced Configurations
to be Included in the MPPM Data Base

<u>Functional Module</u>	<u>First Generation</u>	<u>Advanced</u>
1. Low BTU Gasifier	1,A,1 Lurgi* 1,B,1 Winkler 1,C,1 Koppers Totzek	1,B,2 Westinghouse 1,B,3 BCR 1,B,4 IGT* 1,D,1 Atomics Int.
2. Medium BTU Gasifier- Internal Heat Type	2,A,1 Lurgi* 2,B,1 Winkler	2,B,3 Synthane* 2,B,4 Single-vessel HYGAS 2,C,2 Bi-Gas
3. Medium BTU Gasifier External Heat or Circulating Heat		3,A,1 CO ₂ Acceptor* 3,A,3 Ash-Agglomerating
4. Gaseous-Phase Coal Hydrogenators		4,A,2 Hydrane 4,A,3 COED
5. Liquid-Phase Coal Hydrogenators		5,A,1 H-Coal 5,A,2 Synthoil
6. Solvent Extractors		6,A,1 SRC
7. Chemical Extractors		7,A,1 Battelle
8. Coal Pyrolyzers		8,A,2 TOSCOAL
9. Methane Synthesizers	9,B,1 Multiple-Fixed-Bed*	9,A,1 Tubewall with PGR* 9,A,2 Tubewall without PGR* 9,D,1 Chem Systems
10. Methanol Synthesizers	10,A,1 High Pressure Catalytic	
11. Fischer-Tropsch Synthesizers	11,A,1 Kellogg 11,B,1 Ruhrchemie-Lurgi	
12. Ammonia Synthesizers	12,A,6 Haber Bosch 12,A,7 American (Large)	

TABLE 2.2 (Continued)

<u>Functional Module</u>	<u>First Generation</u>	<u>Advanced</u>
13. Shift/Reverse Shift Synthesizers	13,A,1 Chromium Promoted Iron* 13,B,1 Cobalt-Moly 13,D,1 Reverse Shift	
14. Gas Phase Separators/Purifiers	14,C,4 Benfield* 14,E,1 Rectisol 14,F,2 Selexol	
15. Hydrogen Purifiers	15,C,4 Benfield 15,E,1 Rectisol 15,F,2 Selexol 15,H,1 Methanator 15,J,2 Linde	
16. Coal Preparation	16,A,3 Roll Crusher* 16,B,2 Ball-Race Pulverizer 16,B,4 Ball-Mill Pulverizer*	
17. Mineral Preparation	17,A,2 Roll Crusher 17,B,1 Hammer Mill* 17,B,4 Ball Mill* 17,G,1 Thickener 17,I,1 Dissolver 17,N,1 Centrifuge	
18. Oxygen Producers	18,A,1 Liquid Air Distillation*	
19. Liquids/Suspensions Separators/Purifiers	19,B,1 Pressure Filter 19,C,1 Vacuum Filter 19,D,1 Classifier 19,E,2 Dorr Thickener 19,H,2 Centrifuge 19,J,1 Distillation 19,L,1 Decanter	
20. Hydrotreaters		20,A,1 COED 20,C,1 SRC
21. Liquids/Gases Separators/Purifiers	21,B,1 Condenser 21,D,2 Cyclone 21,F,1 Flash Distillation 21,G,s Distillation	

TABLE 2.2 (Continued)

<u>Functional Module</u>	<u>First Generation</u>	<u>Advanced</u>
22. Hot Gas Cleaning	22,A,1 Cyclone*	22,B,1 High Temp Electrostatic Precipitator 22,D,1 Expanded Bed Filters
23. Oxidation-Reduction Hydrogen Producers		23,A,1 IGT Steam-Iron
24. Conventional (Furnace/Boiler)	24,A,1 Gas Furnace 24,A,2 Oil Furnace 24,C,1 Pulverized Coal Furnace	
25. Fluidized Bed (Furnace/Boiler)		25,A,1 Westinghouse 25,B,1 Pope, Evans, and Robbins
26. Cyclone Furnace	26,A,1 Cyclone Furnace	
27. High Pressure Burners/Furnaces		27,C,1 Solid Fuel Fired
28. Hot Gas Pyrolyzer		28,A,1 MHD Exhaust Suspension Gasifier
29. Direct Coal Burning MHD		29,A,1 Single Stage MHD
30. High Temp Thermo/Turbo-Electric Converters	30,B,1 Gas Turbine	30,A,1 MHD
31. Flue-Gas Clean-Up Processes	31,B,2 Cyclone 31,D,1 Electrostatic Precipitator 31,F,1 Limestone Scrubber 31,G,1 Envirotech 31,I,1 Chemico 31,J,1 Wellman-Lord 31,M,1 Citrate 31,N,1 TVA-EPA	31,R,1 Consolidation Coal
32. Flue-Gas Thermal Energy Recovery	32,A,1 Tubular Feed-Air Heater	31,B,1 Steam Boiler for MHD Exhaust
33. Low-BTU Gas Clean-Up	33,A,1 Cyclone* 33,B,1 Scrubber* 33,E,1 Electrostatic Precipitator	

TABLE 2.2 (Continued)

<u>Functional Module</u>	<u>First Generation</u>	<u>Advanced</u>
34. Mineral Recovery & Waste Treatment	34,D,1 Ammonia Stripping* 34,F,2 Liquid/Liquid Extraction 34,G,1 Evaporation Pond 34,CC,1 Claus Plant* 34,FF,1 Stretford 34,GG,1 Chance*	
35. Turbo-Electric Power Converters	35,B,1 Reaction Turbine	
36. Outlet Cooling	36,D,3 Hyperbolic Cooling Tower	36,F,1 Dry Cooling Tower
37. Gas Turbine/Electric Power Generators	37,A,1 Basic Gas Turbine* 37,A,2 Gas Turbine with Regeneration	
38. Waste Disposal	38,I,2 Landfill* 38,K,1 Stack* 38,L,1 Lagoon*	
39. Demethanators	39,A,1 Methane Reformer	
40. Coal/Chemical Slurry Separators	40,A,1 Centrifugal Filter 40,A,2 Filter Press	
41. Char Preparation	41,A,1 Ball-Mill Pulverizer*	
42. Nuclear Disassociation of Water	42,A,1 Thermal Disassociation	

3. MPPM DESCRIPTION AND METHODOLOGY

In Section 1.4 of this report, we presented a generalized description of the Materials-Process-Product Model. We indicated that it consists of a data base organized by functional modules (with competing--i.e., alternative--configurations within each functional module) and three algorithmic structures:

- A Linking Model (LM) that links selected competing configurations from a series of functional modules to form complete unit processes for converting coal into desired end-products, by-products, and environmentally acceptable waste streams,
- A Process Chain Evaluation Model (PCEM) that compares the costs of these unit processes under the constraints of exogenously specified financial parameters, e.g., taxes, interest rates, raw material costs, and computes the residuals generation and other environmental impacts of the unit process, and
- An Industry Development Model (IDM) that evaluates the cumulative effects of given industry development scenarios and interfaces with other economic models.

The data base structure and the PCEM were developed in the original MPPM foundation and are carried over to the coal-processing technology version of MPPM being developed under this contract but with extensive modifications. The LM was originally part of the PCEM but is given a separate identity here because of the increased complexity of the algorithms required. This increased complexity arises from the variable composition of the intermediate products encountered in transforming coal to desired products. The IDM is a newly defined part of the MPPM and is necessary to perform an interface function between the PCEM and the policy analyst or some larger scale economic model.

In this section we present a more detailed description of the data-base structure and the algorithmic structure of MPPM as we are developing them to meet the requirements of coal-processing technology analysis. The emphasis is on the necessary structure; the limited data

collection and generation undertaken in Phase I was accomplished primarily to illustrate the procedure and prove the feasibility of adapting the MPPM to coal-processing-technology analysis. Further work is required in Phase II to complete and refine the algorithmic structure and to build the data base.

Figure 3.1* presents a schematic of the relationship between the major MPPM components. The PCEM is the heart of the MPPM. Through the use of the PCEM, the relative costs of coal processing alternatives can be established for any given set of environmental constraints, taxing regulations, and other financial ground rules. The LM generates a listing or "library" of feasible processes for the PCEM to evaluate, and the PCEM results form the data input to the IDM scenario calculations.

* Figures and tables are consolidated at the end of each chapter.

3.1 MODULE AND MATERIAL DATA FILES

3.1.1 Data Requirements and Sources

The foldout in the back of this report shows a "road map" of the myriad ways by which useful energy products can be obtained from coal. The depicted routes lead through 42 numbered boxes which we call "Functional Modules". Raw, intermediate, and waste materials are shown by circles on the directed lines leading from module to module. End products are listed on the right side of the diagram.

Associated with each Functional Module are one or more competing configurations, which are collections of equipment potentially capable of performing the function of the module. In general, these configurations are designs that have been proposed or are being used by one or more of the various agencies or companies that are developing coal conversion processes. For instance, the Institute of Gas Technology is developing a multiple-fixed-bed methanator with product gas recycle, while ERDA, at its Pittsburgh Energy Research Center, is developing tube-wall methanators. These are both potentially capable of fulfilling the requirements of functional module No. 9, "Methane Synthesizers", and are "competing configurations". Other hardware designs are also being developed for methane synthesis; and it is probable that designs not yet conceived will become important in the future.

For each competing configuration, a performance data set is required. The data set components are:

- Input-Output materials balance relationships and restrictions
- Net utility requirements (electricity, fuel, steam, and cooling water)
- Capital cost data
- Operating cost data.

The data must be in a form that allows computation of costs, utility requirements, and materials balances as a function of module "throughput" (amount of primary product made by the module per unit time) and other pertinent external parameters, e.g., the pressure of the input gas (if it is a gas) or the composition of the input material, e.g., the amount of methane already present in the input gas to a methane synthesizer. Some of this data, particularly that related to materials input-output balancing, may be common to all competing configurations, but cost data generally will be different for each competing configuration.

The data for each competing configuration is assembled into a standard format file consisting of a descriptive title, a description of the primary input and output materials, a list of process parameter values for a nominal design (e.g., throughput, inlet gas pressure, temperature, fixed capital cost, operating cost parameters) with scaling factors which allow computation of costs for other throughput and design parameters, and a list of materials and utility inputs and outputs with balancing quantities at the nominal design conditions. Specific examples of data files for some competing configurations in Module No. 9, "Methane Synthesizers", are given in Section 3.1.3.

Materials are classified into eight categories:

- (1) Primary raw materials, i.e., coal of various types
- (2) Intermediate materials produced in precursor functional modules, e.g., synthesis gas
- (3) Secondary inputs, e.g., minerals such as dolomite, water, air
- (4) Primary outputs, e.g., SNG, anhydrous ammonia
- (5) By-products and co-products, e.g., sulfur
- (6) Gaseous wastes
- (7) Liquid wastes
- (8) Solid wastes.

A separate file of materials data is included in the MPPM data base. Materials data includes a numerical designation, description,

chemical names, chemical and physical properties (e.g., heat of combustion, molecular weight), and market values (prices).

The list of materials for the original MPPM consisted of 132 numbered items, all of which were taken to be either pure substances, mixtures with fixed proportions, or manufactured items. Some of these will be useful in the present version, but we must also accommodate mixtures with variable proportions of constituents, e.g., synthesis gas and SNG, the input and output of Module No. 9, "Methane Synthesizers". To handle these products we will use a new set of materials, itemized beginning with the number 200, in which the basic item is tabulated in physical units and a series of subscripted items, 200.1, 200.2, etc., are used to designate proportions of constituents. Numbers 200 to 299 will be used for products; 300 to 399 for equivalent intermediate materials; and 400 to 499 for actual intermediate materials. (Each actual intermediate material has an equivalent intermediate material appropriate to that module. The two may, in fact, be identical. Equivalent intermediates are sometimes useful in simplifying material balance computations. Equivalent intermediate materials will be used in the Methanation Example in Section 3.1.3.)

The module data files are completed by gathering engineering data on competing configurations in a form which allows correlation of cost and materials balance data with throughput and a small number of other external parameters of primary importance. The prime source for data of this type is naturally the engineering organization that is developing a particular competing configuration. The ideal form of the data would be in a series of point-designs* which cover the practical range of throughputs and other external parameters. The relationship between costs and external parameters would be deduced from this set of point designs by curve fitting and engineering analysis.

*A "point-design" is simply a complete specification of a configuration at some fixed set of parameters, i.e., at a "point" in parameter space. It would include quantitative material and energy input-output balances and capital and operating costs.

Rough data on the date of availability of major process components will be entered. This data will not be available for each configuration. At the present time, we intend to introduce this constraint at the IDM scenario level of the model.

Ideal data will not always be available, and judgments based on similarities between various equipment designs may be required. Other sources of design data may be drawn upon, such as reports of other ERDA contractors; government agencies, such as the Bureau of Mines; and vendors of preliminary design programs, like ICARUS. It is important to recognize at the outset that authority to obtain the necessary data resides in ERDA itself. The data base to be developed by IR&T will be neither final nor complete, since new methods of accomplishing the requirements of the Functional Modules and new data on known methods are constantly being generated. A continual updating of the data base will be required to maintain the validity of MPPM computations.

3.1.2. Data Validation and Standardization

One of the most important aspects of assembling data on competing configurations is assuring that costing data is derived on a consistent basis for each competing configuration. Functional module boundaries are to some extent arbitrary, and placing particular items of equipment, such as compressors, on one side of the boundary or the other can have a significant effect on comparative costs. Therefore, it is necessary to standardize configuration descriptions and flow sheets, and to recognize the large contributors to cost so that a correct and consistent list of important external parameters is chosen.

Similarly, design data from different organizations needs to be checked for a consistent cost basis. Surprisingly large variations can be found in the cost assigned to rather common items of equipment, such as compressors and pressure vessels. The existence of inaccuracies is not in itself surprising or particularly distressing; preliminary design costing is seldom expected to be more accurate than ± 30 percent for state-of-the-art technology and cost estimates for developmental technology must be expected to be even more uncertain. However, comparability between cost estimates is important and should be obtainable in the ± 20 percent range of uncertainty for closely related configurations.

Our system for building the configuration data sets and for validating and standardizing the data may be summarized as follows:

- Obtain process descriptions, flow sheets, and engineering data.
- Analyze these to identify the principal external parameters that determine costs, effluent characteristics, and utility requirements. Verify conclusions by consultation with developing organization and outside experts.

- Obtain standardized point designs, including cost evaluations, for each configuration to be modeled. The external parameters and throughputs of these designs should cover the full range of practical applications.
- Evaluate these designs for consistency of process chemistry and conditions and costing methods. Modify as appropriate to obtain consistency.
- Correlate point-design costs and material flows with the variations in throughput and other external parameters.
- From these correlations, develop relationships between input and output material quantities and composition, costs, and utility requirements.
- Codify the model into a standard data format.

Another aspect of data standardization concerns utility requirements, particularly steam. In general, at the time a plant is designed, a detailed study of the process heat required or generated at various places is made, and some choices are made as to the grades of steam that should be used for optimum economy, e.g., a high pressure, super-heated steam for turbine drives, and lower pressure saturated steam for process heat requirements. The range of available choices is quite wide and each plant will be designed with a unique selection. At the preliminary design level, appropriate to MPPM costing, a standardized set of choices is required so that steam requirements for entire unit process (assembled from competing configurations in a given sequence of functional modules) can be summarized and the net cost of providing utility steam evaluated. The cost penalty relative to an optimum choice of utility steam service will be well below the uncertainty threshold in the available data.

To standardize calculations as much as possible, we specify the following three grades of steam:

1. Saturated steam at 1200 psia ($T = 567^{\circ}\text{F}$)
2. Superheated steam at 1200 psia ($T = 900^{\circ}\text{F}$)
3. Saturated steam at 120 psia ($T = 341^{\circ}\text{F}$)

The first grade is steam that can be generated in many functional modules (such as methane synthesizers) and can be superheated to the second grade. The second grade is a suitable input to steam turbine drives for centrifugal gas compressors, of which there will be many throughout the unit process plants. The third is a suitable source of process heat for many functions, and is also obtainable as the exhaust of steam turbine drives at relatively little efficiency penalty. The steam rate for a steam turbine with 65 percent turbine efficiency using the superheated steam listed above as an input and exhausting steam to 120 psia backpressure will be about 16 lbs./hr./B.H.P. We assume that steam drives for compressors are so designed, and we will adjust cost data from all sources to reflect these standards.

3.1.3. Representative Module (Methanation)

To clarify the discussion of the last two sections, we will now discuss an example of data collection for some competing configurations. We have identified five apparently viable competing methanator configurations for accomplishing the function of Functional Module No. 9, "Methane Synthesizers". These are listed under Module Group No. 9 in Appendix B. We have assembled sufficient data to formulate data files for three of these configurations:

9,A,1 Tubewall Methanator with Product-Gas Recycle

9,A,2 Tubewall Methanator without Product-Gas Recycle

9,B,1 Multiple-Fixed-Bed Methanator with Product-Gas Recycle

The data files are "models" of these methanators, and we will often refer to them by this terminology. They should be regarded as evolutionary in nature, particularly as regards costs. We are continually searching for improved cost estimates as functions of the throughput and other pertinent input/output variables. All of the competing entries in this module group are in either the research, the development, or the demonstration phases of progression to proven commercial processes. Therefore, we expect changes in process parameters and cost estimates.

The models consist of four separate parts. The first part is concerned with quantitative balancing of flows of input raw materials and output products, by-products, and wastes. The second is concerned with capital costs of the equipment as a function of throughput, input raw materials composition and physical state, and output product specifications. The third is concerned with direct operating costs of the modules vs. designed throughput. (Indirect operating costs will be evaluated for complete unit processes.) The fourth part of the model evaluates utility requirements, e.g., fuel, electric power, steam, and cooling water, as a function of throughput.

(Utility capital and operating costs are determined from aggregated utility requirements for complete plants).

The materials flow parts of the model are almost identical for all three of the methanator configurations considered here. Considerable differences exist, however, in the capital cost parts. Lesser differences occur in the operating cost and utility requirements parts of the models.

In formulating the models reported here, we have followed the methodology described in the previous sections. However, we have had to supplement the procedure in this case by using our own rough design analysis and costing procedures to develop sufficient point-design data. We have had at our disposal five examples of tubewall methanators with product-gas recycle,¹⁻⁵ and two of multiple-fixed-bed methanators with product gas recycle,^{6,7*} from the Bureau of Mines, Process Evaluation Group (BM-PEG) at Morgantown, West Virginia. These did not span a sufficient range of parameters to allow a correlation analysis. In addition, there were sufficient differences in internal process conditions and costing assumptions to make the results inappropriate for direct use in constructing models which would be used for inter-configuration comparisons. (This observation is not meant to be a criticism of the BM-PEG studies, which were done for purposes not directly related to our modeling efforts. It does, however, point up the fact that studies which are undertaken to provide design and cost data for ERDA's use in the MPPM context should be guided by a consistent set of ground rules to promote data compatibility).

To obtain the point-design data for this study, we have undertaken a more detailed analysis of the methanator configurations. We have formulated standardized configuration descriptions and flow sheets, fixing certain key process parameters (e.g., temperatures and dilution levels) and identified costing elements within each configuration. Parametric cost equations for the elements have been developed from various sources, including commercial vendors, and -- where possible -- using element costs from the BM-PEG reports as base cases. We have

*References are listed at the end of this chapter.

computed overall configuration costs as a function of throughput, raw material state (i.e. pressure at which the input gas is delivered), and raw-material composition. This computed data has then been treated as point-design data in the development of the configuration models. Our computed cost data is presented in Appendix C.

This procedure is much too complex and time consuming to be appropriate for use in constructing models for all the modules, and competing configurations within modules, listed in Appendix B. Future modeling will have to depend to a much greater extent on point design data drawn from sources such as process developers, ERDA, and groups like BM-PEG.

3.1.3.1 Module and Configuration Definitions

The product of the "Methane Synthesizer" module is "Substitute Natural Gas" (SNG), as defined in our Proposed Product Specification No. 1 in Appendix A. In essence, the gas is to be 90% Methane delivered at pipeline pressure (1015 psia), temperature (100° F), and water vapor conditions (5.2 grains per 100 ft³). The sulfur content condition for SNG will be automatically met for all methanator configurations because sulfur must be excluded from the input to the methanation catalyst to an even more stringent degree (on the order of one part in 10⁹).

Flow diagrams for the three configurations under consideration are shown in Figures 3.2, 3.3, and 3.4. The equipment items outside the dotted lines are common to all of the configurations. In all cases, the methanation of the input gas is done at the pressure at which the gas is delivered. Initial cost calculations showed that compression of the input gas always results in a larger capital cost for the module as a whole*. The nickel based catalyst is coated on the inside of two inch

*The volume of input gas is always greater than the volume of output gas, so that compression costs tend to be least when all required compression is accomplished on the output stream. Costs of the feed gas (gas-to-gas) heat exchanger and the methanator vessel tend to remain level or increase with pressure. Small savings are realized in catalyst and recycle compressor costs at increased pressures.

diameter tubes in the tubewall methanator,* or is in the form of porous granules in the multiple fixed bed methanator. Pressure drop through the methanator vessel is taken as 15 psi for the tubewall types and 50 psi for the multiple fixed-bed type. Other pressure drops are assumed to be negligible.

The primary reaction catalyzed is the combination of CO and H₂ to form methane and liberate heat.

A second reaction between CO₂ and H₂ can also be catalyzed, but apparently only after the CO methanation is complete. Hence excess hydrogen (over the CO methanation requirements) must be present for this reaction to take place.

Actually reaction (3.2) is the sum of the CO methanation reaction and the so-called water shift reaction.

which also takes place in the methanation vessel. However, the detailed sequences of actual reaction steps are quite different for catalyzed CO methanation and catalyzed CO₂ methanation according to Strakey, et. al.⁸

*A Raney Mickle catalyst (42% nickel and 58% aluminum) in powder form is sprayed on the inside walls of the tubes. It is then activated by leaching with NaOH until 70% of the aluminum is removed.

For modeling purposes, we have assumed that the amount of CO_2 methanated is proportional to the amount of excess hydrogen present, after all the CO has been methanated, i.e.,

$$\begin{aligned}
 f &= \text{fraction of } \text{CO}_2 \text{ methanated} \\
 &= \frac{Q'X'(\text{CO}_2) - Q^{\circ}X^{\circ}(\text{CO}_2)}{Q'X'(\text{CO}_2)}
 \end{aligned}
 \tag{3.4}$$

$$= k [X'(\text{H}_2) - 3 X'(\text{CO})] [X'(\text{CO}_2)]^{-1}$$

with a limiting value of unity. (Symbol definitions are given in Table 3.1.) The value of k is apparently in the range of 0.15 to 0.22, based on stream flow conditions in the two BM-PEG reports where CO_2 methanation was considered. Clearly, it can never be greater than 0.25.

In order to depress the CO concentration in the output of the module to below 0.1%, some excess hydrogen above the minimum 3:1 volume ratio (to the input CO) must be maintained. Assuming that the residence time in the reaction vessel is long enough to allow a close approach to equilibrium conditions in the output of the vessel, the amount of excess hydrogen required will be dependent on the temperature of the exit gas and the pressure maintained in the vessel.

The equilibrium constant for the CO methanation reaction as a function of temperature is shown in Fig. 3.5. From the definition of the equilibrium constant we can show that the minimum concentration of hydrogen in the exit gas must be

$$[x^e(\text{H}_2)]_{\min} = \left(\frac{14.7}{p^e}\right)^{2/3} \left[\frac{1000 x^e(\text{CH}_4) x^e(\text{H}_2\text{O})}{K_p(T^e) (1-x^e(\text{H}_2\text{O}))} \right]^{1/3} \quad (3.5)$$

Putting this in terms of the required volume fraction of hydrogen at the input to the methanator module is rather complex but an approximate solution is

$$\frac{x^i(\text{H}_2)}{x^i(\text{CO})} \geq 3 + A \left(\frac{14.7}{P^i}\right)^{2/3} \left(\frac{1}{K_p(T^e)}\right)^{1/3} \quad (3.6)$$

$$A = 10 \left[\frac{1-2x^i(\text{CO})}{x^i(\text{CO})} \right]^{2/3}$$

In the tubewall methanator, reaction-temperature control and recovery of the thermal energy generated in the methanation reaction is accomplished by boiling "Dowtherm," which surrounds the tubes through which the reactants flow. The pressure in the Dowtherm is maintained at about 150 psia so that the boiling temperature of the Dowtherm is about 750°F, the desired reaction temperature. Exit gas from the methanator at 750°F is used to preheat the input gas to 550°F. The Dowtherm vapor is used to produce Grade 1 steam in a separate boiler (pressure of 1200 psi). Note that for the tubewall configuration, all of the feed gas must be preheated to 550°F. The cost of the gas-to-gas heat exchanger by which this is accomplished is quite large and has important cost implications, as will be discussed in Appendix C.

In the fixed-bed reactor, the exit gas temperature is assumed to be 900°F and heat recovery is accomplished in a water-tube boiler, again generating a Grade 1 Steam. Some heat is extracted from the product gas to preheat a small portion of the feed (probably on the order of 5%) to the methanator. This feed preheater gas-to-gas heat exchanger can thus be made much smaller than for the tubewall methanator with product gas recycle. The temperature over the methanation catalyst is controlled by the introduction of fresh feed between successive beds.

Since the SNG specification on water vapor is equivalent to requiring a 32°F dewpoint, a final dehydration unit is required. This is assumed to be a di-ethylene or tri-ethylene-glycol absorption tower with appropriate regeneration equipment.

A sulfur guard vessel (which must be filled with a sulfur absorption medium, perhaps spent catalyst from the methanator, although certain dangers may exist*) is assumed in all cases to reduce the H₂S input to the methanation vessel to trace amounts.

Many gases which are suitable inputs to the methanator will contain small percentages of ethane, ethylene and higher order hydrocarbons. These will be converted to methane⁸, with appropriate consumption of hydrogen, in the methanator. To simplify the material balance calculations in our model, we assume conversion of all ethane and other higher order hydrocarbons in the actual input synthesis gas to methane, and adjust the input gas quantity and composition to an "equivalent" gas as shown in Table 3.2.

An important internal parameter is the feed dilution level to the methanator. In the BM-PEG reports, the tubewall-methanator-with-product-gas-recycle examples dilute the raw feed with sufficient product gas to bring the CO concentration to within a range of 5.5% to 8.9%, with about 7% as the average. The overall dilution level for the multiple-fixed-bed methanator with product gas recycle was also about 7% in the BM-PEG examples. We have therefore standardized on a dilution of raw feed with product gas to a 7% CO concentration level. This parameter has a pronounced effect on the cost of the feed preheater, the recycle compressor, and the coolers.

During the course of our study, we contacted one of the developers of the tubewall methanator** and were advised that he believes no recycle of product gas is really necessary. We therefore added the tubewall configuration without product gas recycle, since the cost equations were quite similar to those for the configuration with recycle. (The methanator catalyst area remains the same, since it is determined by the CO flow per unit time).

*Nickel carbonyl, a toxic substance, may be formed at low gas temperatures.⁸

**Mr. A.J. Forney, Energy Research Center, Bureau of Mines, Pittsburgh, PA.

A set of restrictions on the input gas is shown in Table 3.3. These should be regarded as necessary but not sufficient. As previously discussed, the $X'(H_2)/X'(CO)$ ratio requirement is due to the $X'(CO)$ restriction on SNG. The required excess hydrogen is different for each configuration due to differences in the temperature of the gas as it exits the methanator vessel and due to the effects of product-gas recycle. The limitations on inert constituents and maximum hydrogen to produce a gas which is 90% methane are given in the next section, where the input-output material balance algorithms are developed. The $X'(CO_2)$ limitation in Table 3.3 is arbitrary.

3.1.3.2 Material Balance Equations

The methanator material flows involve one input gas (the synthesis gas with a properly adjusted H_2 to CO ratio), one output gas (SNG) and one waste stream (condensate). From the discussion of the reaction in the previous section, the output gas quantity and composition can be easily solved for with the results shown in Table 3.4 along with condensate quantity, and thermal power generation.

The requirement that the output gas, after drying, be 90% CH_4 leads, from the equations in Table 3.4, to the following condition on the composition of the input gas:

$$\frac{X'(CH_4) + X'(CO) + fX'(CO_2)}{1 - 3X'(CO) - 4fX'(CO_2) - X'(H_2O)} \geq .9$$

or

$$X'(CH_4) + 3.7X'(CO) + 4.6fX'(CO_2) + .9X'(H_2O) \geq .9 \quad (3.7)$$

This necessary condition is in addition to those listed in Table 3.3.

3.1.3.3 Capital Cost Estimates

As discussed earlier in this section, suitable point-design cost estimates were not readily available in our Phase I work (although we anticipate availability in Phase II). A rather detailed cost study of the competing configurations was undertaken to supply the required data. The details of this study are given in Appendix C.

The important external parameters were quickly identified as

- Output quantity rate, Q° (i.e. "Throughput")
- Input gas pressure, P'
- Effective input gas CO concentration,

$$X_e'(CO) = X'(CO) + f X'(CO_2) \quad (3.8)$$

The first, Q° , clearly sizes the module, while the second, P' , determines the output compressor costs, and also affects the recycle compressor costs, heat exchanger costs, and the amount of catalyst needed. The last, $X_e'(CO)$, determines the degree of methanation required and hence the level of recycle dilution, the amount of catalyst required and the amount of thermal power generated.

In Appendix C the calculated costs are plotted and cross-plotted against these three parameters. A typical curve is shown in Fig. 3.6. Finding a suitable functional approximation to the cost calculations proved rather difficult, especially inclusion of the dependency on inlet pressure, P' . It is necessary to distinguish the case in which the inlet pressure, is equal to the sum of the outlet pressure and the pressure drop across the methanator vessel since a product gas compressor is then unnecessary. Hence a discontinuity appears in the cost as a function of pressure. Since there does not appear to be any practical reason to consider inlet pressures greater than this, we have modeled the cost function by two equations, one for inlet pressures, P' , up to

but not equal to the sum of outlet pressure, P^o , and methanator vessel pressure drop, ΔP , and one for pressures equal to this maximum value. Pressures less than 100 psia were not considered since they appear to be of little practical interest.

The chosen functional form of investment cost, E_m , vs. throughput, Q^o , inlet pressure, P' , and equivalent CO volume fraction of inlet gas, $X'_e(\text{CO})$, is

$$E = K \left(\frac{Q^o}{10.4} \right)^{b_1} \exp \left\{ b_2 \frac{P'}{500} + b_3 \left(\frac{P'}{500} \right)^{1.3} + b_4 \left(\frac{X'_e(\text{CO})}{0.1668} \right)^2 + b_5 \left(\frac{X'_e(\text{CO})}{0.1668} \cdot \frac{Q^o}{10.4} \right) \right\} \quad (3.9)$$

For $P' = P^o + \Delta P$, the equation simplifies since $b_2 = b_3 = 0$. Values of the constants for each competing configuration are shown in Table 3.5. Also shown is the rms difference between the value of E_m computed from Eq. (3.9) and the "point-design" values computed in Appendix C as a percentage i.e.

$$\% \text{ rms deviation} \equiv \sqrt{\frac{1}{N} \sum_n \frac{(E_{mn} - \hat{E}_{mn})^2}{E_{mn}^2}} \times 100$$

Where E_{mn} = n^{th} point design value of E_m
 $\hat{E}_{mn}$ = corresponding value of E_m computed from Eq. (3.9)
 N = number of point-design values

3.1.3.4 Operating Cost Parameters

For each module we consider only direct operating expenses, defined as costs of operating labor, material replacement costs (e.g. catalysts), equipment wearout costs, and costs due to equipment outage.

Indirect operating costs including such factors as overhead, administration, taxes, auxilliary equipment operating costs, and plant maintenance and repair, are specified for complete unit processes.

The parameters that need to be specified include:

- Men per shift at nominal throughput, M_o
- Labor scale exponent, p
- Yearly catalyst replacement cost at design throughput, C_{aro}
- Equipment design lifetime, years, L_m
- Equipment availability factor, F_a

The actual numbers of men per shift, M , is given by

$$M = M_o \left(\frac{Q^o}{10.4} \right)^p \quad (3.10)$$

The catalyst replacement cost includes the cost of new material plus the cost of installation. For the fixed-bed methanator, installation cost is negligible, since the catalyst is purchased as prepared granules or pellets. For the tubewall methanator, installation cost is probably substantial, since the catalyst bearing material must be sprayed on the inside of the tubes, and then chemically treated to bring it to the activated state. In the absence of more definitive estimates, we assume that the installation cost for the tubewall methanator is about equal to the material costs. Yearly catalyst costs, C_{ar} , can be estimated from the cost at the nominal design point by:

$$C_{ar} = C_{aro} \left(\frac{Q'X'_e(CO)}{3.6} \right) \left(\frac{500}{P'} \right) \quad (3.11)$$

Values of M_o , p , C_{aro} , L_m , and F_a 1-7 have been estimated from averages of values given in the BM-PEG reports, and from previous MPPM work. They are shown in Table 3.6.

3.1.3.5 Utility Requirements

The utility requirements are given in Table 3.7. Net saturated steam at 1200 psia is generated and the amount shown is based on the thermal power generated by the methanation reaction with η_s as the efficiency of conversion. A nominal value for η_s can be taken as 0.7. Electric power is principally required for the boiler feedwater pumps and a small (5%) addition is allowed for other pumps such as the dehydrator glycol pumps and the Dowtherm pumps.

Superheated steam at 1200 psia and 900°F is consumed for the compressor drives, and the amount is calculated from the total compressor horsepower required. The turbine exhaust generates saturated steam at 120 psia, but part is used in the dehydration unit to regenerate the glycol absorbant.

Cooling water requirements are based on an 80°F input temperature and an allowed 45°F temperature rise. (Pumping power for cooling water is supplied by the utility module and computed from gross plant requirements for cooling water.)

3.1.3.6 Summary Configuration Description

To complete a configuration model, we codify it to a standard format suitable for program input. The standard format devised for the original MPPM consisted of a brief description, an output description, a list of design parameters (nominal throughput, capital cost, operating cost, and scaling factors), and a list of materials. For the present version of the MPPM, we have modified this format by adding an input description, various input state and design parameters (i.e. inlet pressure P' , inlet temperatures T' , steam generation efficiency, η_s , net module pressure drop, ΔP , CO_2 methanation constant, k), and by deleting various cost parameters (auxiliary equipment costs, overhead cost, and tax cost related items) which we will model at the complete unit process level of aggregation.

The configuration description format is shown in Table 3.8 for the tubewall methanator with product gas recycle. The numbers given are for a nominal design to which the configuration scaling algorithms are normalized. For materials, utility, and energy inputs/outputs, a negative number indicates an input and a positive number an output.

Configuration descriptions for the tubewall methanator without product gas recycle and the multiple-fixed-bed methanator with product gas recycle are given in Tables 3.9 and 3.10, respectively. Only items which have different nominal design values from those given in Table 3.8 are shown.

The algorithms which govern selection of allowable raw material inputs, material balance computations, utility requirements, and scaling of costs are given in the earlier parts of Section 3.1. Table 3.11 is provided to guide the reader to the appropriate tables and equations in the text.

3.2. STRUCTURE OF MPPM ALGORITHMS

3.2.1. Methodology

The previous section has described a functional module and its configurations in detail. Complete unit process routes are made up of sequences of functional-modules, each module producing an output which is the input to its successor. Secondary inputs and outputs (e.g., byproducts or waste flows) give rise to branches on the unit process routes for their creation and further processing. Complete unit processes include module configurations for all operations necessary to convert the primary raw material, coal, into salable products, byproducts, and disposed wastes. The MPPM method of assembling module configurations into complete unit processes is guided by the process "road-map" shown in the foldout inside the back cover of this report.

The procedure for identifying a feasible unit process to produce a given product or product mix from functional-modules consists of stepping along the paths in the road map, opposite to the arrows, from products to modules to precursor modules, selecting at each step those competing configurations within a module that have outputs that are capable of meeting the input specification for each configuration selected in the previous step. Whenever more than one configuration can be selected from a process module, a new possible unit process is established. A unit process is completed when a path to the primary raw material can be completed, and branches for processing all byproducts and wastes are completed. This construction of feasible unit processes is done by the Linking Model (LM). When called upon to do so, the Process Chain Evaluation Model (PCEM) sizes all the configurations in the unit process for a given quantity of output product per unit time, aggregates utility requirements, and sizes a utility module to serve the complete unit process plant. It calculates overall process costs in accordance with a list of exogenous variables, e.g., an inflation index, a tax structure, raw material costs. Process residuals, e.g., released gasses and liquids and material tonnage to landfill, are also calculated.

3.2.2. Data for an Example to Illustrate the Linking Model

As an example of the method of assembling a feasible unit process from a sequence of Functional Modules, consider the end-product "Substitute Natural Gas" (SNG) which is the output of the methanation module considered in the previous section. From the road map we see that Functional Module sequences (i.e., Unit Process Routes) to SNG can be represented as

$$\text{SNG} = \{9\} + \{14\} + \{13\} + \{14\} + \begin{pmatrix} 2 \\ 3 \\ 4 \\ 5 \\ 8 \end{pmatrix} + \{16\} + \text{COAL}$$

Each module will have a number of competing configurations, e.g., module No. 9 has five, module No. 3 has six, module No. 2 has 19.

To illustrate the process in more detail we can consider a restricted subset of all the possible configurations in the above set of modules and trace through the construction of some feasible unit processes. A simple restricted subset is listed in Table 3.12. It contains the three module (No. 9) configurations discussed in Section 3.1., one gas-purification module (No. 14) configuration (plus a default pass-through option), two shift-reaction module (No. 13).

configurations, one configuration from a gasifier module (No. 2), and a coal-preparation-module (No. 16) configuration. We assume the available input to be typical "Pittsburgh Seam" coal. Also shown are the input restrictions and primary input/output relationships for each configuration in sufficient detail for linking purposes. (These are essentially *partial* data files or models of these competing configurations.)

3.2.3 Illustration of the Linking Model

The rules by which process alternatives are judged feasible or infeasible are embodied in a systematic decision rule for linking the competing configurations embodied in the Unit Process routes shown in the road map. In this example we will work backwards from substitute natural gas (SNG) through the alternative process chains to coal, using the restricted subset of competing configurations given in Table 3.12. At the outset there are twenty-four candidates for feasible unit processes,

Starting from the Substitute Natural Gas we proceed to module No. 9, the methanators, and note the input raw material specification. For the three example configurations these input specifications are almost identical, although in general this need not be the case. Proceeding to Module No. 14, gas-purifier, we note that the output of the hot potassium carbonate configuration (14,C,4) is guaranteed to meet the methanator input restrictions on H_2S and H_2O , and, by proper choice of z , on CO_2 . Satisfaction of the remaining methanator restrictions depends on the input to the hot potassium carbonate configuration, while for the pass-through option, satisfaction of all restrictions depends on the input. We flag the conditions which are indeterminate for later checking and proceed to the shift-conversion module (No. 13).

Since all the configurations in the gas purifier module (No. 14) have no input restrictions, both configurations in the shift-conversion module (No. 13) seem to be acceptable. However, shift conversion with a cobalt-molybdenum catalyst (13,B,1) has a high H_2S output. Checking back to the indeterminate condition of the H_2S input to the methanator module through the gas-purification pass-through configuration

(14,Z,1), we see that it will be violated. Thus the linking is not a simple matter of matching outputs to inputs. Rather, consequences operating through several modules must be considered. In this case we had to refer from the shift converter to the methanator to remove invalid embryo-configuration sequences. Sequences growing from the methanator through the pass-through configuration to the cobalt-molybdenum shift converter are therefore discarded.

$$\begin{Bmatrix} 9, A, 1 \\ 9, A, 2 \\ 9, B, 1 \end{Bmatrix} \longleftarrow \{14, Z, 1\} \longleftarrow \{13, B, 1\} \longleftarrow ?$$

Discarded invalid chains

We note further that by proper choice of the selectable parameter, y , of the shift-converter configurations, the input H_2/CO ratio requirement of the methanator modules can be satisfied. Hence this is now a satisfied requirement, rather than indeterminate, and need not be checked again.

Proceeding backward to the second appearance of the gas purification module on the coal process flow diagram, we eliminate further potential sequences. We find that the output of the hot potassium carbonate gas purifier (14,C,4) violates the input requirement for the cobalt-moly shift converter that $X'(H_2S) > 0.001$. Hence embryo sequences of the form

$$\begin{Bmatrix} 9, A, 1 \\ 9, A, 2 \\ 9, B, 1 \end{Bmatrix} \longleftarrow \{14, C, 4\} \longleftarrow \{13, B, 1\} \longleftarrow \{14, C, 4\} \longleftarrow ?$$

are also discarded. Other input conditions for the configurations of the shift conversion module (No. 13) are either satisfied or indeterminate.

We can proceed in this fashion to module No. 2, gasifiers, and module No. 16, coal preparation, checking at each stage the input restrictions of the prior stage and the indeterminate restrictions in previous stages. The input gas composition condition in the methanator state (Table 3.12. I. B. last equation) will be determined to be satisfied or violated when we know the output of the Synthane gasifier configuration (2,B,3). It will be found that none of the processes with the pass-through configuration (14,Z,1) preceeding the methanator can meet the CO_2 restriction and the restriction on methanator input gas composition.

Of the twenty-four original possibilities only nine are found to be feasible processes. These processes are illustrated in Figure 3.7.

In Figure 3.7 we note that the Unit Process with the hot potassium carbonate gas purification configuration preceding the iron-oxide shift converter configuration is probably not competitive with the one with the gas-purification pass-through option preceding the iron-oxide shift converter configuration, since an apparently unnecessary gas-purification step is present. When economic evaluations of the unit processes are made, this will always show up as a cost penalty for the first process relative to the second and inclusion of both unit processes in the library of feasible unit processes need not be of concern. However, once a process has been recognized as being non-competitive, it can be expunged from the process library by an external command.

Each of these unit processes has two adjustable parameters, the z parameter of the gas-purifier and the y parameter of the shift-converter. These are not actually specified in the Linking Model, but are set in the Process Chain Evaluation Model by simply choosing the values which minimize capital cost while allowing satisfaction of all the functional module input restrictions. In some unit processes (e.g., those containing the CO_2 Acceptor Gasifier) it is possible that the methanation input condition will be met with $y = y_e$, implying that no shift conversion is needed. When such a process is economically evaluated, the capital cost of the shift-converter module will be computed as zero, effectively removing the shift-conversion module from the process.

To complete each unit process, module configurations for by-product and waste processing must be added, as well as module configurations for secondary inputs. In the nine unit processes just described, each requires an oxygen input to the synthane gasifier configuration and an acid gas treatment plant for the effluents from the gas purifiers. Char and tar are byproducts from the gasifier which may be evaluated as salable byproducts or used in further process modules. (Waste water treatment for recycling, and generation of steam or cooling water inputs are treated as utility functions.) A complete unit process could appear as shown in Figure 3.8.

The formal statement of the Linking Model algorithm is given in Table 3.13. The intent is to outline a procedure in which the user of the MPPM initiates the first step by selecting a product or product mix and a selection of primary raw materials, i.e., coals of various types. The rest of the algorithm is implemented by the computer program, and a library of feasible Unit Processes is generated. This library is then ready to be subjected to the PCEM algorithms.

3.2.4 The Process Chain Evaluation Model (PCEM)

Having established a "library" or listing of feasible Unit Processes for transforming coal into desired end-products, the next task is to "evaluate" these processes, i.e., determine the product "costs" under specified conditions for each alternative unit process. This procedure involves several steps:

1. PROCESS SIZING

The unit processes as developed by the LINKING MODEL are "feasible" processes in the sense that all configuration inputs and outputs are qualitatively matched. However, each configuration must still be matched quantitatively so that the throughput of each configuration is sufficient to supply, in the end, the desired quantity of product. For some configurations, this will also require a selection of some free parameter, e.g., the parameter y of the configurations Shift Conversion Module, No. 13, used in the example of LINKING MODEL operation. Normally this would be done by an investment cost minimization routine, although some other selection criterion can be chosen with a suitable program modification. In the case of shift conversion, the parameter y would be chosen as the smallest value for which the input specification on the ratio of hydrogen to carbon monoxide at the input to the methanator module configuration, No. 9, is just satisfied. This follows from the presumption that the capital cost of all shift conversion configurations will increase monotonically with y . At the same time quantities of effluents and by-products produced by each configuration for the given quantity of main product (or main product mix) must be evaluated. A "utility" module (or configuration, since only one is modeled) to provide or absorb net fuel, steam, electric power, and cooling water for the sized Unit Process must also be determined. The algorithm that accomplishes these tasks for each Unit Process to be evaluated is the "SIZER".

2. GROSS PROCESS COSTING

After each unit process has been sized, information from the data files of all the module configurations that comprise the process can be used to arrive at the "value added" by the unit process, i.e., by annualizing investment and operating costs. Investment costs are obtained from the investment cost scaling parameters of each module configuration, summed over all module configurations included in the unit process. Similarly, operating costs are obtained from scaled requirements for manpower and materials (i.e., materials which do not enter into the product stream, such as catalysts). Raw material and by-product prices or values are exogenously supplied and held in the materials files described in section 3.1. These are used with the process "value added" to find the gross sales price of the main product (or products), which is just the price that would be demanded in the absence of taxes or market competition, with a specified "venture profit" included. Since investment and operating costs may exhibit scale economies,* the gross product cost will be a function of throughput. The calculation can, of course, be made for any throughput desired by the user of the model. The "GROSS COSTER" is the algorithm that accomplishes these calculations.

3. PROCESS RESIDUALS EVALUATION

As we have specified, the LINKING MODEL adds functional module configurations to each unit process to operate on all waste streams until they are transformed to releasable substances, or are considered non-environmentally degrading. Thus all flue gasses are scrubbed to remove SO_2 , if any is present, to EPA "best available technology" standards. Solid waste disposal, by landfill or other acceptable method, is a configuration and contributes to process costs like any other module. Nevertheless, an evaluation of process residuals is necessary for several reasons: (1) to account for residuals whose discharge is

*That is, the production cost of a unit of product usually decreases as plant size increases due to the introduction of technological, management, and financial economies. Eventually a limit is reached at which the onset of management inefficiency occurs, resulting ultimately in diseconomies of scale.

now permitted (or permitted to some low level) but which may be regulated or penalized in the future (or more stringently regulated), (2) to provide a mechanism to account for residuals not presently recognized as important or for which quantitative data is not presently available. An example of the first is nitrogen oxides discharge, while an example of the second is trace radioactive or heavy metal constituents of coal. The "RESIDUALS EVALUATOR" will be the algorithm that calculates aggregate unit process waste releases and separately computes waste treatment costs. This is a new part of the PCEM specifically added to adapt MPPM to coal processing technology. It will be developed during Phase II of the project.

4. NET PROCESS COSTING

An algorithm called the "NET COSTER" computes realistic "shadow" sales prices for products as determined for each Unit Process. These prices are based on the costs calculated for the desired throughput by the "GROSS COSTER", and an exogenously specified tax structure. Another algorithm called the "TAXER" permits parametric specification of several kinds of charges, taxes, and incentives, including

- Corporate income taxes
- Investment tax credit (a negative tax or incentive)
- Value added taxes
- Effluent charges (materials and waste heat)
- Efficiency surcharges (imposed to reduce resource consumption)
- Payroll taxes

The shadow sales price may be higher or lower than the market price, since market prices are determined by competition and/or government regulation. Thus the shadow price of SNG will most probably be above the regulated (interstate) price of natural gas, but may or may not be above the unregulated (intrastate) price, depending on the exogenously specified material prices and tax structure.

In a sense, the PCEM develops a "ranking" of Unit Processes, based on the exogenously supplied economic environment and an objective

function, e.g., minimum product price. However, the user should bear in mind the level of accuracy in the data; relative cost data for competing configurations within a given module cannot be expected to be more accurate than roughly $\pm 20\%$, while relative costs for configurations in unrelated modules may be even less dependable. Many of the most interesting Unit Processes will include module configurations that are highly speculative in both engineering feasibility and cost estimates. Hence any relative ranking of unit processes must be made in terms of broad bands of uncertainty.

The concept of "objective function" involves several considerations. The factor costs of a process include requirements for capital, raw materials, labor, energy, and effluent disposal. The objective can be to minimize the production cost (i.e., venture cost of sales) any one of the input factor costs (e.g., capital requirements, effluents disposal, etc.), or a collective weighted set of costs. The nature of the objective function can be expected to change with time. For example, the initial emphasis will be placed on bringing a process on-stream and demonstrating feasibility. Subsequently, the emphasis will be shifted to improving cost efficiency. These are, of course, relative--not absolute--shifts in emphasis. Because of the complexity of the interacting factors, it is not possible to definitively identify the objective function for future times. Rather, it must be possible--through use of the PCEM--to reevaluate process alternatives in light of evolving objective definitions.

The term "specification of end products" also involves several considerations. Nearly all energy products serve as "intermediate products" in that they are not ends in themselves, but precursors to the attainment of a set of functional objectives. For example, substitute natural gas (SNG) and syncrude are not valuable per se, but as potential participants in the provision of space heating, energy for transport, process energy, and chemical feedstocks. Even these functional objectives are themselves intermediate steps within the overall economy. The final product for a set of processes must be defined at a level such that all competing processes attain an equivalent end point.

The PCEM evaluations form an essential input to the assessment of the national implications of the coal development strategies as aided by the Industry Development Model (IDM) and other macro-economic and energy supply/demand models.

The evaluation of environmental questions was a principal objective in the original development of the MPPM. The MPPM has already been used to evaluate the effectiveness of effluent taxation strategies in motivating desired pollution control steps within a portion of the chemical industry. Since the PCEM determines the quantity of residual environmental pollutants for each process, environmental effects can be appraised and exogenously incorporated into the process evaluations. The PCEM can address such questions as:

- How will various schedules for utilization of different coal types affect the overall generation of effluents by coal processes?
- How do variations in the process residuals regulations affect the cost of coal processes?
- How do variations in the process residuals regulations affect the processes to be developed?
- What quantities of process residuals are generated by year and by geographic region for a desired product spectrum?

3.2.5 Industry Development Model

The Industry Development Model (IDM) keeps track of the cumulative implications in bringing coal conversion capacity onstream. Each unit process has its individual characteristics--capital, labor, and material requirements; wastes generated; and date of first commercial availability, with estimated rate of growth in plant size. The unit processes are evaluated by the PCEM for alternative economic contexts. As indicated in Figure 3.1, the IDM applies process selection criteria, assesses

process availability, and assembles a set of processes to comply with the designated industry development schedule. On this basis, the IDM compiles a composite industry output spectrum--SNG, coal liquids, electricity, etc.--and the related requirements for capital, labor, and raw materials.

The principal goal of the Industry Development Model (IDM) is aggregative assessment. A number of questions may be posed:

- What is the product spectrum in future year x associated with alternative developmental strategies and schedules for commercial availability of technology?
- What are the capital, material, and labor requirements by year associated with provision of a desired product spectrum? What are the cumulative investments over prior years in each of these areas?
- What quantities of conversion process environmental effluents are generated by year and by geographic region for a desired product spectrum?

These questions, and others, can be handled through use of the MPPM alone and in conjunction with other economic and energy models, as discussed in Chapter 5.

It is useful to consider some of the terms used in the sample questions. "Product spectrum" refers to the fact that many coal-based products--gases, liquids, solids, and direct conversion to electricity--will be developed simultaneously. The precise quantity of each will depend upon their relative value and production costs. The MPPM addresses the cost question, providing inputs regarding product cost to other models, such as Brookhaven's BESOM and ESNS models.*

*BESOM = Brookhaven Energy Systems Optimization Model
ESNS = Energy System Network Simulator

"Alternative developmental strategies" refers to the policy decisions to be made regarding support for coal process development. This involves the quantity and type of coal to be mined, the capital to be made available from the public and private sectors, the environmental constraints to be applied, the taxing policies to be employed, etc. These inputs form the core of the policies to be evaluated.

"Schedules for commercial availability of technology" reflects the fact that there is a substantial time element to be considered in bringing the coal processes to commercial availability. The time element is a function both of the rate of investment and of the technical difficulties to be surmounted. Estimates will be made of the rates at which the technologies seem to be developing. These estimates must be updated as new information becomes available.

The industry development schedule can be specified in a number of ways. The approach presumed in Figure 3.1 is that a capital investment schedule will have been defined, and a weighting placed on the desirability of alternative products, by market prices. Based upon such exogenously supplied data, the IDM selects the best unit process set to satisfy the indicated objectives. The product output spectrum is identified by year, and the industry requirements for capital, etc., are determined. The latter will include prior capital commitments during construction to bring the plant onstream at the desired date.

An alternative way of specifying the industry development schedule is to identify the rate at which specified products, such as SNG or electricity, are to be made available. The IDM then determines the resources--capital, material, etc.--that must be made available by year to accomplish the desired goals.

The need for a type of process is established by year based on the industry development schedule. Each of the evaluated unit processes has an indicated date of first commercial availability. The IDM chooses the

best alternatives from among the available processes to fulfill the specified development schedule. In addition, the IDM estimates the size of each new facility based upon the date of first availability and estimated rate of growth in plant size. Growth in plant size as knowledge of the process is gained and equipment fabrication techniques are perfected is a standard phenomenon in established industries, such as the chemical industry. In the case of coal utilization plants, tremendous quantities of raw materials are involved, e.g., 6,350,000 tons Wyodak seam coal per year to supply 250 MMSCFD SNG via the Synthane process. The implications of mining and shipping such large quantities of coal will play a large role in deciding optimal plant size. Such factors will be considered in establishing the plant size growth rates for the IDM.

Regional considerations are addressed within the IDM. Module configurations will have been differentiated, as necessary, depending upon the type of coal being processed. This applies primarily to the earlier process steps, such as coal preparation and gasification. Thus, variant configurations will be developed for the Synthane medium BTU gasifier which handles Wyodak seam coal, and that which handles Pittsburgh seam coal. The industry development schedule will specify the relative quantities of each type of coal to be utilized. The Synthane process may be evaluated as most promising for use with one coal type, and the CO₂ Acceptor process for use with another. In this fashion, a composite identification of coal development, process employment and waste generation will be assembled by regional location.

3.3 COMPUTER-RELATED EFFORT

IRT will work with Control Data Corporation (CDC) in adapting the prototype MPPM into an efficient computational package. IRT personnel will manage all aspects of the computer program development leading to computational models A and B, (as defined in Section 1.2.3.) with CDC functioning in an advisory capacity. Once model B has been established, the supporting computer group will package the computer programs and carry out associated documentation tasks.

Formats for the storage, retrieval, display, and update of model input data will be determined by CDC analysts. It is currently anticipated that these formats will be designed to be compatible with those used for the Brookhaven energy models.* Corresponding procedures will also be developed to assure that a record of both current and historical inputs is always available to ERDA.

Specifications and appropriate layouts will be developed by CDC for programs required to (1) edit and load data into the MPPM model, and (2) produce output files and reports. Output report formats and options will be based on user requirements determined through coordination with IRT and ERDA personnel.

The last seven months of Phase II will be spent in implementing the MPPM model as an operational package that can be used either on a stand-alone basis or in conjunction with other models. During this period, CDC will develop the *pre- and post-processing programs* previously specified. The MPPM model will then be fully loaded and tested. These tests will exercise all *user options* and will cover a range of assumptions, specified by IRT and ERDA technical personnel.

Program documentation, data and source code listings, cataloged permanent files, and backup data and program tapes will be produced by CDC to complete its task requirements under Phase II.

* See Section 5.1.5 for a discussion of these models.

FIGURE 3.1. RELATIONSHIP OF MPPM COMPONENTS

FIGURE 3.2

Tubewall Methanator with Product Gas Recycle

FIGURE 3.3

Tubewall Methanator without Product Gas Recycle

FIGURE 3.4

Multiple-Fixed-Bed Methanator with Product Gas Recycle

FIGURE 3.5

Equilibrium Constants
for Methanation of CO

FIGURE 3.6

Capital Investment vs. Throughput for
Tubewall Methanator with Product Gas Recycle

$$X'_e(\text{CO}) = 0.15$$

A + P' = 100 psia
B + P' = 300 psia
C + P' = 600 psia
D + P' = 900 psia
E + P' = 1030 psia

FIGURE 3.7

Feasible Coal to SNG Unit Processes

FIGURE 3.8

Complete Unit Process for Coal to SNG

BRANCH MODULE CONFIGURATIONS

- {34, CC, 1} - Claus Plant
- {18, A, 1} - Air Distillation Plant
- {24, A, 3} - Conventional Furnace/Boiler
- {31, D, 1} - Electrostatic Precipitator
- {31, F, 1} - and Limestone Scrubber
- {38, K, 1} - Stack
- {38, I, 2} - Landfill
- {17, F, 4} - Ball Mill for Limestone Preparation

TABLE 3.1

SYMBOLS USED IN METHANATOR MODEL EQUATIONS

Superscript ' denotes equivalent module inputs, e.g., Q' , $X'(CO)$

Superscript " denotes actual module inputs, e.g., Q'' , $X''(CO)$

Superscript ° denotes actual module outputs, e.g., Q° , $X^\circ(CH_4)$

Superscript e denotes outputs from the methanator vessel

Superscript i denotes inputs to the methanator vessel

Q → denotes gas flow quantity in MMSCF/H

Q_{cw} → Cooling water flow in Mgalpm

Q_c → denotes condensate (H_2O) flow rate in MM lbs/H

Q_{sa} → denotes steam flow of "a" grade in M lbs/H, $a = 1, 2, 3$

T_e → denotes thermal power in MMBTU/H

T → Temperature °F

$X(a)$ → denotes volume or mole fraction of gas constituent "a"

ΔP → Pressure drop in methanator vessel, psi

P → Pressure, psia

P_e → Electric power, kw

E_m → Investment cost of complete module

k → Proportionality constant for CO_2 methanation

η_s → Steam generation efficiency

f → Fraction of CO_2 methanated

TABLE 3. 2

Conversion of Actual Input Gas Composition
to Equivalent Input Gas Composition

$$\frac{Q''}{Q'} = \left[1 - \sum_{n,m} \left(n - \frac{m}{2} + 1 \right) X''(C_n H_m) \right]^{-1}$$

$$X'(CH_4) = \frac{Q''}{Q'} \sum_{n,m} n X''(C_n H_m)$$

$$X'(H_2) = \frac{Q''}{Q'} \left[X''(H_2) - \sum_{n,m} \left(\frac{4n-m}{2} \right) X''(C_n H_m) \right]$$

$$X'(CO) = \frac{Q''}{Q'} X''(CO)$$

$$X'(CO_2) = \frac{Q''}{Q'} X''(CO_2)$$

$$X'(N_2) = \frac{Q''}{Q'} \left[X''(N_2) + \sum X''(\text{other inerts}) \right]$$

$$X'(H_2O) = \frac{Q''}{Q'} X''(H_2O)$$

TABLE 3.3

Input Synthesis Gas Restrictions

$$T = 100^{\circ}\text{F}$$

$$X'(\text{H}_2\text{S}) \sim X''(\text{H}_2\text{S}) < 10^{-6}$$

$$X'(\text{CO}_2) < (1/4)X'(\text{CO})$$

$$X''(\text{H}_2\text{O}) < [P']^{-1} \quad (P' \text{ in psia})$$

$$\sum_{\substack{n > 1 \\ m \geq 4}} X''(\text{C}_n\text{H}_m) < .1$$

for 9,A,1 Tubewall Methanator with Product Gas Recycle

$$X'(\text{H}_2)/X'(\text{CO}) \geq 3 + 1.96 \left(\frac{14.7}{P'} \right)^{2/3}$$

for 9,A,2 Tubewall Methanator without Product Gas Recycle

$$X'(\text{H}_2)/X'(\text{CO}) \geq 3 + 0.369 \left[\frac{(1 - 2X'(\text{CO}))}{(X'(\text{CO}))} \right]^{2/3} \left(\frac{14.7}{P'} \right)^{2/3}$$

for 9,B,1 Multiple-Fixed-Bed Methanator with Product Gas Recycle

$$X'(\text{H}_2)/X'(\text{CO}) \geq 3 + 8.44 \left(\frac{14.7}{P'} \right)^{2/3}$$

TABLE 3.4

Material Balance Equations

$$\frac{Q^{\circ}}{Q'} = 1 - 3X'(CO) - 4fX'(CO_2) - X'(H_2O)$$

$$\begin{aligned} Q_c^{\circ} &= \text{condensate generated (MM lbs/Hr)} \\ &= 0.0475 Q' [X'(H_2O) + X'(CO) + 2fX'(CO_2)] \end{aligned}$$

$$X^{\circ}(CH_4) = \frac{Q'}{Q^{\circ}} [X'(CH_4) + X'(CO) + fX'(CO_2)]$$

$$X^{\circ}(H_2) = \frac{Q'}{Q^{\circ}} [X'(H_2) - 3X'(CO) - 4fX'(CO_2)]$$

$$X^{\circ}(CO_2) = \frac{Q'}{Q^{\circ}} (1 - f) X'(CO_2)$$

$$X^{\circ}(N_2) = \frac{Q'}{Q^{\circ}} X'(N_2)$$

$$X^{\circ}(H_2O) = 0$$

$$f = k[X'(H_2) - 3X'(CO)][X'(CO_2)]^{-1} \quad \text{but } \leq 1$$

$$k = 0.20 \text{ (nominal)}$$

$$T_e = \text{Thermal energy released (MMBTU/hr)}$$

$$= Q' [261X'(CO) + 214fX'(CO_2)]$$

$$T^{\circ} = 100^{\circ}\text{F}$$

$$p^{\circ} = 1015 \text{ psia}$$

TABLE 3.5

K AND b COEFFICIENTS FOR CAPITAL COST FUNCTION (EQ 3.8)

 $100 \text{ psia} \leq P' < (1015 + \Delta P) \text{ psia}$

Methanator Type*	K	b_1	b_2	b_3	b_4	b_5	% rms Deviation
Tubewall with PGR	28,219,249	.622902	-1.394095	1.0763094	.59619357	.17375128	7%
Multiple-Fixed-Bed with PGR	52,491,914	.511345	-3.60702	2.500888	.458674	.17938392	7%
Tubewall w/o PGR	28,660,658	.665997	-1.58786	1.131796	.467848	.12919629	5%

 $P' = (1015 + \Delta P) \text{ psia}$

	K	b_1	b_4	b_5	% rms Deviation
Tubewall with PGR	18,785,165	.709785	.75337509	1.4768882	5%
Multiple-Fixed-Bed with PGR	12,883,403	.50745	.54518713	.18424634	3%
Tubewall w/o PGR	13,406,373	.836979	.63603218	.0060981826	2%

*PGR = Product Gas Recycle

TABLE 3.6
OPERATING COST PARAMETERS

M_o	= Number of men per shift @ nominal design	- 6
P	= Labor scale exponent	- 0.25
C_{aro}	= Yearly catalyst replacement costs	
	a) multiple-fixed-bed configuration	- $\$1.7 \times 10^6$
	b) tubewall configuration	- 0.25×10^6
L_m	= Equipment design lifetime years	- 20
F_a	= Equipment availability factor	- 0.9

TABLE 3.7

Utility Requirements for Methanator Module

A. Saturated Steam @ 1200 psia

$$Q_{s1}^{\circ} = 940 \eta_s \left(\frac{Q' X_e' (CO)}{3.6} \right) \quad M \text{ lbs/H}$$

B. Superheated Steam @ 1200 psia and 900°F

1. For tubewall methanator with PGR and multiple-fixed-bed methanator with PGR

$$Q_{s2}' = 963 \left(\frac{Q^{\circ}}{10.4} \right) \left[\left(\frac{1015}{P' - \Delta P} \right)^{0.256} - 1 \right] \\ + 1,981 \left(\frac{Q'}{21.4} \right) \left(\frac{X_e' (CO)}{0.07} - 1 \right) \left[\left(\frac{P'}{P' - \Delta P} \right)^{0.256} - 1 \right] \quad M \text{ lbs/H}$$

2. For tubewall methanator without PGR

$$Q_{s2}' = 963 \left(\frac{Q^{\circ}}{10.4} \right) \left[\left(\frac{1015}{P' - \Delta P} \right)^{0.256} - 1 \right] \quad M \text{ lbs/H}$$

Note: $\Delta P = 15$ psia for tubewall methanator $= 50$ psia for multiple-fixed-bed methanator

C. Saturated Steam @ 120 psia

$$Q_{s3}^{\circ} = Q_{s2}' - \frac{Q^{\circ}}{10.4} \quad M \text{ lbs/H}$$

D. Electric Power

$$P_e' = 1630 \eta_s \left(\frac{Q' X_e' (CO)}{3.6} \right) \quad Kw.$$

TABLE 3.7 (Continued)

Utility Requirements for Methanator Module

E. Cooling Water

1. For tubewall methanator with PGR and multiple-fixed-bed methanator with PGR

$$Q'_{cw} = 33.3 \left(\frac{Q' X_E'(CO)}{3.6} \right) - 10.8 \left(\frac{Q'}{21.4} \right) + 7 \left(\frac{Q^\circ}{10.4} \right) \quad \text{Mgpm}$$

2. For tubewall methanator without PGR

$$Q'_{cw} = 7.4 \left(\frac{Q' X_E'(CO)}{3.6} \right) + 7 \left(\frac{Q^\circ}{10.4} \right) \quad \text{Mgpm}$$

TABLE 3.8

CONFIGURATION DESCRIPTION AND NOMINAL DESIGN PARAMETERS

Module 9, Configuration 9, A, 1, Tubewall

Methanator with Product Gas Recycle.

Output Product: SNG(PPS-1)

Input Raw Material: Synthesis Gas with 3:1 H₂/CO Ratio

ITEM	NOMINAL DESIGN PARAMETER	
1.	Throughput, Q ^o , MMSCFH	10.4
2.	Inlet Gas Pressure, P', Psia	500
3.	Inlet Gas Temperature, T', °F	100
4.	Fixed Capital Investment, 10 ⁶ \$	55.6
5.	Fixed Capital Investment Scaling Constants	
5.1	K	28.22 x 10 ⁶
5.2	b ₁	0.6229
5.3	b ₂	-1.3941
5.4	b ₃	1.0763
5.5	b ₄	0.5962
5.6	b ₅	0.1738
5.7	K	18.79 x 10 ⁶
5.8	b	0.7088
5.9	b ₄	0.7538
5.10	b ₅	1.4769
6.	Direct Labor, men per shift	6
7.	Labor Scale Exponent	0.25
8.	Yearly Catalyst Replacement Cost, 10 ⁶ \$	0.25
9.	Equipment Design Lifetime, Yrs	20
10.	Utilization Factor	0.9
11.	Steam Generation Efficiency, η_s	0.7
12.	Net Module Pressure Drop, ΔP , psi	15
13.	CO ₂ Methanation Constant, k	0.20
14.	Excess H ₂ parameter	1.96

TABLE 3.8 (Continued)

Material, Utility, and Energy Inputs/Outputs

<u>ITEM</u>	<u>CAT</u>	<u>NOMINAL DESIGN PARAMETER</u>	
1	1	Electric Power (KW)	- 1141
2	1	Fuel Energy (MM BTU/H)	0
3.1	1	Grade 1 Steam (M lbs/H)	+ 658
3.2	1	Grade 2 Steam (M lbs/H)	- 222
3.3	1	Grade 3 Steam (M lbs/H)	+ 221
4	1	Cooling Water, (Mgpm)	- 29.5
10	7	Water (M lbs/H)	181.0
200	4	SNG, MMSCFH	+10.4
200.1		Mole fraction, CH ₄	0.9218
200.2		Mole fraction, CO	0
200.3		Mole fraction, H ₂	0.0165
200.4		Mole fraction, CO ₂	0.0247
200.5		Mole fraction, H ₂ O	0
200.6		Mole fraction, N ₂ + Inerts	0.0370
300	2	Equivalent Synthesizer Gas, MMSCFH	-21.4
300.1		Mole fraction, CH ₄	0.2800
300.2		Mole fraction, CO	0.1600
300.3		Mole fraction, H ₂	0.5200
300.4		Mole fraction, CO ₂	0.0200
300.5		Mole fraction, H ₂ O	0.0020
300.6		Mole fraction, N ₂ + Inerts	0.0180
300.7		Equivalent Mole fraction, CO	0.1668
400	2	Actual Synthesis Gas, MMSCFH	-21.4
400.1		Mole fraction, CH ₄	0.2800
400.2		Mole fraction, CO	0.1600
400.3		Mole fraction, H ₂	0.5200

TABLE 3.8 (Continued)

302.4	Mole fraction, CO_2	0.0200
302.5	Mole fraction, H_2O	0.0020
302.6	Mole fraction, N_2 + Inerts	0.0180
302.8	Mole fraction, C_2H_6	0
302.9	Mole fraction, C_2H_4	0
302.10	Mole fraction, C_3H_8	0
302.11	Mole fraction, C_3H_6	0
302.12	Mole fraction, C_4H_{10}	0

etc.

TABLE 3.9

CONFIGURATION DESCRIPTION AND NOMINAL DESIGN PARAMETERS

Module 9, Configuration 9, A, 2, Tubewall

Methanator without Product Gas Recycle

Output Product: SNG (PPS-1)

Input Raw Material: Synthesis Gas with 3:1, H₂/CO Ratio

ITEM	NOMINAL DESIGN PARAMETERS	
4.	Fixed Capital Investment, 10 ⁶ \$	39.3
5.	Fixed Capital Investment Scaling Constants	
5.1	K	28.66×10^6
5.2	b_1	0.6660
5.3	b_2	-1.5879
5.4	b_3	1.1318
5.5	b_4	0.4678
5.6	b_5	0.1292
5.7	K	13.41×10^6
5.8	b_3	0.8370
5.9	b_4	0.6360
5.10	b_5	0.0061
14	Excess H ₂ Parameter	0.369

MATERIAL, UTILITY, and ENERGY INPUTS/OUTPUTS

ITEM	CATEGORY	NOMINAL DESIGN PARAMETERS	
3.2	1	Grade 2 Steam (M lbs/H) -	200
3.3	1	Grade 3 Steam (M lbs/H) +	199
4	1	Cooling Water	14.4

Note: Only items different from Table 3.8 are listed.

TABLE 3.10

PROCESS DESCRIPTION AND NOMINAL DESIGN PARAMETERS

Module 9, Configuration 9, B, 1, Multiple-Fixed-Bed

Methanator with Product Gas Recycle.

Output Product: SNG (PPS-1)

Input Raw Material: Synthesis Gas with 3:1, H₂/CO Ratio

ITEM	NOMINAL DESIGN PARAMETER	
4.	Fixed Capital Investment, 10 ⁶ \$	40.8
5.	Fixed Capital Investment Scaling Constants	
5.1	K	52.49 x 10 ⁶
5.2	b ₁	0.5113
5.3	b ₂	-3.6070
5.4	b ₃	2.5009
5.5	b ₄	0.4587
5.6	b ₅	0.1794
5.7	K	12.88
5.8	b ₃	0.5075
5.9	b ₄	0.5452
5.10	b ₅	0.1842
8	Yearly Catalyst Replacement Cost, 10 ⁶ \$	1.7
12	Net Module Pressure Drop, P, psi	50.0
14	Excess H ₂ Parameter	8.44

MATERIAL, UTILITY, and ENERGY INPUTS/OUTPUTS

ITEM	CATEGORY	NOMINAL DESIGN PARAMETERS	
3.2	1	Grade 2 Steam (M lbs/H) -	-299
3.3	1	Grade 3 Steam (M lbs/H) +	+298

Note: Only items different from Table 3.8 are listed.

TABLE 3.11
METHANATOR MODULE ALGORITHMS

- A. Equivalent Synthesis Gas Computation
 See Table 3.2
- B. Input Gas Restrictions
 See Table 3.3 and Equation 3.7
- C. Input Gas Quantity and SNG Composition Computation
 See Table 3.4
- D. Fixed Capital Investment Scaling
 See Equations 3.8 and 3.9
- E. Operating Cost Parameter Scaling
 See Equations 3.10 and 3.11
- F. Utility Requirements Scaling
 See Table 3.7

TABLE 3.12
Functional-Module Configurations - Subset for Feasible
Unit Process Construction Example using the LM

I. Module No. 9, Methanation

A. Configurations

1. Tubewall Methanator with Product Gas Recycle (9,A,1)
2. Tubewall Methanator without Product Gas Recycle (9,A,2)
3. Multiple-Fixed-Bed Methanator with Product Gas Recycle (9,B,1)

B. Input Raw Material Restrictions

$$X'(H_2S) \sim X''(H_2S) < 10^{-6}$$

$$X'(H_2)/X'(CO) \geq 3 + 1.9 \left(\frac{14.7}{P'} \right)^{2/3} \quad (9,A,1)$$

$$X'(H_2)/X'(CO) \geq 3 + 0.37 \left(\frac{1-2X'(CO)}{(X'(CO))^{2/3}} \right) \left(\frac{14.7}{P'} \right)^{2/3} \quad (9,A,2)$$

$$X'(H_2)/X'(CO) \geq 3 + 8.1 \left(\frac{14.7}{P'} \right)^{2/3} \quad (9, B, 1)$$

$$X''(H_2O) < [P']^{-1} \quad (P' \text{ in psia})$$

$$X'(CO_2) < (1/4)X'(CO)$$

$$\sum_{\substack{n > 1 \\ m \geq 4}} X''(C_n H_m) < 0.1$$

$$X'(CH_4) + 3.7X'(CO) + 4.6fX'(CO_2) + .9X'(H_2O) \geq .9$$

(Input gas composition restriction)

TABLE 3.12

Functional-Module Configurations - Subset for Feasible
Unit Process Construction Example using the LM
 (Continued)

C. Input/Output Relationships

Material Balance Equations

$$\frac{Q^o}{Q^i} = 1 - 3X'(CO) - 4fX'(CO_2) - X'(H_2O)$$

$$\begin{aligned} Q_c^o &= \text{condensate generated (MM lbs/Hr)} \\ &= 0.0475 Q^i [X'(H_2O) + X'(CO) + 2fX'(CO_2)] \end{aligned}$$

$$X^o(CH_4) = \frac{Q^i}{Q^o} [X'(CH_4) + X'(CO) + fX'(CO_2)]$$

$$X^o(H_2) = \frac{Q^i}{Q^o} [X'(H_2) - 3X'(CO) - 4fX'(CO_2)]$$

$$X^o(CO_2) = \frac{Q^i}{Q^o} (1 - f) X'(CO_2)$$

$$X^o(N_2) = \frac{Q^i}{Q^o} X'(N_2)$$

$$X^o(H_2O) = 0$$

$$\begin{aligned} f &= k[X'(H_2) - 3X'(CO)][X'(CO_2)]^{-1} \quad \text{but } \leq 1 \\ k &= 0.20 \text{ (nominal)} \end{aligned}$$

$$\begin{aligned} T_e &= \text{Thermal energy released (MMBTU/hr)} \\ &= Q^i [261X'(CO) + 214 fX'(CO_2)] \end{aligned}$$

II. Module No. 14, Gas Purification

A. Configurations

1. Hot Potassium Carbonate (14,C,4)
2. Pass-Through (Output=Input) Default (14,Z,1)

TABLE 3.12
Functional-Module Configurations - Subset for Feasible
Unit Process Construction Example using the LM
(Continued)

B. Input Raw Material Restrictions

None

C. Input/Output Relationships (14,C,4)

1. If $X'(H_2S) > 10^{-6}$

$$X^o(H_2S + \text{other sulfurous gases}) = .99 \times 10^{-6}$$

$$X^o(H_2O) = \frac{1}{p^o}, T^o = 100^\circ F$$

$$p^o = p' - 30 \text{ psia}$$

$$X^o(CO_2) = \text{MIN} \left\{ \begin{array}{c} 5 \left(\frac{X'(CO_2)}{X'(H_2S)} \right) X^o(H_2S) \\ Z \end{array} \right\}$$

$$X^o(\text{each other constituent}) = \frac{Q'}{Q^o} X'(\text{each other constituent})$$

$$\frac{Q^o}{Q'} = \frac{1 - X'(H_2S + \text{other sulfurous gases}) - X'(H_2O) - X'(CO_2)}{1 - X^o(H_2O) - X^o(CO_2)}$$

where Z is a selectable parameter $0.01 < Z$

2. If $X'(H_2S) < 10^{-6}$

$$X'(H_2S) = X'(H_2S)$$

$$X^o(CO_2) = Z$$

other equations as above

III. Module No. 13, Shift Conversion

A. Configuration

1. Chromium Promoted Iron Oxide Catalyst (13,A,1)
2. Cobalt-Moly Catalyst (13,B,1)

TABLE 3.12
Functional-Module Configurations - Subset for Feasible
Unit Process Construction Example using the LM
 (Continued)

B. Input Raw Material Restrictions

1. Chromium Promoted Iron Oxide 13,A,1 → None
2. Cobalt-Moly 13,B,1 → $X'(H_2S) \geq 0.001$

C. Input/Output Relationships

$$\frac{X^o(H_2)}{X^o(CO)} = y$$

where y is selectable over the following range

$$y_e \leq y \leq 20 \quad \text{where } y_e \equiv \frac{X'(H_2)}{X'(CO)}$$

$$P^o = P' - 15 \text{ psia}$$

$$T^o = 100^\circ\text{F}$$

$$X^o(H_2O) = 1/P^o$$

$$X^o(CO) = \frac{1 + y_e}{1 + y} \frac{Q'}{Q^o} X'(CO)$$

$$X^o(CO_2) = \frac{Q'}{Q^o} \left[X'(CO_2) + \frac{y - y_e}{y + 1} X'(CO) \right]$$

$$\frac{Q^o}{Q'} = \frac{1 + \frac{y - y_e}{y + 1} X'(CO) - X'(H_2O)}{1 - X^o(H_2O)}$$

$$X^o(\text{each other constituent}) = \frac{Q'}{Q^o} X'(\text{each other constituent})$$

IV. Module No. 2, Medium BTU Gasifiers - Internal Heat Type

A. Configuration

1. Synthane Process (2,B,3)

TABLE 3.12
Functional-Module Configurations - Subset for Feasible
Unit Process Construction Example using the LM
(Continued)

B. Input Material Restrictions*

1. $Y'(H_2O) \leq 0.05$

particle size $\rightarrow$ 70% through 200 mesh

C. Input/Output Relationships

For Pittsburgh Seam coal

$$\frac{Q^o}{S^o} = 0.071 [1 - Y'(H_2O)] \text{ MMSCFH/ton coal}$$

$$X^o(H_2) = 0.175 \quad X^o(C_2H_6) = 0.005$$

$$X^o(CO) = 0.105 \quad X^o(H_2S) = 0.003$$

$$X^o(CO_2) = 0.182 \quad X^o(N_2) = 0.005$$

$$X^o(CH_4) = 0.154 \quad X^o(H_2O) = 0.371$$

$$P^o = 990 \text{ psia} \quad T^o = 275^\circ F$$

V. Module No. 16, Coal Preparation

A. Configuration

1. Ball Mill (with facilities for receiving, storing, crushing, drying, and controlling dust, as necessary) (16,D,4)

B. Input Raw Material Restrictions

None

C. Input/Output Relationship

For $Y'(H_2O) \leq 0.05$

$$\frac{S^o}{S^i} = 0.95$$

For $Y'(H_2O) > 0.05$

$$\frac{S^o}{S^i} = 0.95[1.05 - Y'(H_2O)]$$

Output particle size $\rightarrow$ 70% through 200 mesh

* $Y(a)$ = wt. % of component a

S^i = input coal rate

S^o = output coal rate

TABLE 3.13

Algorithm for Feasible Unit Process Construction (Linking Model)

The user initiates the algorithm by selecting a product(s) and raw material(s). The computer then proceeds to:

1. Select and order, by Index N_1 , Stage 1 modules and competing configurations which produce the selected product: Set $N_1 = 1$.
2. For the N_1 th configuration of Stage 1, select and order by Index N_2 , Stage 2 modules and competing configurations which may produce the input raw material required by the N_1 th module of Stage 1: Set $N_2 = 1$.
3. For the N_2 th configuration of Stage 2 compare its output to the input specifications of N_1 th configuration of Stage 1. Each specification is either:
 - violated; Set $N_2 = N_2 + 1$ and repeat Step 3
 - satisfied
 - indeterminate - depends on input to N_2 th configuration - flag for later check.
4. For N_2 th configuration, select and order by Index N_3 , Stage 3 modules and competing configurations which may produce the input raw material required by the N_2 th module: Set $N_3 = 1$.
5. For the N_3 th configuration of Stage 3, compare output to input specifications of N_2 th configuration of Stage 2. If any violated, Set $N_3 = N_3 + 1$ and repeat. If none violated, check indeterminate specifications of N_1 th configuration of Stage 1. If any now violated, Set $N_3 = N_3 + 1$ and repeat.
6. Continue until primary raw material is reached. Record current sequence as a feasible unit process. Increment last index $N_k = N_k + 1$ until k th stage list is exhausted. Then reset $N_k = 1$ and increment $N_{k-1} + 1$. Continue until all feasible processes are identified.
7. For each feasible unit process identify effluents, byproducts, and secondary input streams. For each such stream, order and index a list of process-module configurations that might process or supply that material. Build-up side chains in same manner as primary chain. Record all feasible side chains as variants under primary chain.

References for Chapter 3

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4. APPLICATION OF MPPM TO POLICY ANALYSIS OF COAL RD&D PROCESS

4.1. ENERGY RD&D POLICY PLANNING

The Energy Reorganization Act of 1974 which created ERDA, placed upon the Administrator, among his other duties, the responsibilities for:

"exercising central responsibility for policy planning, coordination, support, and management of research and development programs respecting all energy sources in relation to near-term and long range needs, policy planning in regard to meeting those requirements, undertaking programs for the optimal development of the various forms of energy sources, managing such programs, and disseminating information resulting therefrom;"

To meet these responsibilities ERDA must combine both RD&D priority planning and the formulation of basic energy policy itself. In many cases energy policy analysis and the setting of energy RD&D priorities have a mutual influence on each other, insofar as the setting of RD&D priorities will influence the type of fuels developed and the structure of energy use. For example, if the U.S. were to formulate a policy decision that for environmental reasons, electrified mass transit for urban areas should be given primary emphasis, the impact on RD&D priorities would be significant. Following such a decision, research funds that might otherwise be spent on developing clean coal-based liquid fuels for combustion in vehicular engines would be directed to develop advanced electric power generation technology. However, such a policy decision would be unlikely to occur in the first place, in the absence of reliable evidence as to the relative technological promise and costs of the competing technologies.

Because of this interdependency, energy policy formulation and the setting of energy RD&D priorities will require a continuous cycle in which preliminary policy formulations influence RD&D priorities,

and RD&D results in turn cause revisions of policy formulations. This interactive character is central to RD&D policy planning and creates the need for a way of quickly and easily retesting and re-evaluating earlier results as later and more reliable data are obtained and as technological breakthroughs develop.

4.2. COAL-RELATED RD&D POLICY PLANNING

RD&D planning related to coal requires resolution of the same kinds of issues that must be resolved in planning for other fuels: technological feasibility, capital and operating costs, environmental effects. To the extent that coal is to be used in the direct production of space or process heating or cooling, its utilization would involve relatively few process steps (Functional Modules). When, however, coal is to be converted into a liquid, gaseous, or alternative solid fuel, and this fuel is then used to produce electrical or mechanical power, the energy system becomes a complex chain and the functions of each module in the unit process route typically can be fulfilled by any of several different alternative configurations. This same characteristic is even more true when the coal-related policy planner considers not only the energy systems based on coal, but the processes that could transform coal into feedstocks for industrial chemicals, pharmaceuticals, fertilizers and plastics.

The MPPM identifies 42 of these functional modules, as a convenient format for describing all existing or postulated coal-based energy or chemical systems. The number of alternative configurations within individual functional modules ranges from one to eighteen, with a plurality including at least five.

For these reasons, the policy-maker dealing with coal-based RD&D will have to keep track of a relatively large number of candidate module configurations competing for RD&D support. A very large proportion of these utilize rapidly changing technologies, and many of them yield products that have the capability of substituting for one another.

Variations in projected input costs or other limiting factors can cause realignments into new optimum unit processes. It is also characteristic of unit processes and/or configurations that many of them are based in whole or in part upon proprietary concepts upon which both technical and cost data are not always fully available. As a result, constantly changing configuration data is, in general, available for evaluation-- hopefully improving in quality.

To summarize, four conditions are characteristic of coal-related RD&D policy planning: a large number of candidate unit processes, many technologies in a state of rapid evolution, many products susceptible to substitution for one another with the optimum dependent on marginal changes in the economic environment, and continually changing (hopefully improving) data reliability.

4.3. COAL RD&D PRIORITY ASSESSMENT

Although what follows is in part generally applicable to RD&D planning, it is especially important as applied to coal-related planning because of the circumstances set forth above. The RD&D policy maker will almost certainly need a dynamic plan that will change with the passage of time as the apparent relative utility of competing configurations changes. He must be aware that these technologies will bear different relative importance to one another depending upon the data of a projected use and the anticipated constraints under consideration.

The RD&D planner will only be able to distribute a single year's budget once among the candidate technologies. Before making the distribution he will wish to rank order the candidate technologies according to the criteria that seem to him most persuasive at that time. He will always be uncertain to a large degree about what the actual future constraints will be upon the coal-based technologies among which he must allocate his limited current resources. For this reason he will probably wish to test the sensitivity of any rank ordering of competing candidate technologies to changes in the economic environment and to changes in cost parameters (within their perceived accuracy limits).

This entails not only looking at the existing systems, but also postulating new systems that could exist if one or another missing technological link could be supplied. To perform this function, it would be extremely useful to have a method by which to determine to what degree the rank ordering of currently definable systems would be changed by the postulated achievement of what would otherwise be a missing link, so as to permit the construction of a new hypothetical candidate system. In making up the hypothetical system, in turn, the planner would be helped by a tool that would permit him to estimate what the cost and performance specifications of the missing configuration would be.

4.4. USE OF MPPM IN COAL-RELATED POLICY DECISION MAKING

The foregoing discussion has outlined the general activities of the RD&D policy maker. The MPPM gives a common format and consistent data base for analyses; it also embodies the calculational capability through which identified systems can be compared to one another and analyzed for sensitivity to changes in data and economic variables. The procedure is computerized so that the many variables embodied in evaluating all the candidate technologies can be dealt with quickly and inexpensively in order to permit repeated testing of the consequences of various possible alternative situations and policies.

4.4.1. Policy Questions Suitable for MPPM Analysis

Questions that are relevant to policy decisions on coal-process technology RD&D fall into two general categories: 1) those related to aggregative efforts, and 2) those related to the sensitivity of relative rankings of technological options to changes in the economic environment and/or changes in the data base. Examples of questions in the aggregative assessment category include:

- "What are the aggregate investment requirements, using the best available process, to produce middle distillate oil from coal by the amount required to meet 25% of U.S. residential heating demand by 1990?"

- "What mix of SNG unit process will require the smallest capital investment per unit output, given a certain availability schedule for coal by type, to provide a substitute for one third of the United States' anticipated demand for natural gas, by 1985? What would be the result if the goal were two-thirds by 1995?"
- "Given a forecast of anticipated demand for polyurethane elastomers for 1985, what would be the demand for coal, and for coal-based products, required to meet the demand for chemical feed stocks now obtained from hydrocarbon fuels? What would be the cost of raw materials per unit output?"
- "What will be the cost of controlling the process residuals that would be generated by producing low molecular weight liquid hydrocarbon mixtures at the scale necessary to supply one-third of the anticipated United States automobile fuel demand for 1995?"
- "Determine the increase over time in installed capacities for coal-derived methanol production that could be achieved for a specified capital investment schedule."
- "What investment schedule is necessary to achieve a desired capacity for coal-derived methanol production? How should this investment be allocated between Eastern and Western U.S. for a given regional demand structure and interregional transportation cost?"

Some examples of policy related questions in the sensitivity analysis category might be

- "What is the most significant obstacle to the potentially least costly coal based middle distillate oil production to meet 25% of the United States residential heating requirements by 1990? What would be the cost consequences of relying on a less than optimum process based on existing technology?"

- "What coal conversion unit processes are the most promising candidates to meet a given projection of demand for anhydrous ammonia of the United States fertilizer industry in 1990? How do changes in raw material costs affect relative process rankings?"

As may be readily observed from these examples, there is a good deal of overlap in the two categories of policy questions. Thus to arrive at an estimate of aggregative investment costs using a "best" process for middle distillate oil, one must define "best". This, in turn, implies some kind of sensitivity analysis.

4.4.2. MPPM Policy Analysis

A detailed sequence of operations to use the MPPM to analyze the production of middle distillate oil from coal would be as follows:

- Raw material sources (coal types and availability by region) would be specified, probably in a series of scenario variations. Demand for middle distillate oil for residential space heating would be projected (by the analyst, aided by a macro-economic model). Economic/environmental variables, including interest rates, tax structure, raw material prices, by-product prices, venture-capital profit expected, and maximum investment per plant, would have to be specified by the user, perhaps in several alternate combinations.
- The MPPM algorithms would be exercised starting with the Linking Model to construct a "library file" of feasible unit processes that could lead from the specified raw materials to middle distillate oils. The various parts of the PCEM would operate on this list to evaluate and rank the unit processes.

- At this point, outputs available to the analyst would be:
 - a list of feasible unit processes
 - a list of configurations used
 - process throughput at optimum and maximum (may be identical) plant size for each feasible unit process
 - product cost for each unit process
 - process residuals and cost of waste treatment for each unit process
 - by-products made available from each unit process and amounts credited against unit process costs
 - time-phased availability of each unit process, based on availability of component module configurations.
- The analyst can now answer the first question given under the sensitivity analysis category, i.e., he can recognize the "potentially least costly" process for production of middle distillate oil, compare its time phase availability to other less-than-optimum processes, and recognize the pacing module configurations; and he can assess the cost penalty of using the processes with earlier availability. These results can be further tested against variations in economic parameters and configuration cost data by rerunning the PCEM against a chosen subset of the feasible unit process library file.
- By choosing a process selection criterion, development schedule (or using the process availability times obtained in the previous step), the IDM can now be used to address the middle distillate oil question under the aggregative assessment category. Results available to the analyst would include:
 - List of unit processes chosen, paired with raw material usage by region.
 - Product cost by unit process and by region, and national average costs.

- Residuals generated by unit process, by region, and nationally. Similarly for waste processing costs.
- By-product production by unit process, by region, nationally, and amounts credited against unit process costs.

All of these results can be recomputed at any stage using redefined scenario variables. The list of unit processes to be considered at each iteration can be shortened or lengthened by external command. The MPPM does not make decisions for the analyst. It provides data and computational results in a form from which the analyst can recommend and justify RD&D policy decisions.

In evaluating the MPPM, it will also be important to be aware of one function it cannot perform by itself: the model will not estimate the amount of construction material, such as stainless steel or copper, required by a particular unit process. The MPPM does not contain information on the materials composition of production equipment. By itself it will not compare the materials used to construct the process equipment of alternative technologies. It will be possible to link the model to input-output models which compute such demands on the basis of average demand coefficients for industry segments, e.g., materials consumption of the chemical industry per dollar of new plant construction. One such model is "INFORUM" a component of "SEAS", the EPA-sponsored macro-economic model.

4.5. SUMMARY

The policy maker concerned with setting RD&D priorities for coal based technology and making associated policy decisions will be working with a very much larger number of variables and a much less well-defined data base than his counterparts dealing with other energy supply technologies. He will need a comprehensive mechanism for repeatedly re-analyzing his alternatives as his data base improves, and as technological

advances occur. He will also wish to consider a number of competing criteria and possible future technical, economic and environmental developments in deciding his research priorities. To satisfy these needs he will require a systematically organized, internally consistent data base and a computational capability through which to apply his chosen criteria repeatedly and--therefore quickly and inexpensively--to compare the relative and absolute merits of the candidate technologies he must evaluate. The aim of MPPM is to provide such a tool.

5. MPPM USE WITH OTHER COMPUTATIONAL MODELS

Operating as a self-contained model, the MPPM generates comparative assessments of coal technology alternatives, thereby facilitating the evaluation of coal RD&D policy. Linking the MPPM to general economic energy models will reveal the influence of coal RD&D policy decisions on other sectors of the economy. This linkage will also provide exogenous information regarding coal process tradeoffs. Such joint evaluations increase the scope of the MPPM system and show the important causal linkages between coal technology options and economic events.

The purpose of this chapter is to review other existing energy and economic models as candidates for integration with the MPPM. In the first section, several models of interest are reviewed in detail and an evaluation of their advantages and disadvantages is given. The second section shows the relationship of each of the models studied to an overall description of U.S. energy supply and demand. Emphasis is given to the role of the MPPM, and the chapter concludes with a description of several possible approaches to usefully integrating the MPPM with other models.

5.1. ENERGY MODELS

The following energy models are reviewed in this section:

- Project Independence Evaluation System (FEA/PIES)
- University of Illinois Energy Input-Output Tables
- Strategic Environmental Assessment System (SEAS)
- Dartmouth System Dynamic Coal 1, Fossil 1
- Brookhaven Energy System (BNL)
- Bechtel Source-to-Use Economics
- Bechtel-NSF Energy-Supply Model
- Other Models

5.1.1. Project Independence Evaluation System (FEA/PIES)

5.1.1.1. Abstract

Project Independence was created in response to the Arab oil embargo of 1973. The model was supposed to provide a "blueprint" for energy independence of the U.S. by 1980, but finally was designed to provide a tool for measuring and evaluating various policies having an impact on:

- development of alternative energy sources;
- vulnerability to import disruptions;
- economic growth, inflation, and unemployment; and
- environmental, social, and regional effects.

The model includes eight scenarios representing a range of possible energy situations for the United States in 1985. The methodology used, schematized in Figure 5.1, can be explained as follows:

- a macroeconomic model generates such variables as GNP, unemployment, inflation, population;
- these variables, combined with the use of a 24 sector input-output table and other techniques, enable the user to compute the total energy demand split between the industrial, residential, commercial and transportation sectors;
- these total demands in energy are then disaggregated by the use of market share functions, and demand elasticities are derived at the same time for each fuel;
- supply curves by regions and fuels have been obtained through judgmental evaluation of experts, as well as the availability of critical resources (materials, capital, manpower, etc.);
- this information is then combined in an integrating model which combines the two sets of curves and optimizes the transportation of energy flow by iterative use of a linear programming algorithm.

5.1.1.2. Inputs

The model does not require any inputs other than the modification of existing parameters in order to study alternative scenarios. Nevertheless, there are some possibilities of furnishing more detailed data from other models (industrial demand in energy, etc.), as will be described in Section 5.2.

5.1.1.3. Outputs

The model gives the following outputs for 1977, 1984, 1985, and for the two scenarios of "Business as Usual" and "Accelerated Development":

- description of the U.S. energy system under the scenario studied;
- demand in energy from various sectors;
- market clearing price for each fuel in each region;
- transportation pattern of the energy flows;
- level of activity of each form of energy; and
- requirements in resources, materials, capital, and manpower.

5.1.1.4. Types of Questions Addressed

The Project Independence energy model has been developed to help solve the following problems:

- evaluation of alternative energy sources at the national level;
- impact of world fuel prices on the U.S. energy system;
- evaluation of inter-fuel substitution in terms of the impact of cost and availability of resources;
- evaluation of inter-regional competition for fuels; and
- environmental impact associated with each energy system.

5.1.1.5. Advantages and Disadvantages

The Project Independence Evaluation System relates macro-economic projection of energy demand with microtechnological evaluation of the energy supply system. This combination facilitates consistent energy projections. Moreover, the model presents enough detail for the assessment of short-term inter-fuel substitution, and the regionalization of the demand and supply curves gives a good framework for the study of inter-regional competition. On the other hand, the time-frame defined for the model (1973, 1985) provides few opportunities for the evaluation of technologies which will not be on a large commercial scale by 1985, such as most of the advanced coal conversion processes. This presents a serious limitation for considering the model as an RD&D planning tool.

The model is weaker in its evaluation of potential bottlenecks in the transportation system, and the acceptability of environmental or social effects associated with some form of energy. The demand elasticity curves are reliable for small changes in demand, but they break down for drastic changes in demand. This limitation can be acceptable within the short time frame of the model, but could be a problem if longer term projections have to be made. Finally, a problem inherent with the optimization used in the methodology is that the real energy system is not optimum, and therefore the energy price could be underestimated or the demand overestimated. To summarize, the Project Independence Evaluation System must be considered a good comprehensive tool for analyzing short-term energy policies, but is of little help in evaluating RD&D projects to be on a large commercial scale after 1985.

References

Federal Energy Administration Project Independence Report, *Project Independence*, November 1974.

5.1.2. The University of Illinois Energy Input/Output Models

5.1.2.1. Abstract

The Illinois energy input-output table has been created to compute the values of the total direct and indirect energy embodied in any good or service. The indirect component of this total demand may be important. Thus, in one study using this model, the results indicate that the auto manufacturer itself uses only about 6% of the total energy necessary to produce and market a car¹-- the remaining energy being used at earlier steps to manufacture components required by the car manufacturers (steel, windows, etc.).

The input-output technique has been chosen for two reasons:

- (1) The conceptual framework of the input-output models takes into account the steps involved in the complex manufacture/sales chain.
- (2) A large body of data was already available from the U.S. Department of Commerce at a fairly high level of detail (367 sectors of the economy).

The basic I-O table has then been implemented with a set of energy coefficients which determines the amount of energy products required by unit of output of each sector. The energy products used in the table are:

- coal
- crude oil
- refined petroleum
- electricity
- natural gas

The resolution of the system (which consists mainly of the computation of the inverse matrix of input coefficient $(I-A)^{-1}$, followed by the multiplication of this matrix with the matrix of energy coefficients) gives the amount of energy required for the manufacture of each type of goods and services, with the relative shares

of the five forms of energy described above. These results have been computed for the 1963 and 1967 (BEA) I- Tables. ²

A special version of the Illinois I-0 table has been designed to permit the interface of the model with the Brookhaven energy system model.³ The great improvement of this new approach (which will be described extensively in Section 5.2.), is to replace the energy technology coefficients, which were given in terms of specific energy form (coal, gas, etc.), by energy coefficients given in terms of basic energy demand (BTU used), letting the Brookhaven optimization model compute the optimal fuel mix to satisfy these demands.

5.1.2.2. Inputs

The inputs required by the Illinois energy input-output model depend on the problem of the user:

- No inputs are necessary to compute the energy required for the manufacture of specific goods.
- A vector of final demand is required for the computation of the total energy demand in a specific year for interfacing with the Brookhaven model.

5.1.2.3. Outputs

Depending on the inputs furnished, the outputs can be:

- Energy demand, in terms of energy products, (coal, gas, etc.) for the manufacture of each good or service represented in the model.
- Total energy demand in terms of energy products required by the total industry in a specific year.
- Total basic energy demand and equivalent optimal fuel mix obtained through interfacing with the Brookhaven model.

5.1.2.4. Types of Questions Addressed

The model in this original or modified form can help to solve the following problems:

- What is the total energy required by an automobile or other equipment through its lifetime? This can be computed using the energy required for the manufacture, maintenance, insurance, garage, tires, etc., given by the energy coefficients.
- What is the total demand in energy required by a sector of the industry? This can be determined by the same type of computation for all the sections of a group.
- What is the total demand in energy in a specific year, consistent with GNP or other projections for the same year?
- What is the impact of conservation measures in the industry energy usage?

5.1.2.5. Advantages and Disadvantages

The original version of the I-0 table of the University of Illinois presents a very useful tool for the evaluation of the direct and indirect energy requirement of specific products or services. Its high level of disaggregation (367 sectors) enables the user to perform a detailed comparative evaluation of energy intensiveness. On the other hand, the formulation of energy requirements in terms of energy products and the problems encountered in the inconsistency between flow of dollars and flow of BTUs does not permit the user to compare BTU requirements. The modified version of the model presents several advantages. First, it permits the projection of energy demand consistent with the projection of other macroeconomic variables. Second, its structure--separating energy products, energy supply sectors, and industrial sectors--facilitates the evaluation of the industrial requirements of alternative energy policies, as well as the evaluation of various fuel mixes. It also permits the evaluation of policies such as conservation measures in industrial energy use, or technological changes. The only drawback of the method of computing BTU requirements instead of product

requirements is that in some cases substitutions are not possible and certain forms of energy must be used for technical reasons. How this problem is taken into account is not fully explained.

References

1. "An Energy I-O Matrix for the United States, 1963", User's Guide by R. Herendeen, March 1973, CAC Document #69.
2. "Energy Cost of Goods and Services, 1963, 1967," R. Herendeen, C.W. Bullard, November 1974, CAC Document No. 140.
3. "A Two-Level Iterative Model for Estimating Inter Fuel Substitution Effects," BNL 19863, Brookhaven National Laboratory, Upton, New York, 1973.

5.1.3. Strategic Environmental Assessment System (SEAS)

5.1.3.1. Abstract

The Strategic Environmental Assessment System has been designed as "a collection of interdependent models for forecasting the state of the environment resulting from alternative environmental policies and socio-economic trends."¹ The different modules incorporated in SEAS, and their inter-relations, are shown in Figure 5.2. Of particular interest in this study are the modules concerned with energy projections, namely INFORUM and ENERGY. These modules, which forecast the direct and indirect industrial demand in energy, coupled with two additional modules (in the process of development) which will forecast the energy demand of the transportation and residential and commercial sectors, enable SEAS to forecast energy demands consistent with macro-economic variable projections.

The different modules work as follows:

- The INFORUM module consists of a macroeconomic variable generator which forecasts variables such as population, disposable income, labor force, and money supply--and which, in turn, serves to define a vector of final demand for a 185 sector I-0 table. This vector of final demand represents the components of GNP, such as personal consumption expenditures, government purchases, capital investment, inventory changes, and imports. This vector of final demand associated with the I-0 table gives the value of the level of activity for each of its 185 industrial sectors studied.
- The ENERGY module computes the equivalent energy required to allow these levels of activity. These amounts are obtained through the use of energy coefficients which give the amount of energy required by unit of output

for each sector. When the levels of activity of the sectors are known, therefore, the equivalent amounts of energy required are computed.

- The additional residential/commercial and transportation modules will compute the energy required by these sectors, taking into account the projection of activity of passenger miles travelled and stock of such existing equipment as electrical appliances, as well as the type of cars in service.

The INFORUM and ENERGY modules are fully developed and can give projections up to the year 1990 or 2000. The residential/commercial and transportation sectors are in the process of development.

5.1.3.2. Inputs

The SEAS model does not require any inputs but can accept alternative parameters such as:

- GNP components or final demand sectors from other projections. Currently, SEAS can be run with the macro-economic forecast from Chase Econometric Associates or the "low productivity" scenario developed by Clopper Almon, Jr.
- Change in the I-O coefficients concerning technological changes in processes or interfuel substitution.

5.1.3.3. Outputs

The outputs of the SEAS model are:

- Level of activity of the 185 sectors of the I-O tables;
- Demand in energy by fuel type, consistent with macro-economic projections. This demand is formulated for each category--industrial, residential, commercial, and transportation.

- Other effects--e.g., environmental or social, not directly related to the energy demand.

5.1.3.4. Types of Questions Addressed

The SEAS model originally designed for the evaluation of environmental impacts can be useful in evaluating the following questions:

- What is the direct and indirect demand in energy by fuel type required by the industrial sector?
- What is the demand for energy products or energy use (BTU required) of the transportation sector by mode of transport (auto, bus, rail, air, etc.)?
- What is the demand for energy products or energy use of the residential and commercial sector, by type of usage (space heating, air conditioning; etc.)?

5.1.3.5. Advantages and Disadvantages

SEAS is a reliable model for the mid-term projection of energy demand. This demand is based on the projection of macroeconomic variables and, therefore, should be considered a potential input to the more detailed model of energy supply and demand, which could, in turn, feed back information concerning modification of coefficients. Such developments are already in process and will be emphasized in Section 5.2.

Another favorable feature of the model is that it can forecast the energy demand not only in terms of energy products, but also in terms of BTUs, letting other more detailed models define the optimal type of fuel to employ in each specific case.

An area which is not fully explained in the model is its ability to cope with conservation measures induced by the energy price. Finally, a disadvantage of the model--one which is found in most of the models of this type--is the lack of interaction between energy price and energy demand either through the interaction of elasticities or through the modification of the projection of the macroeconomic variables (effect of energy price on GNP growth).

References

Strategic Environmental Assessment System, Executive Summary for EPA, September 1975, Booz, Allen & Hamilton, Inc.

Version IV - SEAS Residential/Commercial Module, by Ralph Doggett, November 1975. IR&T Document.

Version IV - SEAS Transportation Module, by Marc Narkus-Kramer, November 1975. IR&T Document.

5.1.4. Dartmouth System Dynamic Coal 1, Fossil 1

5.1.4.1. Abstract

The purpose of the Dartmouth System Dynamic (DSD) modeling project is to develop a tool capable of evaluating the social, political, and environmental implications of the introduction of new fossil fuel conversion technologies during the energy source transition period of 1975 to 2010.

The objective of the "System Dynamic Methodology" is not to give a precise long-term prediction of such a complex technological transition, but to facilitate understanding of the complex dynamic interactions within the energy system, and the delays inherent in any technological transition. The model uses the system dynamic methodology developed by J. Forrester¹, and will cover the period 1950-2010, so as to permit a validity test on the period 1950-1975. The time period limits the dynamic phenomena to be considered in the model.

The following phenomena will be introduced:

- growth in energy demand;
- interfuel substitution;
- fossil energy depletion;
- adjustment to changing energy prices;
- development of new technologies; and
- environmental restrictions on energy use.

The level of detail with which each of the elements will be treated will have to be a trade off between a risk of misrepresentation of the phenomena for an aggregated model, and a problem of data gathering for a disaggregated model. In some cases, the problem will be solved by interfacing with other models.

The structure of Fossil 1, which is a proposed extension of the existing Coal 1, is given in Figure 5.3.

5.1.4.2. Inputs

The following inputs may be provided to the model:

- Macroeconomic parameters, GNP, population, etc.;
- Data concerning different RD&D policies such as performance data for advanced coal conversion processes associated with required transportation costs; and
- Energy and non-energy-related policy scenarios.

5.1.4.3. Outputs

The outputs associated with these inputs are:

- Nature and time of potential energy shortages;
- Economic and environmental impact index; and
- Relative share of energy use (coal, gas, electricity).

5.1.4.4. Types of Questions Addressed

The primary purpose of this model is to provide a useful tool for analyzing the effects of alternative technological options, and to help isolate the complex secondary and tertiary effects of various RD&D policies. The scenarios which could be studied by the model are threefold:

- Evaluation of the effects of exogenous variables (GNP growth, population, etc.) on energy policy decisions;
- Evaluation of various RD&D policies and identification of areas requiring intense development effort; and
- Evaluation of the influence of other fossil energy policies, such as natural gas price deregulation, amendment to the Clean Air Act, etc., on the energy system.

5.1.4.5. Advantages and Disadvantages

The Dartmouth System Dynamic model represents the interaction of the different components of influence in the U.S. energy system.

Its strength is its capacity to consider, in a dynamic frame, the economic, environmental, social, and political constraints which could slow down the expected development of coal conversion technologies, and thereby create energy shortages between now and the year 2010. The DSD is one of the few models which explicitly permit the user to judge the desirability of various RD&D projects and to evaluate the additional legislative measures required for the overall feasibility of the system. On the other hand, the fact that the model is aggregated at a national level does not permit analysis of the inter-regional fuel competition. But as mentioned before, the interaction of the DSD with other disaggregated models should partly overcome this problem. There is some uncertainty as to whether the parameters employed in the model description are sufficiently realistic, and it would be interesting to know the sensitivity of the solutions to the value of these estimated parameters (estimate of time lags, rate of discovery, etc.).

References

1. J. Forrester, "Industrial Dynamics," Cambridge, Mass. MIT 1961.
2. Dennis L. Meadows, "Mid Term Technology Assessment System: A Dynamic Simulation Model of the U.S. Fossil Energy Transition (1975-2010)," February 1975, Thayer School of Engineering, Dartmouth College.

5.1.5. Brookhaven National Laboratory Energy Models (BNL)

5.1.5.1. Abstract

The Brookhaven Energy Model has been designed to describe the processing, delivery, and use of energy in the U.S. and to permit technological assessment and policy analysis. The core of the model consists of the "energy model data base" (EMDB) associated with a network which represents the flow of energy, step by step, from extraction to end use. The network, schematized in Figure 5.4., consists mainly of a supply file and a demand file linked together by the exchange of energy products, including electricity, low or high BTU gas, fuel, etc. With each of the steps (extraction, conversion, transportation) involved in the processing or use of the energy, is associated a set of 41 parameters. These data concerning the efficiency, cost, environmental impact, and health hazards give a quantitative evaluation of the effect associated with the running of each process. The network and data base can be used in two different ways:

- The system has its own projection of demand, energy use, and flow of energy through the network, for several base years (1977, 1985, 2000, 2020).
- The user can choose to study the overall economic or environmental effect associated with the perturbation of some of the components (variation in the final demand or in processes).
- The user can also use a linear programming optimization routine called BESØM, which will design the "best" economical or environmental process combination, taking into account constraints on resource availability and effluent limitations.

Several other routines enable the user to modify or extract some data from the data base.

5.1.5.2. Inputs

As described before, the inputs depend on the problem of the user, who may choose to furnish or default any of the following:

- Final demand in energy use disaggregated by industrial, residential, commercial, and transportation sectors. This demand has to be formulated in terms of energy use (space heating, passenger miles travelled) in order to allow for substitution.
- Process allocation within an activity (for transportation of coal: percentage of coal transported by train, percentage by barge, percentage by slurry pipelines).

5.1.5.3. Outputs

The outputs provided give summary results sorted by the following categories:

- The energy flow for each process, and the associated environmental effects;
- The energy flow and effect at an activity level (transportation of coal by all means).

5.1.5.4. Types of Questions Addressed

Depending on the inputs furnished, the BNL can help to answer the following questions:

- What are the economic and environmental impacts of candidate energy policies?
- What are the substitutions or technological changes likely to take place in the energy "product" usage, e.g., competition of electricity or natural gas for space heating?
- What are the desirable technological changes in the energy conversion processes, e.g., competition of different synthetic gases?
- Coupled with an I-O table, the BNL model can use energy projections consistent with macro-generation of

GNP and beedback-adjusted I-0 coefficients representing technological changes and inter-fuel substitution.

5.1.5.5. Advantages and Disadvantages

The BNL's strongest feature is its evaluation of technology changes on the supply side as well as on the utilization side. It therefore represents a useful tool in the evaluation of alternative RD&D projects. It can also be considered a powerful accounting system for computing the environmental, economic, and social impacts of national energy mixes. One of the major weaknesses of the model is its lack of regionalization. This presents a problem for analysis of inter-regional competition of fuels, as well as for evaluation of transportation requirements. Another disadvantage is the model's lack of dynamic effect. The optimum or other solutions generated are static solutions for different years, and the desirability of these solutions for earlier or later years is not taken into account. Consequently, the model does not take into account the existing facilities and the time lags involved in the substitution. Finally, there is a lack of price sensitivity for the resource evaluation in the optimization routine. BNL is attempting to remedy all of these problems, and the modified version should provide an interesting tool for evaluation of RD&D projects. Present work being done to couple I-0 models like the Hudson-Jorgenson or the I-0 of Illinois with the BNL should lead to a useful technique for estimating substitution effects.

References

"Brookhaven Energy System Optimization Model" E-A Cherniavsky, December 1974. BNL 19569 Brookhaven National Laboratory, Upton, NY 11973

"Reference Energy System and Resource Data for Use in the Assessment of Energy Techniques," AET 8, April, 1972, Associated Universities, Inc.

5.1.6. Bechtel Energy Source-to-Use Model

5.1.6.1. Abstract

The purpose of the Bechtel Energy Source-to-Use Model was to provide a tool for "evaluating the relative economics of various systems of delivering clean coal energy from the mine to the energy user."¹ In order to do so, the model emphasized the study of coal or coal-related energy transportation systems: coal transportation by barge, train, slurry pipelines, or the transportation of synthetic gas or electricity. To permit a detailed evaluation of the transportation system requirement, as well as to take advantage of the regional definition of effluent limitations, the model has been regionalized to the 243 Air Quality Control Regions (AQCR).

The methodology employed can be explained by the following steps:

- For each AQCR region, the following information is given:
 - coal production capacity, cost, BTU content, sulfur content;
 - demand in energy products, including electricity, high and low BTU gas, etc.
 - coal conversion processes data; and
 - effluent limitations.
- Between each of the regions, the transportation cost and capacity are given for each form of energy transportation.
- Taking the above information into account, a linear programming algorithm computes the optimal transportation flow between regions. The optimum is relative to overall transportation and conversion cost, and must fulfill the constraints defined for each region.

The model can be used to study mid-term (75 to 95) scenarios, and is now in the last stage of development.

5.1.6.2. Inputs

The model has its own set of input data, but the following inputs can be used for this study of scenarios:

- the energy product demand disaggregated to AQCR regions (electricity, gas, etc.);
- regionalized data concerning coal conversion technologies;
- data concerning the transportation systems of coal or coal-related products.

5.1.6.3. Outputs

The outputs of the model are of the following nature:

- amount of coal, electricity, gas, etc. shipped by various modes of transportation;
- amount of coal processed in each region;
- constraints on the solution, and marginal benefit associated with the extension of the constraints (e.g., benefit of expanding the production capacity in a region).

5.1.6.4. Types of Questions Addressed

The Bechtel Source-to-Use model can help to answer the following questions:

- Which combinations of coal conversion processes and transportation modes provide the least costly methods of deriving clean energy from coal in each region?
- What are the marginal economic benefits of increasing the level of activity for a particular technology?
- How do combinations of coal conversion and transportation processes compete with non coal-related energy?

- How sensitive are the least costly technological methods of deriving clean energy from coal to
 - . environmental regulations?
 - . transportation capacities?
 - . coal production capacities?
 - . energy demand projections?

5.1.6.5. Advantages and Disadvantages

A strength of the model is its capacity for comparative evaluation of energy transportation systems and their relative contribution to the U.S. distribution network. The high level of regionalization (243 AQCR) can be considered either an advantage or a disadvantage. The advantage is that it permits a precise evaluation of the transportation requirements by type and by fuel, but there is a disadvantage in the need to gather the data at such a level of detail. The demand in energy production, as well as the production capacity or the resource availability at such a level of detail, can be difficult to obtain. Another type of input difficult to assess is the transportation capacity, as this value depends strongly on such considerations as loading and unloading at the end of lines. Finally, the "realism" of the model could be greatly improved if the resource constraints could be replaced by price-sensitive supply curves. This would transform the problem from a linear to a quadratic one; but this problem could still be solved by iterative application of LP, and would reflect more accurately the real behavior of the energy system. In any case, this model can provide useful information concerning transportation requirements to other more aggregated models.

References

1. "Clean Coal Energy - Source to Use Economics," Phase I Report, R&D Report #111, from Bechtel Corporation, California, May 1975.

5.1.7. Bechtel/NSF-Energy-Supply

5.1.7.1. Abstract

The Bechtel/NSF-Energy-Supply model has been designed to study the feasibility of proposed U.S. energy policies, with regard to resource requirements associated with the construction and operation of energy supply and transportation facilities. The time range covered by the model (1975 to 1990) allows the evaluation of alternative mid-term energy policies. The model is essentially a systematic planning method involving the following steps:

- the user chooses a candidate future energy mix for the years 1977, 1980, 1985, 1990;
- a computer program calculates the additional energy facilities to be put on line each year to meet the demand;
- at user specification, the model locates the energy facilities in 14 regions and designs the transportation network required to link these facilities to the 11 demand regions; and
- the program then calculates the annual requirement of capital, manpower, and materials for each energy and transportation facility from initial commitment to plant startup, and throughout its economic life.

Figure 5.6. shows the interaction among the 66 energy facilities. The model is fully operational and has been tested on the "President's Energy Program."

5.1.7.2. Inputs

The system has been designed to allow flexible inputs at different levels of decisions. The user has to specify:

- the relative amounts of energy products required (electricity, low or high BTU gas, . . .) or fuel mix, for at least one of the following years: 1977, 1980, 1985, 1990.

The user may specify or default:

- process allocation coefficients for each of the final fuels;
- energy facility location coefficients;
- regional demand coefficients;
- interregional fuel flow rules; and
- interregional transportation modal split coefficients.

5.1.7.3. Outputs

The outputs, like the inputs, are flexible and can be specified to the convenience of the user. The outputs consist of the annual requirements of resources belonging to the following categories:

- manpower requirements (man-years);
- capital, material and equipment (dollars); and
- selected major material and equipment (physical units).

This information can be given for part or all of the 66 energy facilities and 25 transportation modes, and on a national or regional level of detail.

5.1.7.4. Types of Policy Questions Answered

Provided that the required inputs are furnished, the following questions can be answered:

- What energy and transportation facilities must be constructed to implement a candidate national energy program?
- What is the annual requirement in manpower, material, and capital required for the energy program?
- What would be the equivalent amount required for a specific industry or a specific region?
- What are the relative requirement tradeoffs between energy policies?

5.1.7.5. Advantages and Disadvantages

The main advantages of the model are its high level of detail concerning the resource requirements of the different facilities involved in the model, and its transparency to the user. The manipulation of the data is quite straightforward and enables the user to interface with the model at different levels of decision and, therefore, to check the validity of the results. A less appealing feature is the way the transportation problem is taken into account. The regions defined in the model are large, and there may be some uncertainty about the accuracy of the transportation data, particularly that which concerns intra-regional transportation. Another aspect of the model which could be considered a disadvantage is the lack of constraint on resources. The model will compute the resource requirements independently of their feasibility. Consequently, if a solution appears infeasible after a first analysis, an iterative procedure is required in order to change the solution to a feasible one. Hopefully, this adjustment can be achieved by interaction with other models, as will be described later.

In summary, this model can be considered a good planning tool for energy assessment.

References

"The Energy Supply Planning Model," M. Carasso, Bechtel Corporation, August 1975.

Final report to NSF, Volumes I and II.

5.1.8. Other Energy Models

The various energy models described above were the ones assigned in the Task Force. Nevertheless, it appeared useful to us to review, albeit briefly, other models available which could interface directly with the MPPM or with other models. The comparative evaluation of the models of the two groups will be done in Section 5.2. The time constraint does not enable us to present a detailed description of these models, but the following list should provide the reader with adequate references for a more detailed analysis.

- HUDSON-JORGENSEN - "U.S. energy policy and economic growth, 1975-2000"
The Bell Journal of Economics and Management Science,
Autumn, 1974, p. 461; or for a more condensed
description, "Survey of Regional Energy Model,"
Argonne National Laboratory
- SRI-GULF - "SRI-GULF Energy Model - Overview of Methodology,"
Edward G. Gazalet, January, 1975, SRI Publications.
- LORENDAS - "Long-Range-Modeling of Worldwide Energy Development
and Supplies: Outline of Formulation and Applications,"
L.A. Rapoport, July, 1975, Virginia Polytechnic
Institute and State University, Blacksburg, Virginia.
- JAMES JUST - "Impact of New Energy Technology Using Generalized
Input-Output Analysis," Proceedings of MIT, MIT Press,
February, 1973.
- ICARUS - "COST" Cost Oriented System Technique Users' Manual
and "Chemical Engineering Deskbook", October 21, 1974
p. 115.
- BATELLE/COLUMBUS - "A Proposal to Develop Energy Price and Availability
Projections," Batelle Columbus Laboratories, April,
1973.

5.2. MODELS INTERACTION

In the preceeding section (5.1), we gave a description of the models of interest in this study. In this section, we give a general description of the energy supply and demand system, and the relative position of the models in this system. We then proceed to a comparative evaluation of their characteristics, and conclude by giving several examples of models interaction involving the MPPM.

5.2.1. General Description of the Energy System and Place of the MPPM

A possible representation of the energy supply and demand system is shown in Figure 5.7. This figure emphasizes particularly the interaction between supply and demand and the different steps involved in this interaction.

- The origin of the energy demand in a specific year can be related to the projection of macroeconomic variables for the same year (GNP growth, population, employment etc.). These projections serve to define a vector of final demand for the I-0 Table(1). This final demand vector represents the different components of the GNP, as personal consumption expenditure, government spending, industrial investment, stock variations, and net imports.
- The I-0 Tables then compute the overall industrial level of activity required to meet the demand, and the equivalent direct and indirect energy used in the process(2). At this step, the demand in energy is formulated in terms of non substitutable energy use (industrial steam, space heating, number of passenger miles travelled).
- This demand in energy use is then converted to the demand in energy products (electricity, gas, fuels, etc.). The models dealing with this step make possible the study of interfuel substitution in meeting the energy demand, and take into account the conversion efficiency of each process (e.g., space heating by electric heater compared to space heating by gas burner). The output of this step is the definition of the fuel mix(3).

- The last step involves the combination of three activities: first the transportation of the energy products from the processing plant to the demand location; then the conversion of the energy as raw material (coal, crude oil, etc.) to energy products; and finally the transportation of the raw materials from the supply region to the processing plant. The outputs of this phase are the total requirements of energy raw materials consistent with the projections of macroeconomic growth(4). The models involved in this step can evaluate alternative RD&D projects in the overall energy context.

Figure 5.7. locates each of the models studied in this system. These models can deal with the same sector at different levels of aggregation. As an example, the transportation sector can be very aggregated as in the Brookhaven model, or very detailed as in the Bechtel source-to-use models.

The problems encountered with these more aggregated models is that they place their emphasis on the structural aspect of the problem and are dependent on the availability of processing data of a particular level of aggregation. Because such data are often impossible to obtain, serious deficiencies may appear in the results. The problem is well summarized by James Just in his article on "Impact of New Energy Technology Using Generalized I-O Analysis:"

"When dealing with new technologies such as coal gasification, there are many competing processes that perform the same function or yield the same product. In developing technological coefficients to represent such technology, it is important to make sure that the coefficients are representative of all the processes, so that any conclusions from such a study are not sensitive to the exact process chosen."

The same difficulty is mentioned in the report of the Bechtel/NSF Energy Supply model:²

"It was the intent of the modeling effort to include environmental effluent data resulting from the operation of energy facilities, consumption of waters, and requirements of land resources. The efforts made to obtain such data were only partially successful."

One strength of the MPPM lies in its flexibility regarding the level of aggregation of the data. This model can evaluate processes, taking into account such differences as regional data concerning cost of labor and material, or effluent limitations, or even differences in the tax structure of the region. Integrated with other models like the Brookhaven energy system, the MPPM can furnish more aggregated conversion coefficients to other models. This flexibility of the MPPM allows the user to study the impact of new technologies in the overall system, taking advantage of the precision of engineering studies.

The second of the two large diagrams provided at the back of this report shows a more detailed representation of the MPPM's direct and indirect interaction with other models. Some of the interactions already in the process of development will be given in examples in Section 5.2.3. The possible combinations have to be considered with the time frame, as well as other characteristics, in mind. Table 5.1. shows the time frame of each model, and the following section will be devoted to the comparative evaluations of these models.

5.2.2. Comparative Evaluation of the Models

In most cases, a decision problem concerning a new energy conversion technology, such as coal gasification, is very difficult or impossible to isolate from the energy system with which it must operate. The complexity of the energy system represented in the tables of the previous section shows that the economics of end use, transportation, and resource production will play a major role in determining what resources are produced, how they are transported, and how they are used. The remainder of the section will consider the characteristics that a comprehensive model of energy supply or demand should cover. Summary tables will then indicate the comprehensiveness of the model studied with regard to these characteristics. The conclusion of this analysis is that few models--if any--cover the spectrum of these characteristics, but that this spectrum can be covered through the combination or interaction of several models.

5.2.2.1. Characteristics of the Demand Side of Energy Models

- Energy demand projections: the forecast of energy demands can be done through the use of econometric projections, judgment projections, macroeconomic projections coupled with an I-O model, or a combination of these techniques. The last of these is important as it permits consistent projections with macro-growth projections (GNP growth, population, etc.), and facilitates the study of scenarios where these variables can be changed.

- Impact of energy price on demand. This impact can be represented at different levels: first, the influence of energy price on the projection of the macroeconomic variables; then the influence of energy price on total energy demand; and finally the influence of energy price on the relative share of each form of energy. The first level is achieved by no existing model, while the last raises questions about the results obtained, since the elasticities based on past series data can no longer be true when drastic changes occur.

- Form and level of aggregation of the energy demand. The energy demand can be formulated either as a demand in energy products (gas, electricity, fuels, etc.) or in terms of energy use (space heat, industrial steam, passenger miles travelled, etc.). The second form is more desirable, as it provides the opportunity to study interfuel competition to meet this demand. This interfuel substitution is usually evaluated in the supply side of the energy models.

The PIES, SEAS, Hudson-Jorgenson, Illinois I-0, and SRI-Gulf models deal with the demand side of the energy system, and their positions with regard to these characteristics are summarized in Table 5.2.

5.2.2.2 Characteristics of the Supply Side of Energy Models

- Dynamics. A non-dynamic model that characterizes the energy system only at specific points in time cannot reflect important changes in technology and demand, or the effect of depletion of the resource base. Moreover, static solutions in specific years do not assure the consistency of the feasibility of the overall solution.

- Supply & Demand characteristics: The influence of price on supply and demand of resources is an asset for a model; but on the other hand, the difficulty involved in creating these curves and checking their reliability can outweigh their value.

- Interfuel Substitution. The ability of a model to cope with detailed interfuel substitution is primary, if this model has to be able to evaluate alternative technological processes. As an RD&D tool, such a model should be detailed enough to permit precise evaluation of processes in the manufacture, as well as in the use, of energy products (electricity, gas, etc.). Data concerning specific processes can be obtained by detailed models such as the MPPM, and can be easily integrated in the model.

- Regionalization and Transportation. The regionalization of the energy supply and demand associated with the important costs of moving energy in any form will play an important part in the evaluation

of processes and locations. Moreover, the interregional competition for fuel is a determining factor in the solution of the overall energy system.

- Supply and Demand Integrating Model. Several approaches can be used to relate supply and demand characteristics. The model can serve to identify overall feasible solutions of the dynamic network (DSD, SRI), or to optimize the energy system in specific years (BNL, PIES, Bechtel source-to-use). The optimization approach seems appealing but does not assure the overall desirability of the solution, and can provide erroneous solutions. The real energy system can be far removed from ideal competition.

- Other Considerations. Some limitations concerning the environmental implications of the system, as well as the social and industrial changes implied by the solution, must be taken into account. Some of the models consider these limitations implicitly in consideration for the solution, while others simply keep track of them. Table 5.3. summarizes the results of this comparative evaluation.

The first conclusion of this study is that none of the models can deal adequately with all of the desirable features. This does not imply that an effort should be made toward the creation of such a model, as it would be very difficult or impossible to create at the proper level of detail for each characteristic, and could hardly compete with extremely detailed models designed for a specific problem.

On the other hand, a wide spectrum of these characteristics can be covered by interacting the models. The Models Interaction diagram in the back of the report shows that the same type of data can be obtained through different routes in the energy network. The combination chosen by the user will depend on the specific questions he has to answer, and on the evaluation of the relative tradeoffs involved in using one model rather than another. Tables 5.2. and 5.3. can help the user to select the characteristics he would like his model to include, and then to select the models to be interacted.

The following section will be devoted to the description of several integrations of models involving the use of the MPPM.

5.2.3. Integration of the MPPM with Other Models

The general description of the energy system and the comparative evaluation of the models give the energy policy analyst the ability to design a combination of models to meet specified requirements. Not all of the paths described in the Models Interaction diagram are possible or even desirable. Some major incompatibilities can occur when more than two models are interacted, even if every single interaction between one model and another is feasible (the time range of the models may not be consistent, etc.). The first task of the user will therefore be to check the compatibilities. However, some of these paths involving the MPPM are already in the process of development, some at the conceptual stage, others at the preoperational stage. The remainder of this section will present three of these developments.

5.2.3.1. SEAS/BNL/Bechtel-Energy-Supply

The way the Strategic Environmental Assessment System (SEAS), the Brookhaven Energy System (BNL), the Bechtel/NSF-Energy-Supply-Model, and the Material-Process-Product Model (MPPM) will interface, is shown in Figure 5.8. and can be described as follows:

- Macroeconomic variables will be projected by the macro generator of the INFORUM module and converted to the projection of a final demand vector for the 185 sector I-O Table. The resolution of this I-O Table will forecast the industrial demand in energy consistent with the initial projections. Two other modules will forecast, for the same period of time, the energy demand coming from the residential/commercial and transportation sectors. The outputs of the SEAS model will therefore be the annual energy demand, formulated in terms of non-substitutable energy use (industrial steam, space heating, etc.).

- The Material-Process-Product Model will perform a comparative evaluation of the advanced coal conversion processes on a detailed basis; assess the requirements of each of these processes in terms of products, manpower, energy, land and water use; give detailed data on waste composition; and summarize these data for the initial construction of the plants as well as for their operation.

● The Brookhaven Energy System will take the energy demand from the SEAS model , and the data concerning conversion processes from the MPPM, and will compute the fuel mix composition (gas, electricity, fuels, required) and the energy base product requirement (coal, crude oil, etc.). The Brookhaven Model will also give information on the other impacts associated with the energy system (environment, social, etc.). No use of the optimization routine is planned, for the reasons explained earlier. The Brookhaven Model, with its high level of detail, will be used to convert non-substitutable energy demand in the demand for intermediate and primary energy products.

● The Bechtel Energy-Supply Model will take as input the fuel mix defined by the BNL model and the process data generated by the MPPM , to determine the annual requirements in energy and transportation facilities. Finally, this model will compute, in a very detailed way, the annual requirements of manpower, capital, and resources necessary for the creation and operation of these facilities.

● The last step in the chain consists of a comparison of the amount of labor, material, and capital for the energy sector initially forecasted in the SEAS model, with the computed amount induced by the linking of the models. This comparison will permit a test of consistency on the overall projection.

This combination illustrates the advantages gained in the linkage of models with various levels of aggregation. The SEAS model, or part of it, is aggregated at a macro level. The Brookhaven Model operates at an activity level (such as gasification by the Lurgi process), and the MPPM and Bechtel Models operate at a micro engineering level (such as comparison of methanators in the Lurgi process). Finally, the feed-back of information is a test of consistency in the use of these models.

5.2.3.2. DSD/MPPM/Bechtel Source-to-Use

The Dartmouth System Dynamic (DSD), the Material Process Product Model (MPPM) and the Bechtel Source-to-Use Model, are designed to interface in a loop form, described in Figure 5.9.

- First, the DSD model will generate input data for the MPPM and the Bechtel Source-to-Use Model, such as aggregate demand, fuel mix, price of resources, etc.
- The MPPM, taking into account the costs and other data generated by the DSD model, will evaluate advanced coal conversion technologies in the same way as described in the previous section.
- The Bechtel Source-to-Use Model will combine the aggregate demand and fuel mix generated by DSD, with the coal conversion data generated by the MPPM, adding the transportation component to the system. Once the network is solved, the output of the Bechtel model will be the aggregated coal conversion data with transportation costs included. (The share of transportation in the total cost is of primary importance.)
- The DSD will then take these coefficients and solve the system in a dynamic way, and assess the overall feasibility of the solution over time.

This second example shows how a model which places its particular emphasis on the structural aspect of the problem can take advantage of more detailed study for the evaluation of some of its parameters.

5.2.3.3. Illinois I-0/BNL/MPPM

The coupling of the Illinois Energy Input-Output Table with the Brookhaven Energy Model has been the object of previous studies.³ The addition of the MPPM to this coupling could provide more accurate information to the user. The modified version of the Illinois I-0 Table consists of a matrix partitioned into four input and output

groups. These groups, which are schematized in Figure 5.10., are the resource supply sector (R), the secondary energy form (S) (electricity, gas, etc.), the basic energy demand (B) (space heating, process heat, etc.), and the industrial sector (I). This configuration enables the Illinois I-O model to forecast the total demand in energy use, and the BNL model to define the optimal fuel mix necessary to meet this demand. The interaction of the models can be described as follows:

- The modified Illinois I-O Table associated with a vector of final demand for a specific year forecasts the demand in basic energy need (space heating, process heat, etc.).
- The MPPM, as described previously, gives detailed data concerning advanced coal conversion technologies.
- The optimization routine of the Brookhaven model (BESØM), taking into account the energy demand and the advanced processes, computes the optimal fuel mix required to meet this demand.
- Technological coefficients concerning the process involved in the manufacture of the fuel mix are then computed and fed back into the Illinois Model (A_{rs} , A_{sp} coefficients).
- These changes involve a change in industrial requirements through the A_{IR} and A_{IP} coefficients, which finally is converted to a change in the initially projected energy demand.
- The process is then iterated, until no major changes occur in the basic energy demand.

The iterative coupling of models has the advantage of evaluating the impact of alternative energy policies on the industry requirement, and can provide accurate energy demand initially based on GNP projections. On the other hand, the choice of the optimization routine (BESØM) for the definition of the fuel mix requires a precise evaluation of processes. Erroneous data, such as excessive costs or requirements for a process, could exclude this process from the potential candidates. The Material

Process Product model, because of its high level of detail in the analysis, can preclude this kind of problem.

References

1. "Impact of New Energy Technology Using Generalized Input-Output Analysis," James E. Just. ENERGY. Proceeding on Energy Demand, Conservation and Institutional Problems. February, 1973. p 119
2. Bechtel/NSF Energy Supply Model, August, 1975. Chapter 6, p. 32, Volume I.
3. "Coupled Energy System - Economic Models," K.C. Hoffman. Proceeding of the Conference on Energy Modeling and Forecasting, June, 1974. p 27, Lawrence Berkley Laboratory. LBL.3635

5.3. COMPUTER RELATED EFFORT

As discussed in Section 3.3 regarding Phase II MPPM development, IR&T suggests that a computer support group be utilized in conducting the MPPM policy analysis-oriented calculations to be made in conjunction with the large economic/energy model configurations just discussed. The support group's major tasks* during the 12-month Phase III period will be to link the MPPM to the large computational configurations; to use the resulting system to run several alternative scenarios defined by ERDA; to develop update procedures for systems maintenance; and to train ERDA personnel in the use of the system.

The exact models to be linked, and the feasibility of implementing the required linkages, will be determined by IR&T and the support group during Phase II. Two general approaches will be considered in determining the most practical means of linking the models.

One approach would be to bring all of the models into a common computer facility. Each model could then be run in proper sequence, and the resulting intermediate files could be passed from one model to the next. This method would be the most ideal for efficiency and control of system runs. However, it could entail high initial conversion costs, as well as continual updating problems.

The second approach would be to establish the necessary links through data file compatibility. In this approach, data files needed for input to the MPPM would be generated by each model at its current operational site and sent to the support group for processing. Similarly, output files from the MPPM model would be produced by the support group and transmitted to those facilities at which the receiving models are operational. File layouts and transformation programs would be designed by the support group during Phase II to assure that compatible formats are available both for input to the MPPM model and for entry into other models fed by MPPM.

* The discussion of computer-related tasks was provided by Control Data Corporation (CDC), an organization skilled in this type of computer application.

By the end of Phase II, all design specifications for the input/output file layouts and transformations required to link the various models will have been completed. The support group will then proceed to Phase III with the coding, debugging, and validation of all linkage software. Upon successful validation of each individual link, tests will be performed to validate all possible link combinations available in the integrated system. Several scenarios will be prepared for this purpose; each scenario will be jointly constructed by the support group, IR&T and the ERDA staff. The format of all output reports will be designed concurrently with the development of the test scenarios. These scenarios will be designed to show the effects of alternative capital investments, manpower requirements, product outputs, energy requirements, other resource or material requirements, and efficiencies of various system configurations.

Data base updating will also be examined to ascertain what data has to be revised and with what frequency. This necessity of updating is of critical importance to maintaining a relevant, viable integrated model reflecting the current status of all exogenous data. The detailed analysis that was conducted during Phase II will have done much to determine the frequency of data updating with respect to each model linked with the MPPM. Techniques for performing the updating operation will be developed and verified as being efficient and timely. As an example, the special-purpose programs used to extract data from the various model output files could be run on a periodic basis commensurate with the production update runs of each model.

Training of ERDA personnel in the use of the integrated system comprises an important part of the support group's commitment to the project. The MPPM model itself depicts many complicated processes relating to the coal industry, with associated data bases consisting of parameters unique to each process. In addition, the user must understand the complex involvement of the interfaces with the other models. To simplify system operations, the support group will produce a comprehensive user's manual. The contents of the manual will be:

- System Narrative - a description of how the models interface
- Input Preparation - a description of scenario preparation procedures
- Output Samples - output reports obtained from previous production runs with detailed explanation of their interpretation
- Source Code Listing - the entire source code with special purpose software included
- Running Instructions- a complete set of operational instructions

The support group will also hold technical seminars to familiarize ERDA personnel with all aspects of the integrated system. In addition, the support group will prepare material for IR&T's final report which will present all details of the operation and updating of the integrated system, a complete description of the interactions of the various components of the system, tabular output of all scenarios used to validate the model, and a specification of the procedures necessary to maintain all data bases in a current status.

FIGURE 5.1.
The FEA Project Independence Evaluation System

———— DIRECT FLOW

----- FEEDBACK

NOTE: ALL MODULES PRODUCE REPORTS OUTPUTS AND
INPUTS TO POST-PROCESSOR

FIGURE 5.2.
SEAS System Flow Chart

DENAND SECTOR

FIGURE 5.3.
Dartmouth System Dynamic
FOSSIL 1

REFERENCE ENERGY SYSTEM, YEAR 1977

Figure V-2

FIGURE 5.4.
The Brookhaven Energy System Network

5-45

FIGURE 5.5.
Bechtel Energy Source to Use Model

FIGURE 5.7.
Relative Position of the Models in the Energy Supply and Demand System

FIGURE 5.8.
SEAS/BNL/MPPM/Bechtel-NSF Interaction

FIGURE 5.9.

DSD/MPPM/Bechtel Source to Use Interaction

FIGURE 5.10.
Illinois Energy I-O Table/BNL/MPPM Interaction

TABLE 5.1.
Time Frame of the Models

*Not defined explicitly, depends on the inputs available.

TABLE 5.2.

CHARACTERISTICS OF THE DEMAND SIDE OF ENERGY MODELS

MODELS	ENERGY DEMAND PROJECTIONS	PRICE SENSITIVE DEMAND	FORM AND AGGREGATION OF ENERGY PROJECTIONS
Project Independence Evaluation System "PIES"	Macro growth model from Data Resource + 24 sector I-0 Table for industrial demand and econometric equations for Residential/Commercial/Transportation.	Price elasticities between fuels obtained through past series data but no overall demand elasticity.	Total demand for Residential/Commercial/Industrial/Transportation sectors then disaggregated by market shares in electricity and specific fuel demand.
Strategic Environmental Assessment System "SEAS"	Macro model from INFORUM or Chase Econometric + 185 sector I-0 Table + econometric and stock functions.	Not considered.	Demand in terms of physical units as industrial steam or number of passenger miles for Industrial/Residential/Commercial/Transportation.
Hudson Jorgensen	Macro growth model from Data Resource + 9 sector I-0 Table where I-0 coefficients are estimated by econometric equations.	Energy price defines the total energy demand relative to labor demand, capital demand, or other non-energy inputs.	Total energy demand then disaggregated by fuel types by market share equations.
University of Illinois Energy I-0 Table	Macro growth model + 364 sector I-0 Table + econometric equations.	Not considered in original version. Interfuel substitution or elasticities induced in modified version coupled with BNL.	Original version: demand in terms of products (coal, electricity, gas, ...). Modified version: demand in terms of physical units (BTU).
Stanford Research Institute Gulf Oil	Price sensitive demand curves for several years obtained through expert judgement.	Taken into account by the individual fuel demand curves which emphasize fuel substitution but exclude total energy demand elasticity.	Demand curves in terms of usable energy (space heat, industrial steam, etc.) for Industrial/Residential/Commercial/Transportation sectors.

TABLE 5.3.

CHARACTERISTICS OF THE SUPPLY SIDE OF ENERGY MODELS

MODELS	DYNAMIC ASPECT	SUPPLY & DEMAND ELASTICITIES	INTER FUEL SUBSTITUTION		REGIONALIZATION & TRANSPORTATION	METHOD USED IN THE INTEGRATING MODEL OF SUPPLY AND DEMAND	OTHER CONSIDERATIONS
			FOR ENERGY PRODUCTS (ELECTRICITY, GAS)	FOR ENERGY USE (SPACE HEATING, INDUSTRIALIZATION)			
Brookhaven National Laboratory (BNL)	In the present version is static with a dynamic version in process.	Not considered. In the BESOM routine the supply and demand are rigid constraints.	Very flexible. Computed by BESOM in the comparative evaluation of paths leading from raw material to energy products.	Very flexible. Computed by BESOM in the comparative evaluation of paths leading from energy product to energy use.	BESOM is not yet regionalized. Transportation costs to be taken from other studies.	Linear programming associated with rigid constraints.	The environmental impact for some products (NO _x , SO _x) is taken as a constraint for the solution.
"SRI-GULF"	Incorporated by introduction of lag functions and all the solutions for # years computed in the same time.	Supply and demand curves given by fuel type and regions.	Not fully explained, but seems induced by comparative evaluation of paths leading to the same product.	Same as for energy products.	Regionalized to 8 demand regions and 11 supply basins. Interregional transportation costs are computed.	Iterative resolution of supply and demand curves through the interface with the network.	Requirements on secondary industries (specialized equipment) influence the solution.
"PIES" Project Independence Evaluation System	Not considered. Static solutions for specific years.	Supply curves given by expert judgment. Demand curves by extrapolation of computed elasticity around the first demand projections.	Considered in the resolution of the system by LP but not flexible for study of technological changes.	Considered through the use of relative market share. Function of fuels relative energy prices.	Regionalization of the data depends on the fuel studied. Transportation costs are computed.	Linear programming associated with price sensitive constraint. Quadratic problem solved by iterative process.	Environmental, social financial impact are computed but do not interact with the solution.
"DSD" Dartmouth System Dynamic	The whole methodology is based on the dynamic aspect, resource usage, social behavior etc.	Introduced through the interaction of causal loops.	Considered through relative share of the market plus the interfacing with detailed models for technological changes.	Not considered. The demand is formulated in terms of energy products.	Not considered. Given implicitly by the interface with other models.	System dynamics.	Environmental, social institutional impacts influence the solution.
Bechtel Source House	Not considered.	Supply and demand are rigid constraints for the LP algorithm.	Very flexible and taken into account by comparative evaluation of technological processes associated with transportation costs.	Not considered. Same as above.	High level of regionalization (243 AQCR) plus very detailed evaluation of the overall transportation network by fuel type.	Linear programming associated with rigid constraints.	Environmental constraint on SO ₂ emissions.
Bechtel Energy Supply	Not really dynamic but the resolution of the system gives consistent solutions for all the years.	Demand is fixed by the inputs. Supply required are computed without constraints.	Considered if specified in input coefficients for the fuel mix.	Not considered. Same as above.	Optional 14 supply, 11 demand regions. Aggregate transportation costs computed.	Planning method with no constraints on supply.	Not considered.

6. PROJECT ORGANIZATION

The project is separated into three phases. This report represents the final task of Phase I. A synopsis of Phase I accomplishments is given in Section 1.2.3. Descriptions of the work to be completed in Phases II and III, as well as of the project organization, computer-related support, and brief biographical descriptions of project staff, are given in this chapter. The work of Phase III is separate and distinct from that of Phase II and will be undertaken as warranted by the success achieved in Phase II and authorized by ERDA.

6.1. WORK PLAN

6.1.1. Phase II

Twelve tasks will be accomplished in Phase II. A listing of these tasks, their timelines for performance, and the staff participation allocation among these tasks, is shown in Figure 6.1. The tasks are broken out into subtasks in Table 6.1. Completion of the Phase II tasks will achieve the first five project objectives discussed in Section 1.2., i.e.;

- 1) Extend the Materials-Process-Product Model to coal process technology
- 2) Assemble the coal process data base
- 3) Generate the library of feasible "economic unit processes" for conversion of coal to desired end products
- 4) Evaluate the unit processes within the context of coal RD&D policy scenarios
- 5) Conduct sensitivity analyses of the evaluation results

Three successive incremental steps will be taken to accomplish the Phase II objectives. The first increment of nine months will be devoted to establishing a Model A prototype version of the coal-based MPPM.

This model will include unit process routes leading to SNG, low-BTU gas, medium-BTU gas, and on-site electrical/mechanical energy. Tasks 2.1. to 2.4. are associated with the establishment of Model A. They include: developing the process data base, establishing the necessary computer programs, and conducting a feasibility demonstration of model use. The same sequence of steps in the second increment of six months will be repeated to develop a Model B version of the MPPM at the end of fifteen months. Model B will have a much larger data base, including representative configurations for all 42 coal-process functional modules (see Road Map at back of report). This model will include approximately three-quarters of the total Phase II data base. The final increment of 3 months in Phase II will be to complete the data base and, with the help of the computer support group, to make any programming revisions necessary for computing efficiency.

At the conclusion of Phase II the MPPM will be delivered to ERDA as a documented working computer program for internal use in RD&D policy analysis as described in Chapter 4. It will include the Linking Model (LM), the Process Chain Evaluation Model (PCEM) and the Industry Development Model (IDM) as described in the earlier chapters of this report. The data base will include the Materials and Utilities file and models of approximately 125 competing configurations. The data base will, of course, be expandable and subject to modernization as new and better data on technological alternatives becomes available.

The models will have been exercised through a limited set of scenarios to evaluate competing unit processes for conversion of coal to end products. Sensitivities of the evaluations to scenario variations and data uncertainties will be assessed for unit processes which appear to be most promising from an economic criterion.

Documentation will include quarterly progress reports and a final report which will contain descriptions of the computer programs and the data base. Letter-type monthly technical and financial reports will also be submitted.

6.1.2. Phase III

There are seven tasks in the twelve month Phase III that concludes the project. These tasks lead to the accomplishment of the sixth objective in Section 1.2.--use of the coal-based MPPM in conjunction with large scale energy/economic computer models to conduct evaluations of coal-process RD&D policy options within an enlarged energy/economic context. The timeline for task accomplishment and staff participation allocations are shown in Figure 6.2. The seven tasks are broken out into subtasks in Table 6.2.

The Phase III tasks form three general groups. First, it will be necessary to establish data-file compatibility with those models selected for joint computations. Next, the scenarios must be designed, run, and analyzed. Finally, project documentation, including a guide for joint use of models will be developed.

6.2. STAFF PARTICIPATION

The organizational chart for IRT staff participation, as well as for consultants and subcontractors, is given in Figure 6.3. Dr. James Cummings-Saxton is the Project Manager, Dr. Robert Roig is the Deputy Project Manager, and Dr. Robert U. Ayres is Executive Consultant. As shown, there are two principal areas of staff participation. Phase II emphasis will be on engineering analysis and on computer model development. Phase III emphasis will be on policy analysis.

Drs. Cummings-Saxton and Roig have responsibility for conduct of the Engineering Analysis aspects of the study. The methodology for functional module analysis developed during Phase I will be applied to the diverse types of competing configurations. Necessary working relationships will be developed with the engineering organizations that can provide essential data inputs. An additional engineering analyst--M. Narkus-Kramer--will be added to the project to undertake the organization and assessment of the large quantities of engineering data being entered into the MPPM data base. Jack Dart, Wilburn Schroeder, and Robert Capell serve as expert consultants for the engineering analysis.

Leslie Ayres heads the computer programming effort within Computation and Analysis. Control Data Corporation will take over a large portion of the Computation and Analysis workload after December 1976. Nickolaus Leggett assists in data gathering and analysis. Edward Ayres acts as Technical Editor for the project.

The background of participating IRT staff and consultants have been summarized into brief paragraphs in Section 6.4.

6.3. COMPUTER RELATED SUPPORT

As discussed in Section 3.3, Control Data Corporation (CDC), an organization with prior experience and competence in packaging and documenting large computer models, will provide computer-related support during Phase II development of the MPPM. Funding to CDC will be managed through a subcontract to IR&T in order to facilitate a joint effort.

The transformation of all IR&T prototype programs and design criteria to flowcharts and programming specifications will be the responsibility of a CDC analyst. This analyst will be assigned to the project commencing in the fifth month and will continue to prepare detailed programming specifications through the ninth month.

Two CDC programmers will be assigned full time to the Phase II effort, under the direction of the CDC analyst, starting in the tenth month. Their responsibility through the sixteenth month will be to code, debug, validate and document the MPPM model.

In Phase III, CDC will be involved in the development of software and interface programming. Scenario testing will take place after the first six months of Phase III. It is intended that Phase III will conclude with CDC developing user guides to all interfaced models, and leading training sessions on utilization of MPPM alone and with other models.

6.4. STAFF RESUMES

Short biographical sketches of project personnel are given in the following paragraphs. Complete resumes have been previously provided to ERDA. The participation of each individual is shown in Figure 6.3.

6.4.1. IR&T Staff

JAMES CUMMINGS-SAXTON

Dr. Cummings-Saxton will be the project manager. He is a chemical engineer specializing in materials/energy flow studies of the major industrial sectors. He acted as Project Manager of a recent study of the economic impact of water-pollution-abatement costs upon the chemicals processing industry (for the National Commission on Water Quality). He also served as Project Manager of a major study of the use of fuels and feedstocks in the industrial chemicals industry, under contract to the Federal Energy Administration. He conducted an analysis of the effect of process change on industrial chemicals' solid waste generation (for EPA). He has contributed to the continuing development of EPA's Strategic Environmental Assessment System, a regionalized environmental model used to forecast the emissions, stocks, levels of recycling, and other quantified activities of all industrial sectors.

Dr. Cummings-Saxton received his Ph.D. in chemical engineering from the University of California at Berkeley. He was a supervisor in the Bellcomm Division of Bell Telephone Laboratories from 1966 until joining IR&T in 1972. He studied at MIT in Summer, 1971, in the area of modeling, simulation, and optimization of chemical processes. He is a Fellow of the American Institute of Chemists, and a member of the American Institute of Chemical Engineers. He is listed in American Men of Science, Physical and Biological Sciences; Who's Who in the South and Southwest; and the Dictionary of International Biography.

His writings include *Industrial Energy Study of the Industrial Chemicals Group*, prepared for FEA under Contract No. 14-01-0001-1654 (August 30, 1974), with Marc Narkus-Kramer et. al.; *Solid Waste Generation in the Industrial Chemical Sector: The Effect of Process Change, Potential for Resource Recovery and Cost of Improved Disposal*, prepared for ORM, EPA under Contract No. 68-03-0138 (October 4, 1973), with Marc Narkus-Kramer; and *Materials-Process-Product Model, A Feasibility Demonstration Based on the Bottle Manufacturing Industry*, prepared for the National Science Foundation under Contract No. NSF-C-652 (December 11, 1972) with Robert Ayres and Martin Stern.

ROBERT W. ROIG

Dr. Roig will act as Deputy Project Manager. He is an electrical engineer who has specialized in analysis of large scale systems and interdisciplinary technological problems. At IR&T, Dr. Roig managed an investigation into the economic and technical impacts of changing automobile materials composition, with particular emphasis on resource recovery problems. Dr. Roig also served as Project Manager of IR&T's analysis of petroleum product end-uses by region and industry (for FEA), and has done extensive work in the study of technological substitution trends.

Dr. Roig worked with General Research Corporation (GRC), IR&T's parent company from 1968 to 1974. He was Director of GRC's Dayton Operations, where he directed studies of aircraft and RPV systems. His work at GRC Washington Operations and Santa Barbara Operations has included ballistic missile defense studies (involving engagement logic development, engagement simulations, radar sensor capabilities, and tropospheric refraction effects); "SAFEGUARD" and "Hardsite" systems analyses and syntheses; strategic weapon systems analyses for the Arms Control and Disarmament Agency; and other projects.

Before joining GRC, Dr. Roig was a member of the technical staff of the Mitre Corporation. He received his Sc.D. in Electrical Engineering from Massachusetts Institute of Technology in 1968.

ROBERT U. AYRES

Dr. Ayres will be an Executive Consultant to the project. A mathematician and economist, he has played a leading role in the development of economic modeling and forecasting techniques for long-range planning and policy analysis in both government and business. He has directed a number of projects in which dynamic input-output models (including IR&T's "Materials-Process-Product Model" and EPA's "Strategic Environmental Assessment System") have been used to study the future impacts of technological change--particularly with respect to the supply and demand for critical materials, food, and energy in the U.S. and world economies.

Dr. Ayres has served as a consultant on science policy and the economics of technological change for a wide range of institutions, including the Organization for Economic Cooperation and Development (OECD), the National Academy of Science, the United Nations, and several departments of the U.S. government. He has conducted major forecasting studies for the governments of West Germany and France.

He is the author of more than fifty publications. His books include *Technological Forecasting and Long-Range Planning*, McGraw-Hill Book Company, 1969; and *Aspects of Environmental Economics: A Materials Balance - General Equilibrium Approach*, with Allen V. Kneese and Ralph C. d'Arge, Resources for the Future, Inc., Johns Hopkins University Press, 1970. His articles and papers include "Food," *Science Journal*, Associated Iliffe Press Limited, London, October 1967; "Technology and Prospects for World Food Production," Hudson Institute, HI-640-DP, Harmon-on-Hudson, New York, 1966; "Forecasting by the Envelope Curve Technique," J. Bright (ed.), *Technological Forecasting for Business and Government*, Prentice Hall, 1968; and "A Model for Resource Allocation in Materials Processing in R&D," with Christine Ralph and Marvin J. Cetron, *Industrial Application of Technological Forecasting and Its Use in R&D Management*, John Wiley and Sons, Inc., New York, 1971. He received his Ph.D. in mathematical physics from the University of London in 1958.

LESLIE AYRES

Ms. Ayres will do the computer systems programming for the project. She is a senior computer sciences specialist who came to IR&T in 1970 from the Univac Division of Sperry Rand Corporation. At IR&T she has participated in a number of mathematical modeling and simulation efforts, most recently the development and application of a major environmental model--the Strategic Environmental Assessment System (SEAS Model)--for the Environmental Protection Agency.

At Univac she was a Senior Systems Analyst and Data Processing Consultant. Her work there included the design and implementation of a limited nationwide computerized election system, the design and programming of an assembly-language-to-language translator; and the design and preparation of master files for the Defense Documentation Center Information Retrieval System.

Before joining Univac in 1962, she was a member of the technical staff of the G. C. Dewey Corporation; a Senior Programmer with IBM; and a Programmer with the Massachusetts Institute of Technology and the United Aircraft Corporation.

Ms. Ayres is co-author of "ESP: A Computer-Aided System to Facilitate Projections of Inter-Related Variables", Resources for the Future, 1971; and "A Model for Strategic Allocation of Water Pollution Abatement Funds," with Ivars Gutmanis and Charles Schultze, Brookings Institution, 1970.

MARC NARKUS-KRAMER

Mr. Narkus-Kramer will assist in the engineering analysis tasks of Phases II and III. He is a physicist specializing in environmental/energy modeling. He has been a principal contributor to the development of EPA's Strategic Environmental Assessment System (SEAS), a regionalized national forecasting model which has been used by four different U.S. government agencies to study the long-range impacts of alternative economic, environmental, and energy policies.

He has served as Project Manager of IR&T's contract to develop a comprehensive new energy module for SEAS, as well as of an earlier project involving the development of a materials resource (STOCKS) module.

Narkus-Kramer has also contributed to IR&T's energy related studies of the industrial chemicals industry and the nuclear power industry. He is co-author of FEA's *Industrial Energy Study of the Industrial Chemicals Group*, and author of chapters in *Electric Power Consumption and Human Welfare*, (AAAS) and *The Pentagon Watchers*, Doubleday, 1970.

Before joining IR&T in 1972, Mr. Narkus-Kramer taught six terms of physics laboratories and several courses on the History of Science and Einstein's Theory of Relativity at the University of Michigan.

NICHOLAUS E. LEGGETT

Mr. Leggett will assist in data gathering and analysis for the project. He is a political scientist whose professional and personal interests have focused on the relationships between the political process and the development of technology. The draft thesis for his Ph.D. (in political science) at Johns Hopkins University is concerned with the influences of changing social values on the productivity of inventors. The research for this thesis included an extensive survey of patent-holders, along with a statistical analysis of patent data. He is himself the holder of two U.S. patents (#3,280,929 and #3,280,930) on steering and propulsion systems for air cushion vehicles.

At IR&T, Mr. Leggett has worked in two major studies of material and energy flows in the chemical industry. In the first project, The Industrial Energy Study of the Industrial Chemicals Group (conducted for the Federal Energy Office), Mr. Leggett developed data on the energy and feedstock needs of the producers of major chemicals. In the second project, The Economic Impact of Water Pollution Control Costs Upon the Chemical Processing Industries (for the

National Commission on Water Quality), he traced the influence of water pollution control costs on the prices of chemicals--and on the activities of sectors that use these chemicals.

Mr. Leggett has also performed analyses of the probable impacts of innovations in automobile safety and insurance on future markets for automobiles, as part of a 34-country study, The World Automotive Industry to 1995, recently completed by IR&T and Business International, Inc., under the sponsorship of forty industrial clients.

Mr. Leggett graduated from Wesleyan University in 1968 with a B.A. in Government, and has subsequently completed his graduate studies at Johns Hopkins University. He is a licensed commercial radio operator, as well as a licensed hot air balloon pilot who has also built and operated a ground-effect machine using his own patented steering and propulsion systems.

EDWARD AYRES

Mr. Ayres will act as technical editor for the project. He is a professional writer and editor, experienced in both technical writing and the preparation of technical material for general readers. He is the author of The Economic Impact of Conversion to a Nonpolluting Automobile (U.S. Department of Transportation, 1969), an input-output study; What's Good for GM (Aurora, 1970), an exposition of the economic, ecological, and social impacts of the automobile industry, with a foreword by Senator Gaylord Nelson; and the opening chapter of Montgomery at the Mid-Million Mark, a demographic study commissioned by the County Executive of Montgomery County, Maryland.

Mr. Ayres has worked as a writing consultant to scientists and professionals in the fields of technology assessment, long-range forecasting, and economic analysis. He is experienced in the preparation of publishable research reports, and has written or edited final reports and articles for publication by a wide range of clients including M.I.T. Technology Review, Harvard University Health Services, the U.S. Department of Transportation,

the National Science Foundation, the Organization for Economic Cooperation and Development (OECD), the Greater Philadelphia Publishing Company, the U.S. Army Corps of Engineers, and others. He is currently working as a full-time technical and promotional writer for International Research and Technology Corporation.

6.4.2. Consultants

JACK C. DART

Mr. Dart will primarily assist in the process analysis tasks of Phase II. He is a chemical engineer and consultant to the chemical, petrochemical, and petroleum industries, specializing in catalytic processes. His consulting firm, J. C. Dart & Associates, has conducted economic and engineering studies of processes for the production of synthetic ammonia, methanol, hydrogen, formaldehyde, and sulfuric acid, as well as of catalytic cracking, catalytic reforming, catalytic desulfurization, dehydrogenation, and alkylation processes.

Dart is also engaged in studies involving process selection based upon economic studies of various processes to optimize overall project economics. He is a former Director of Houdry Process Corporation, which licenses such processes as Houdriforming, Houdrybutane dehydrogenation, Detol, and Litol. Before becoming Director, he served as Director of Development, General Manager of Research and Development, and Vice President and General Manager of the Chemicals Division. Before joining Houdry, he supervised a group responsible for petrochemical engineering process R&D for ESSO Research and Engineering Company.

Dart received his A.B. from Albion College in 1934, his B.S.E. from the University of Michigan in 1935, and his M.S.E. from the University of Michigan in 1937. His papers on process technology and process economics have been published in *Chemical Engineering Progress*, *The Oil and Gas Journal*, *Petroleum Refiner*, *Chemical Processing*, and *Engineering Digest*.

WILBURN C. SCHROEDER

Professor Schroeder will help in the analysis of coal processes to develop competing configuration descriptions. He is a chemical engineer with extensive experience in the development of processes for combustion and utilization of fuels; production of chemicals from gas, oil, oil shale, and coal; conversion of solid fuels to gaseous and liquid fuels; gasification of fuels; development of underground gasification processes for coal and shale; evaluation and direction of experimental programs on fuels and chemicals; and economic studies of fuels and interrelationships between fuels.

Dr. Schroeder is a professor of Chemical Engineering at the University of Maryland and a former Assistant Director of the U.S. Bureau of Mines, in charge of research and development. He has served as a consultant to the Bureau of Mines, Office of Coal Research, Atomic Energy Commission, National Academy of Engineering, Spencer Chemical Company, El Paso Natural Gas Company, and others.

He received his B.E. in Chemical Engineering from the University of Michigan in 1930, his M.S.E. from the University of Michigan in 1931, and his Ph.D. from the University of Michigan in 1933. He is a member of the American Chemical Society and a Fellow of the American Institute of Chemical Engineers.

ROBERT CAPELL

Mr. Capell will also assist in the MPPM-oriented analysis of coal processes primarily during Phase II. He is a civil engineer with extensive experience in industrial research and development and corporate planning, as well as in technological forecasting and assessment. As a petroleum industry consultant, he has published many papers and holds nine U.S. patents in the fields of catalysis, petroleum wax technology, and absorbent manufacture of usage. He is a past president of the Pittsburgh Section, American Institute of Chemical Engineers.

TABLE 6.1
PHASE II TASK LIST

<u>TASK NO.</u>	<u>DESCRIPTION</u>
2.1.	ASSEMBLE MODEL A DATA BASE
2.1.1.	Compile Materials/Utilities (M/U) Properties File
2.1.1.1.	Define Properties File Characteristics
2.1.1.2.	Assemble M/U Thermophysical Data
2.1.1.3.	Identify M/U Mixture Compositions
2.1.1.4.	Define Mixing Rule for Mixture Properties
2.1.2.	Develop Configuration Descriptions
2.1.2.1.	Obtain Configuration Data
2.1.2.2.	Analyze Data
2.1.2.3.	Develop Analytical Models
2.1.2.4.	Compare Models' Characteristics with Configuration Descriptions
2.1.2.5.	Modify Analytical Models, if Necessary
2.2.	ESTABLISH LINKING MODEL (LM)
2.2.1.	Develop Road-Mapping Subprogram
2.2.1.1.	Define Algorithms
2.2.1.2.	Code/Debug Subprogram
2.2.2.	Develop Linking Model
2.2.2.1.	Define Algorithm
2.2.2.2.	Code/Debug Program
2.2.2.3.	Validate
2.3.	ESTABLISH PROCESS CHAIN EVALUATION MODEL (PCEM)
2.3.1.	Develop Sizer Subprogram
2.3.1.1.	Define Algorithm
2.3.1.2.	Code/Debug Subprogram
2.3.2.	Develop Gross Coster Subprogram
2.3.3.	Develop Net Coster Subprogram
2.3.4.	Develop Taxer Subprogram
2.3.5.	Develop Residuals Evaluator Subprogram

Subtasks as Per
Those of 2.3.1.

TABLE 6.1
(Continued)

<u>TASK NO.</u>	<u>DESCRIPTION</u>
2.3.6.	Assemble Subprograms to Form PCEM
2.3.6.1.	Define Algorithm
2.3.6.2.	Code/Debug Program
2.3.6.3.	Validate
2.4.	CONDUCT FEASIBILITY DEMONSTRATION FOR MODEL A
2.4.1.	Conduct Comparative Process Evaluations Using Model A
2.4.2.	Compare With Literature Results
2.4.3.	Modify Model A, if Necessary
2.4.4.	Assess Effect of Data Uncertainties
2.5.	ASSEMBLE MODEL B DATA BASE
2.5.1.	Extend Materials/Utilities Properties
2.5.1.1.	Modify Properties File Characteristics, if Necessary
2.5.1.2.	Assemble M/U Thermophysical Data
2.5.1.3.	Identify M/U Mixture Compositions
2.5.2.	Develop Configuration Descriptions
2.5.2.1.	Obtain Configuration Data
2.5.2.2.	Analyze Data
2.5.2.3.	Develop Analytical Models
2.5.2.4.	Compare Models' Characteristics with Configuration Descriptions
2.5.2.5.	Modify Analytical Models, if Necessary
2.6.	ESTABLISH INDUSTRY DEVELOPMENT MODEL (IDM)
2.6.1.	Define Type of Developmental Scenarios
2.6.2.	Assemble Data Base for Developmental Scenarios
2.6.3.	Define IDM Algorithms
2.6.4.	Code/Debug Program
2.6.5.	Validate

TABLE 6.1
(Continued)

<u>TASK NO.</u>	<u>DESCRIPTION</u>
2.7.	CONDUCT FEASIBILITY DEMONSTRATION FOR MODEL B
2.7.1.	Conduct Comparative Process Evaluations Using PCEM
2.7.2.	Perform Scenario Evaluations Using IDM
2.7.3.	Assess Results
2.7.4.	Modify Model, if Necessary
2.7.5.	Assess Effect of Data Uncertainties
2.8.	COMPLETE MPPM DATA BASE
2.8.1.	Extend Materials/Utilities Properties File
2.8.1.1.	Modify Properties File Characteristics, if Necessary
2.8.1.2.	Assemble M/U Thermophysical Data
2.8.1.3.	Identify M/U Mixture Compositions
2.8.2.	Develop Configuration Descriptions
2.8.2.1.	Obtain Configuration Data
2.8.2.2.	Analyze Data
2.8.2.3.	Develop Analytical Models
2.8.2.4.	Compare Models' Characteristics with Configuration Descriptions
2.8.2.5.	Modify Analytical Models, if Necessary
2.9.	ESTABLISH FUNCTIONAL COMPUTER DESIGN
2.9.1.	Develop Flowcharts
2.9.2.	Prepare Detailed Programming Specifications
2.9.2.1.	Develop Design Specifications for Data Processing
2.9.2.2.	Define Formats for Handling Input/Output Data
2.9.2.3.	Establish Procedures for Maintaining Historical Data Record
2.9.2.4.	Define Program Specifications for Data Manipulation and Report Generation
2.10.	FINISH PROGRAMMING
2.10.1.	Develop Programs as Specified
2.10.2.	Complete Final Coding and Debugging
2.10.3.	Conduct Demonstration Tests Exercising All User Options

TABLE 6.1
(Continued)

<u>TASK NO.</u>	<u>DESCRIPTION</u>
2.11.	DOCUMENT PROGRAM
2.11.1.	Product Program Documentation
2.11.2.	Write Program Description
2.12.	PROJECT AND TECHNICAL MANAGEMENT
2.12.1.	Planning and Project Organization
2.12.2.	Prepare Monthly [•] and Quarterly [◇] Reports
2.12.3.	Prepare Task Completion Reports [▲]
2.12.4.	Prepare Phase II Draft Final Report
2.12.5.	Incorporate ERDA-Suggested Modifications
2.12.6.	Issue Phase II Final Report [■]

TABLE 6.2
PHASE III TASK LIST

<u>TASK NO.</u>	<u>DESCRIPTION</u>
3.1.	DEVELOP COMPATIBLE SOFTWARE
3.1.1.	Review Other Models' Input/Output Structure
3.1.2.	Negotiate Compatibility Adjustments
3.1.3.	Establish Data File Compatibility
3.2.	CONDUCT SYSTEM TESTS
3.2.1.	Perform Joint Model Evaluation
3.2.2.	Debug System
3.2.3.	Validate System
3.3.	RUN SCENARIOS
3.3.1.	Define Scenarios
3.3.2.	Develop Exogenous Data
3.3.3.	Perform Scenario Evaluations
3.3.4.	Analyze Results
3.4.	DEVELOP DATA UPDATE PROCEDURES
3.4.1.	Review Data File
3.4.2.	Select Final Data Format
3.4.3.	Define Algorithm
3.4.4.	Code Program
3.4.5.	Debug Program
3.4.6.	Validate
3.5.	DEVELOP USER'S GUIDE FOR INTEGRATED MODELS
3.5.1.	Fully Document Program
3.5.2.	Prepare Draft User's Guide
3.5.3.	Utilize in Training Program
3.5.4.	Prepare Final User's Guide

TABLE 6.2
(Continued)

<u>TASK NO.</u>	<u>DESCRIPTION</u>
3.6.	CONDUCT TRAINING PROGRAM
3.6.1.	Present Scenarios on MPPM Use
3.6.2.	Demonstrate with Sample Problems
3.6.3.	Furnish Consulting Service
3.7.	PROJECT AND TECHNICAL MANAGEMENT
3.7.1.	Planning and Project Organization
3.7.2.	Prepare Monthly● and Quarterly◇ Reports
3.7.3.	Prepare Task Completion Reports▲
3.7.4.	Prepare Phase III Draft Final Report,
3.7.5.	Incorporate ERDA-Suggested Modifications
3.7.6.	Issue Phase III Final Report■

FIGURE 6.1
PHASE II TASK TIMELINES AND STAFFING

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FIGURE 6.2
PHASE III TASK TIMELINES AND STAFFING

FIGURE 6.3

Project Organization Chart

*The numbers in brackets identify the Phase II task participation of each individual. For example, 1/2 designates Tasks 2.1. and 2.2. These are seen in Table 6.1. to be, respectively: Assemble Model A Data Base, and Establish Linking Model (LM). Further information for each individual is given in the resumes presented in Section 6.4.

APPENDICES TO
MATERIALS-PROCESS-PRODUCT ANALYSIS
OF COAL PROCESS TECHNOLOGY

By

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Final Report
for
Project Phase I

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APPENDIX A
PRODUCTS AND PROPOSED PRODUCT SPECIFICATIONS
FOR USE IN MPPM ANALYSIS OF COAL PROCESSING TECHNOLOGY

LIST OF PRODUCTS

A. ENERGY PRODUCTS

- High Temperature Thermal Energy ($T > 400^{\circ}\text{F}$)
- Low Temperature Thermal Energy ($T < 400^{\circ}\text{F}$)
- Base/Intermediate Load Electric Energy
- Peak Load Electric Energy
- On-Site Electric (Mechanical) Energy

B. MATERIAL PRODUCTS

- Low-BTU Gas (Hot or Cold) (PPS #3)*
- Medium-BTU Gas (PPS #2)
- Substitute Natural Gas (SNG) (PPS #1)
- Anhydrous Ammonia
- Methanol
- Oxygenated Hydrocarbon Mixtures
- Low Molecular Weight Gaseous Hydrocarbon Mixtures (PPS #6)
- Aromatic Mixtures
- Low Molecular Weight Liquid Hydrocarbon Mixtures
- Middle Distillate Oils (Low Sulfur No. 2 Distillate Fuel Oil Equivalent) (PPS #7)
- Clean Liquid Boiler Fuel (Low Sulfur Residual Oil Equivalent) (PPS #4)
- Clean Solid Boiler Fuel (PPS #5)

C. BY-PRODUCTS

- Sulfur/Sulfur Compounds
- Ammonia/Ammonia Compounds
- Aggregates
- Gypsum
- Argon
- Nitrogen
- Carbon Dioxide

*Proposed Product Specification (PPS)

PROPOSED PRODUCT SPECIFICATION #1

Substitute Natural Gas (SNG)

T = 100°F; P = 1015 psia

Composition Limits

$H_2O \leq 0.015\% \text{ Vol.}$ (5.2 grains/100 SCF)

$SO_x + H_2S \leq 0.003\% \text{ Vol.}$ (1 grain/100 SCF)

$CO \leq 0.1\% \text{ Vol.}$

$CH_4 \geq 90\% \text{ Vol.}$

Remainder H_2 + Inert Gases (N_2 , CO_2 , etc).

Intended Applications

- Input to existing natural gas pipeline network for delivery to all present customers of natural gas pipelines without requirement for adjustment of burners.

PROPOSED PRODUCT SPECIFICATION #2

Medium BTU Gas

$T = 100^{\circ} \text{ F}; 15 \text{ psia} \leq P \leq 1015 \text{ psia}$

Composition Limits

$\text{H}_2\text{O} \leq 0.1\% \text{ Vol.}$

$\text{SO}_x + \text{H}_2\text{S} \leq 0.01\% \text{ Vol}$

$200\% \text{ Vol} \geq \text{CO} + \text{H}_2 + 3\text{CH}_4 + 5\text{C}_2\text{H}_6 \geq 90\% \text{ Vol.}$

Remainder Inert (N_2 , CO_2 , Ar, etc)

Intended Applications

- Peaking electric power gas-turbine generators
- Medium distance delivery to industrial and electric utility users by dedicated (special) pipeline.

PROPOSED PRODUCT SPECIFICATION #3

Low BTU Gas

$$100^{\circ}\text{F} \leq T \leq 3000^{\circ}\text{F} ; \quad \text{psia} \leq P \leq 1015 \text{ psia}$$

Composition Limits

$$\text{H}_2\text{O} \leq 10\% \text{ Vol.}$$

$$\text{SO}_2 + \text{H}_2\text{S} \leq 0.01\% \text{ Vol.}$$

$$90\% \text{ Vol.} \geq \text{CO} + \text{H}_2 + 3\text{CH}_4 + 5\text{C}_2\text{H}_6 \geq 40\% \text{ Vol.}$$

Remainder Inert (N_2 , CO_2 , Ar, etc.)

Intended Applications

- Clean boiler fuel for on-site electric power generation (base load).
- Short distance delivery to industrial and electric utility users by dedicated pipeline.
- Gas/turbine/generators for peak load and on-site electric power.

PROPOSED PRODUCT SPECIFICATION #4

Clean Liquid Boiler Fuel (Low Sulfur Residual Oil Equivalent)

T, P = Ambient

Viscosity @ 100°F; 350 sec. (min.), 750 sec (max.)
by Saybolt Universal Viscometer

Flash Point 130°F

Gravity, °API 16 (min.)

Composition Limits

$H_2O \leq 1.0\% \text{ Wt.}$

$S \leq 0.6\% \text{ Wt.}$

$Ash \leq 0.15\% \text{ Wt.}$

$C \geq 84\% \text{ Wt.}$

H/C Ratio $\geq 10\%$ by Wt.

Heat value will be approximately 18,500 BTU/lb (54 lbs/10⁶ BTU)

Intended Applications

- Boiler fuel for base/intermediate load electric power generation with no sulfur clean-up and no particulate clean-up of flue gas required.
- General purpose boiler fuel for industrial use and commercial/institutional space heating.

PROPOSED PRODUCT SPECIFICATION #5

Clean Solid Boiler Fuel (General Grade and Special Grade)

T, P = Ambient

Melting Point $>400^{\circ}\text{F}$

Crushable and pulverizable

Composition Limits

$\text{S} \leq 0.8\% \text{ wt.}$

$\text{Ash} \leq 0.13\% \text{ wt. special grade}$

$\text{Ash} \leq 2.7\% \text{ wt. general grade}$

$\text{C} \geq 95\% \text{ wt.}$

Heat value will be approximately 13,400 BTU/lb ($74.5 \text{ lbs}/10^6 \text{ BTU}$).

Intended Applications

- Boiler fuel for base/intermediate load electric power generation with no sulfur clean-up and 95% particulate clean-up of flue gas for general grade. For special grade, no particulate clean-up of flue gas required.
- General purpose boiler fuel for industrial use and commercial/institutional space heating. (Installations with over $250 \times 10^6 \text{ BTU/hour}$ capacity will require 95% particulate clean-up of flue gas when using general grade).

PROPOSED PRODUCT SPECIFICATION #6

Low Molecular Weight Gaseous HydroCarbon Mixtures

T = Ambient; 15 psia < P ≤ 1015 psia

Composition Limits

$$C_1H_4 + C_2H_b + C_3H_c + C_4H_d \geq 90\% \text{ Vol}$$

$$C_1H_4 \leq 20\% \text{ Vol}$$

$$H_2O \leq 0.015\% \text{ Vol}$$

$$SO_x + H_2S \leq 0.003\% \text{ Vol}$$

$$CO \leq 0.1\% \text{ Vol.}$$

Remainder H_2 + Inert

Intended Applications

- Chemical industry (Ethylene, Propylene, Butadiene Manufacture) Feedstock
- Bottled gas for heating, cooking, crop drying, etc.
- Supplementary input to natural gas utility networks.

PROPOSED PRODUCT SPECIFICATION #7

Middle Distillate Oil (Low Sulfur No. 2 Distillate Fuel Oil Equivalent)

T,P = Ambient

Kinematic Viscosity @ 100°F; 2.0 centistokes (min), 3.6 centistokes (max).

Gravity, °API, 30 (min)

Flash Point, 100°F (min)

Pour Point, 20°F (max)

90% Distillation Temperature, 540°F (min), 640°F (max)

Composition Limits

$H_2O \leq 0.1\% \text{ wt.}$

$S \leq 0.1\% \text{ wt.}$

Ash - Trace quantities only

$C \geq 84\% \text{ wt.}$

H/C ratio $\geq 12\% \text{ wt.}$

Uncombined Carbon Residue $\leq 0.35\% \text{ wt.}$ (determined from remainder after 90% distillation)

Heat value will be approximately 19,500 BTU/lb (51 lbs/10⁶ BTU)

Intended Applications

- General purpose domestic heating oil.

APPENDIX B
CATALOGUE OF MODULE CONFIGURATIONS FOR MPPM ANALYSIS
OF
COAL PROCESSING TECHNOLOGY

LIST OF FUNCTIONAL MODULES AND SUB-GROUPS

1. Low-BTU Gasifiers
 - 1.A. Fixed Bed
 - 1.B. Fluidized Bed
 - 1.C. Entrained Flow
 - 1.D. Molten Bath Bed
2. Med. BTU Gasifiers - Internal Heating Type
 - 2.A. Fixed Bed
 - 2.B. Fluidized Bed
 - 2.C. Entrained Flow
 - 2.D. Molten Bath Bed
3. Med. BTU Gasifiers - External Heat or Circulating Heating Medium Type
 - 3.A. Fluidized Bed
 - 3.B. Molten Bath Bed
 - 3.C. Nuclear Heat Source
4. Gaseous Phase Coal Hydrogenators
5. Liquid Phase Coal Hydrogenators
6. Solvent Extractors
7. Chemical Extractors
8. Coal Pyrolyzers
9. Methane Synthesizers
10. Methanol Synthesizers
11. Fischer-Tropsch Synthesizers
12. Ammonia Synthesizers
13. Shift/Reverse Shift Reactors
14. Gas Phase Separators/Purifiers
15. Hydrogen Purifiers
16. Coal Preparation Processes

17. Mineral Preparation Processes
18. Oxygen Producers
19. Liquids/Suspensions Separators/Purifiers
20. Hydrotreaters
21. Liquids/Gasses Separators/Purifiers
22. Hot Gas Cleaning Processes
23. Oxidation - Reduction Hydrogen Producers
24. Conventional Furnaces/Boilers
25. Fluidized Bed Furnaces/Boilers
26. Cyclone Furnace
27. High Pressure Burners/Furnaces
28. Hot-Gas Pyrolyzer
29. Direct Coal Combustion MHD
30. High Temperature Thermo/Turbo Electric Power Converters
31. Flue Gas Clean-Up Processes
32. High Temperature Flue Gas Thermal Energy Recovery and Partial Clean-Up Processes
33. Low-BTU Gas Thermal Energy Recovery and Clean-Up Processes
34. Mineral Recovery and Waste Treatment Processes
35. Turbo-Electric Power Converters
36. Outlet Cooling
37. Gas Turbine/Electric Power Generators
38. Waste Disposal
39. Demethanators
40. Coal/Chemical Slurry Separators
41. Char Preparation Processes
42. Water Dissociation via Nuclear Energy

FUNCTIONAL MODULE #1

Definition: Low-BTU Internal Heat Gasifiers - Thermal energy required for gasification obtained by internal oxidation of part of coal. Product gas is low-BTU intended for boiler use nearby. Air and Steam inputs.

	Sub-Group	Configuration	Process Name	Process Flowsheet	Equipment Schematic	Advanced	PRIORITY	Out of Date
							State of Art	
B-3	1,A,1	Fixed Bed	Lurgi		X		X	
	1,A,2	Fixed Bed	Wellman-Galusha	X	X		X	
	1,A,3	Fixed Bed	USBM Stirred Bed	X	X	X		
	1,A,4	Fixed Bed	GE Gas			X		
	1,A,5	Fixed Bed	Thyssen Galoszy					X
	1,A,6	Fixed Bed	McDowell-Wellman	X			X	
	1,B,1	Fluidized Bed	Winkler	X	X		X	
	1,B,2	Fluidized Bed	Westinghouse-Coal Gas for Elec. Power	X		X		
	1,B,3	Fluidized Bed	Bituminous Coal Res. Low-BTU Fuel Gas			X		
	1,B,4	Fluidized Bed	IGT-U-Gas		X	X		
	1,C,1	Entrained Flow	Koppers-Totzek		X		X	
	1,C,2	Entrained Flow	Texaco		X			X
	1,C,3	Entrained Flow	Babcock and Wilcox (DuPont)		X			X
	1,C,4	Entrained Flow	Combustion Engineering Low-BTU Gas for E.P.			X		
	1,C,5	Entrained Flow	Foster-Wheeler-Gas for Combined Cycle			X		
	1,D,1	Molten Bath Bed	Atomics Int. Molten Salt Furnace	X		X		

FUNCTIONAL MODULE #2

Definition: Internal Heat Gasifiers - Thermal energy required for gasification obtained by internal oxidation of part of coal. Oxygen and steam inputs.

	Sub-Group	Configuration	Process Name	Process Flowchart	Equipment Schematic	Advanced	PRIORITY	Out of Date
							State of Art	
B-4	2,A,1	Fixed Bed	Lurgi	X	X		X	
	2,A,2	Fixed Bed	Wellman-Galusha		X		X	
	2,A,3	Fixed Bed	USBM Stirred Bed		X	X		
	2,A,4	Fixed Bed	GE Gas			X		
	2,A,5	Fixed Bed	Thyssen-Galoszy					X
	2,B,1	Fluidized Bed	Winkler		X		X	
	2,B,2	Fluidized Bed	COED Stage 4, Reactor	X		X		
	2,B,3	Fluidized Bed	SYNTHANE	X		X		
	2,B,4	Fluidized Bed	Single Vessel HY-Gas	X		X		
	2,B,5	Fluidized Bed	B of M Fluid-Bed Gasifier			X		
	2,C,1	Entrained Flow	Koppers-Totzek	X	X		X	
	2,C,2	Entrained Flow	Bigas	X		X		
	2,C,3	Entrained Flow	Texaco		X			X
	2,C,4	Entrained Flow	Babcock and Wilcox (DuPont)		X			X
	2,C,5	Entrained Flow	Rummel		X			X
	2,C,6	Entrained Flow	Panindco					X
	2,C,7	Entrained Flow	Combustion Engineering				X	
	2,D,1	Molten Bath Bed	Kellog (NaCO ₃)	X		X		
	2,D,2	Molten Bath Bed	Atgas (Iron)	X	X	X		

FUNCTIONAL MODULE #3

Definition: External Heat Gasifiers - Thermal energy required for gasification obtained from air combustion of part of coal input in a separate chamber or other means. Thermal input to gasification chamber by circulation of heated material between combustion chamber and gasifier or by conduction. Air and steam inputs.

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	<u>Out of Date</u>
						<u>State of Art</u>	
3,A,1	Fluidized Bed	CO ₂ Acceptor	X		X		
3,A,2	Fluidized Bed	ICI Moving Burden					X
3,A,3	Fluidized Bed	Ash - Agglomerating (Battelle-Union Carbide)	X	X	X		
3,B,1	Molten Bath Bed	Rummel Double-Shaft Slag Bath Gasifier		X			X
3,C,1	Nuclear Heat Source				X		
3,D,1	Other External Heat Sources	IGT Electrothermal Gasifier	X		X		

FUNCTIONAL MODULE #4

Definition: Gaseous Phase Hydrogenators - Gasification by direct mixing of coal particles with hydrogen or hydrogen rich gas - additional heat required, if any, supplied from external source. Hydrogen or hydrogen rich gas (i.e., synthesis gas) inputs.

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowsheet</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	
						<u>State of Art</u>	<u>Out of Date</u>
4,A,1	Fluidized Bed	HY Gas	X		X		
4,A,2	Fluidized Bed	HYDRANE	X	X	X		
4,A,3	Fluidized Bed	COED - Stage 2 & 3 Reactor	X		X		
4,A,4	Fluidized Bed	Gulf-General Atomic/Stone and Webster			X		

FUNCTIONAL MODULE #5

Definition: Liquid Phase Hydrogenators - Gasification and/or liquification by direct mixing of coal particles suspended in a liquid medium with hydrogen (or a hydrogen-rich gas). Hydrogen (or hydrogen-rich gas) and liquid suspension medium inputs. Additional reaction heat required, if any, supplied from an external source.

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowsheet</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	<u>Out of Date</u>
						<u>State of Art</u>	
5,A,1	Liquid Suspension	H-Coal	X		X		
5,A,2	Liquid Suspension	Synthoil	X		X		
5,A,3	Liquid Suspension	Corsol $ZnCl_2$	X		X		
5,A,4	Liquid Suspension	CSF			X		
5,A,5	Liquid Suspension	Bergius	X				X

FUNCTIONAL MODULE #6

Definition: Solvent Extractors: coal dissolved in a solvent, usually in the presence of hydrogen or a hydrogen rich gas. (Similar to Group 5 except that hydrogenation is carried forward to only a minor extent and no catalyst is used). Hydrogen and liquid suspension medium inputs. Additional heat as required from an external source.

B-8	<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowsheet</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	<u>Out of Date</u>
							State of Art	
	6,A,1	Liquid Suspension	Solvent refined coal (SRC)	X		X		

FUNCTIONAL MODULE #7

Defintion: Chemical Extractors: Coal is slurried with a chemical solution which dissolves ash and sulfur from the coal. Liquid suspension medium and mineral (chemical) inputs. Heat as required from an external source.

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<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowsheet</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY <u>State of Art</u>	<u>Out of Date</u>
7,A,1	Liquid Suspension	Chem-Thermal Extraction- Battelle	X		X		
7,B,1	Liquid Suspension	TRW	X		X		

FUNCTIONAL MODULE # 8

Definition: Pyrolyzers - Decomposition of coal by input of externally supplied heat in an inert atmosphere. Heat input.

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowsheets</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	<u>Out of Date</u>
						<u>State of Art</u>	
8,A,1	Fluidized Bed	COED Stage 1 Reactor	X		X		
8,A,2	Fluidized Bed	TOSCOAL	X		X		
8,A,3	Fluidized Bed	Garret Res. & Dev.	X		X		

FUNCTIONAL MODULE #9

Definition: Methane Synthesizers - Convert synthesis gas to SNG (PPS #1) by catalytic methanation of CO and H₂ input - Synthesis gas with a adjusted H₂/CO ratio.

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowsheet</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	
						<u>State of Art</u>	<u>Out of Date</u>
9,A,1	Tubewall with PGR*	ERDA-Pitts.	X		X		
9,A,2	Tubewall without PGR	ERDA-Pitts.	X		X		
9,B,1	Multiple-Fixed Bed with PGR	IGT	X		X		
9,C,1	Fluidized Bed				X		
9,D,1	Liquid Phase	Chem Systems			X		

*Product Gas Recycle

FUNCTIONAL MODULE # 10

Definition: Methanol Synthesizers - Industrial Process for
Producing Methyl Alcohol

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	<u>Out of Date</u>
						State of Art	
10,A,1	High Pressure Reaction Catalytic Conversion	Synthesis from Hydrogen and Carbon Monoxide	X			X	
10,B,1	Distillation of Hardwood	Hardwood Distillation					X
10,C,1	By-Product of Acetaldehyde Production by Hydrocarbon Oxidation	By-Product				X	

FUNCTIONAL MODULE # 11

Definition: Fischer-Tropsch Synthesizers - Convert synthesis gas to a variety of light hydrocarbons and oxygenated hydrocarbons which are separated by distillation.

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowsheet</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	
						<u>State of Art</u>	<u>Out of Date</u>
11,A,1	Suspended Catalyst	Kellog (Sasol)	X			X	
11,B,1	Fixed Bed Catalyst	Ruhrchemie-Lurgi (Sasol)				X	

FUNCTIONAL MODULE # 12

Definition: Ammonia Synthesizers - Convert synthesis gas to anhydrous ammonia.

	<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	
							<u>State of Art</u>	<u>Out of Date</u>
B-14	12,A,1	Promoted Iron	DuPont					X
	12,A,2	Promoted Iron	Claude				X	
	12,A,3	Promoted Iron	Casale				X	
	12,A,4	Doubly Promoted Iron	American 300 ATM					X
	12,A,5	Promoted Iron	Fausser-Montecatini				X	
	12,A,6	Promoted Iron	Haber-Bosch				X	
	12,A,7	Doubly Promoted Iron	American (Large) 150 ATM				X	
	12,A,8	Iron Cyanide	Mont Cenis				X	

FUNCTIONAL MODULE # 13

Definition: Shift/Reverse Shift Reactors - Adjust H₂/CO ratio in synthesis gas to desired level. Inputs - synthesis gas and steam.

<u>Sub-Group</u>	<u>Catalyst</u>	<u>Function</u>	<u>Process Flowsheet</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	
						<u>State of Art</u>	<u>Out of Date</u>
13,A,1	Chromium Promoted Iron Oxide	Raise H ₂ /CO ratio	X			X	
13,B,1	Cobalt Molybdenum	Raise H ₂ /CO ratio			X		
13,C,1	Copper-Zinc	Raise H ₂ /CO ratio				X	
13,D,1	Chromium Promoted Iron Oxide (at high T)	Lower H ₂ /CO ratio				X	

FUNCTIONAL MODULE # 14

Definition: Gas Purification - Removal of impurities. Principally acid gasses (CO₂ and H₂S) from a gas stream.

	Sub-Group	Configuration	Process Name	Process Flowchart	Equipment Schematic	Advanced	PRIORITY	Out of Date
							State of Art	
B-16	14,A,1	Alkanolamine Absorbent	Ethanolamine Processes	X			X	
	14,B,1	Aqueous Ammonia Absorbent	Selective Hydrogen Sulfide Removal	X			X	
	14,C,1	Alkaline Salt Solution	Seaboard (Koppers Co.)	X				X
	14,C,2	Alkaline Salt Solution	Vacuum Carbonate Process (Koppers Co.)	X				X
	14,C,3	Alkaline Salt Solution	Tripotassium Phosphate Process (Shell)	X				X
	14,C,4	Alkaline Salt Solution	Benfield Process (Hot Potassium Carbonate)	X			X	
	14,C,5	Alkaline Salt Solution	Catacarb Process (Eickmeyer)	X			X	
	14,E,1	Physical Absorbtion in Cold Methanol	Rectisol (Lurgi)	X			X	
	14,F,1	Physical Absorbtion in Organic Solvent	Fluor Solvent Process	X			X	
	14,F,2	Physical Absorbtion in Organic Solvent	Selexol Process (Allied Chemical)	X			X	
	14,F,3	Physical Absorbtion in Organic Solvent	Purisol Process (Lurgi)	X			X	
	14,G,1	Physical & Chemical Solvent	Sulfinol (Shell)	X			X	
	14,Z,1	Pass-Through Option	Default					

FUNCTIONAL MODULE # 15

Definition: Hydrogen Purifiers - Chemical and Physical Methods for Removing H₂S, CO, CO₂ and Other Impurities from a Gas that is Primarily Hydrogen.

B-17	<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY <u>State of Art</u>	<u>Out of Date</u>
	15,A,1 - 15,G,1 - Identical to Module 14							
	15,H,1	Fixed Bed Methanator (for Trace CO Methanation)	Methanator	X			X	
	15,I,1	Copper Liquor Scrubbing	Girdler				X	
	15,J,1	Cryogenic Liquid Methane Scrubbing	Linde				X	
	15,J,2	Cryogenic Liquid Propane Scrubbing	Linde				X	
	15,K,1	Palladium Diffusion	Union Carbide				X	

FUNCTIONAL MODULE # 16

COAL PREPARATION PROCESSES

Definition: Systems Used to Convert the Raw Coal to a Form Suitable for Combustion or Conversion

(To Form an Actual Configuration, A Crusher, Grinder, Washing and/or Dryer Linked Together to Form a Functional Whole)

PRIORITY

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	<u>State of Art</u>	<u>Out of Date</u>
16,A,1	Crusher	Blake Crusher		X		X	
16,A,2	Crusher	Gyratory Crusher		X		X	
16,A,3	Crusher	Toothed Roll Crusher		X		X	
16,B,1	Grinder	Impactor		X		X	
16,B,2	Grinder	Ball-Race (Raymond Mill) Pulverizer		X		X	
16,B,3	Grinder	Roller Mill		X		X	
16,B,4	Grinder	Ball Mill		X		X	
16,C,1	Washing	Washing				X	
16,D,1	Dryer	Fluidized Bed Dryer				X	
16,D,2	Dryer	Rotary Kiln				X	
16,E,1	Preoxidation Treatment of Coal with Air or Oxygen and Steam	Pretreatment to Prevent Caking				X	
16,F,1	Mixing of Pulverized Coal with Oil	Paste Preparation				X	

Mineral Preparation - Convert raw minerals to a form suitable for use in coal conversion processes. (Actual Configurations for Mineral Preparation will consist of a Grinder or crusher and Additional Equipment as required.)

PRIORITY

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	<u>State of Art</u>	<u>Out of Date</u>
17,A,1	Crusher	Gyratory Crusher		X		X	
17,A,2	Crusher	Roll Crusher		X		X	
17,B,1	Grinder	Hammer Mill				X	
17,B,2	Grinder	Ball-Race Pulverizer		X		X	
17,B,3	Grinder	Roller Mill		X		X	
17,B,4	Grinder	Ball-Mill		X		X	
17,C,1	Evaporation	Evaporator				X	
17,D,1	Cooling	Cooler				X	
17,E,1	Furnace	Melting				X	
17,F,1	Rolling Under Heat	Rolling				X	
17,G,1	Thickener	Thickener		X		X	
17,H,1	Flotation	Flotation		X		X	
17,I,1	Dissolver	Agitated Dissolver		X		X	
17,J,1	Crystallization	Vacuum Crystallizers		X		X	
17,K,1	Leaching	Leaching		X		X	
17,L,1	Activated Carbon	Treatment with Activated Carbon				X	
17,M,1	Pressure Filter	Pressure Filter				X	
17,N,1	Continuous Centrifuge	Dewatering				X	
17,O,1	Steam-Heated Dryer	Dryer				X	

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FUNCTIONAL MODULE # 18

Definition: Oxygen Producers - Processes for the making of Oxygen

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<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	<u>Out of Date</u>
						State of Art	
18,A,1	Air Liquifaction and Distillation	Air Separation Plant	X			X	
18,B,1	Electrolysis of Water	Electrolysis					X

FUNCTIONAL MODULE # 19

Definition: Liquids, Suspensions/Separators/Purifiers - Methods for separating (a) Solids Suspended in Liquids and (b) components of liquids.

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	<u>Out of Date</u>
						<u>State of Art</u>	
19,A,1	Screen Across the Flow	Strainer				X	
19,B,1	Pressure Filter	Pressure Filter-Thickener		X		X	
19,C,1	Vacuum Filter	Rotary-Drum Vacuum Filter		X		X	
19,D,1	Classifier	Rake Classifier		X		X	
19,E,1	Flocculation and Sedimentation	Settling Tank		X		X	
19,E,2	Flocculation and Sedimentation	Thickener with Mechanical Agitation (Dorr Thickener)		X		X	
19,F,1	Hydraulic Separation	Sink & Float System		X		X	
19,G,1	Flotation	Air-Lift Cell		X		X	
19,H,1	Centrifugal Separation	Sludge Separator		X		X	
19,H,2	Centrifugal Separation	Continuous Filtering Centrifuge		X		X	
19,I,1	Evaporation	Evaporation				X	
19,J,1	Distillation	Distillation Column		X		X	
19,K,1	Gravity Separation of Immiscible Fluids	Cone Bottom Settling Tank				X	
19,L,1	Gravity Separation of Immiscible Fluids	Continuous Decanter (Centrifugal)		X		X	

FUNCTIONAL MODULE # 20

Definition: Hydrotreaters - Equipment to Combine Hydrocarbon Liquids Derived from Coal with Hydrogen Under Heat and Pressure to Increase H/C Ratio and API Gravity, and Remove Sulfur (as H₂S). Inputs Hydrogen and Hydrocarbon Mixture.

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	
						<u>State of Art</u>	<u>Out of Date</u>
20,A,1		COED Hydrotreating	X		X		
20,B,1		CONSOL Hydrotreating	X		X		
20,C,1		SRC Hydrotreating	X		X		

FUNCTIONAL MODULE # 21

Definition: Liquid/Gas Separators/Purifiers - Removal of undesired components from liquid/gas streams.

	<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	<u>Out of Date</u>
							State of Art	
B-23	21,A,1	Electric Field Removal of Particulates	Electrostatic Precipitator		X		X	
	21,B,1	Condensers	Surface Condensers		X		X	
	21,B,2	Condensers	Direct Contact Condensers				X	
	21,C,1	Gravity Settling Chamber	Gravity Settling Chamber		X		X	
	21,D,1	Cyclone Separator	Cyclone Separator		X		X	
	21,E,1	Entrainment Separators	Entrainment Separators				X	
	21,F,1	Drum	Flash Distillation		X		X	
	21,G,2	Column	Distillation Column		X		X	

FUNCTIONAL MODULE # 22

Definition: Hot Gas Cleaning Processes - Removal of particulates and/or H₂S from the output of a gasifier with gas retaining substantially all thermal energy.

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	<u>Out of Date</u>
						<u>State of Art</u>	
22,A,1	Inertial Separation	Cyclone Separator		X		X	
22,B,1	Electric Field Particulate Removal at High Temperature	Electrostatic Precipitators		X	X		
22,D,1	Expanded Bed Filters	Expanded Bed Filters			X		
22,E,1	H ₂ S Absorbers	Hot Iron Oxide Absorption (USBM)			X		

FUNCTIONAL MODULE # 23

Definition: Hydrogen Production alternative oxidation (with Steam or Water)
and reduction (with Low BTU Gas) of an intermediate chemical.
Steam or Water and Low BTU Gas Inputs.

<u>Sub-Group</u>	<u>Intermediate Chemical</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY <u>State of Art</u>	<u>Out of Date</u>
23,A,1	Iron Oxide	IGT Steam Iron	X		X		

FUNCTIONAL MODULE # 24

Definition: Conventional Furnaces/Boilers Used to Produce Steam (or Other High Temperature Working Fluid) for Turbines or Other Applications Where High Temperature (Up to About 1200 F) Thermal Energy is Required. Air, Fuel, and Working Fluid Inputs.

B-26

<u>Sub-Group</u>	<u>Fuel</u>	<u>Configuration</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	<u>Out of Date</u>
						State of Art	
24,A,1	Gas		X			X	
24,A,2	Oil		X			X	
24,A,3	Solid (Coal)		X			X	

FUNCTIONAL MODULE # 25

Definition: Fluidized Bed Furnaces/Boilers - Direct combustion of coal in fluidized bed for same purposes as conventional furnaces (Module #24).

PRIORITY

State
of
Art

Out
of
Date

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>		
25,A,1	Fluidized Bed At 10 ATM	Westinghouse Pressurized Fluidized Bed	X		X		
25,A,2	Pressurized Fluidized Bed	Argonne National Laboratory			X		
25,A,3	Pressurized Fluidized Bed	Bcura, Ltd.			X		
25,A,4	Pressurized Fluidized Bed	Combustion Power Company			X		
25,B,1	Atmospheric Pressure Fluidized Bed	Pope, Evans & Robbins Atmospheric Pressure Fluidized Bed	X	X	X		

B-27

FUNCTIONAL MODULE # 26

Definition: Cyclone Furnace - Partial oxidation of coal in air with simultaneous removal of particulates to produce a high-temperature low-BTU gas for use in MHD or other high temperature converter.

<u>Sub-group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Process Schematic</u>	<u>Advanced</u>	PRIORITY	
						<u>State of Art</u>	<u>Out of Date</u>
26,A,1	Rotary Flow of Coal and Air	Cyclone Furnace		X		X	

FUNCTIONAL MODULE # 27

Definition: High Pressure Furnaces - Combustion of coal or coal derived fuels at high pressures (750 psia) for energy conversion in MHD or other high temperature converter.

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowsheet</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	<u>Out of Date</u>
						<u>State of Art</u>	
27,A,1	Gas Fixed				X		
27,B,1	Liquid Fuel Fired				X		
27,C,1	Solid Fuel Fired				X		

FUNCTIONAL MODULE # 28

Definition: Hot-Gas Pyrolyzer - Pyrolysis of coal in high-temperature exhaust gas to produce a low-BTU gas for energy conversion in MHD or other high temperature converter.

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	<u>Out of Date</u>
						State of Art	
28,A,1	Reaction of CO ₂ + H ₂ O MHD Exhaust with Coal	Suspension Gasifier			X		

FUNCTIONAL MODULE # 29

Definition: Direct Coal Burning MHD Converter - Burns Coal
(or Other Solid Fuel) Directly with Preheated Air to
Produce Very High Temperature Working Fluid for MHD Section.

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	<u>Out of Date</u>
						<u>State of Art</u>	
29,A,1	Single-Stage		X		X		

FUNCTIONAL MODULE # 30

Definition: High Temperature Thermo/Turbo Electric Power Converters; Extract Electric/Mechanical Power from High Temperature Working Fluids ($T \geq 1200^{\circ}\text{F}$).

<u>Sub-Group</u>	<u>Type</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	
					<u>State of Art</u>	<u>Out of Date</u>
30,A,1	MHD	X		X		
30,B,1	Gas Turbine			X		

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FUNCTIONAL MODULE # 31

Flue Gas Clean-Up Processes

Definition: Devices for the removal of particulates, sulfur dioxide, and other pollutants from the stack gas after the thermal energy has been extracted from the coal.

To Form an Actual Configuration a Particulate Removal Device Will Be Connected to an SO₂ Removal Device.

PARTICULATE REMOVAL

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Flowsheet</u>	<u>Schematic</u>	<u>Advanced</u>	PRIORITY	<u>Out of Date</u>
						State of Art	
31,B,1	Inertial Separation	Impaction Separators	X	X		X	
31,B,2	Inertial Separation	Cyclonic Separators		X		X	
31,C,1	Filter	Cloth Filter		X		X	
31,D,1	Air-Ionization	Electrostatic Precipitator		X		X	
31,E,1	Liquid Contact Area	Liquid Scrubbers		X		X	

FUNCTIONAL MODULE # 31

SO₂ REMOVAL

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowsheet</u>	<u>Schematic</u>	<u>Advanced</u>	PRIORITY	
						<u>State of Art</u>	<u>Out of Date</u>
31,F,1	Lime and/or Limestone	Limestone Scrubbing	X	X		X	
31,F,2	Lime and/or Limestone	Gibbs & Hill Lime Scrubber	X	X		X	
31,F,3	Lime and/or Limestone	Combustion Engineering Limestone Injection & Lime Scrubbing	X	X			X
31,G,1	Double-Alkali	Envirotech		X		X	
31,G,2	Double-Alkali	FMC/Link Belt	X			X	
31,G,3	Double-Alkali	ADL + Combustion Equipment Associates	X			X	
31,G,4	Double-Alkali	General Motors	X			X	
31,H,1	Sodium Carbonate	Sodium Carbonate Scrubbing	X			X	
31,I,1	Magnesium Oxide	Chemico/Basic	X	X		X	
31,J,1	Wellman-Lord	Davy Powergas	X			X	
31,K,1	Catalytic Oxidation	Monsanto		X		X	
31,L,1	Cupric Oxide	Shell International		X		X	
31,L,2	Copper Oxide	Bureau of Mines	X				X
31,M,1	Citrate Process	Pfizer-McGee-Peabody (Bureau of Mines)	X			X	

FUNCTIONAL MODULE # 31

SO₂ REMOVAL (Continued)

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowsheet</u>	<u>Schematic</u>	<u>Advanced</u>	PRIORITY	<u>Out of Date</u>
						<u>State of Art</u>	
31,N,1	Ammonia Absorption	TVA-EPA	X			X	
31,O,1	Calsox-Aqueous Ethanolamine	Monsanto		X			X
31,P,1	Activated Carbon	Westvaco		X		X	
31,P,2	Activated Carbon (Coal)	Foster-Wheeler	X			X	
31,Q,1	Ionics SO ₂ Removal	Stone & Webster		X		X	
31,R,1	Potassium Formate	Consolidation Coal	X		X		
31,U,1	Sulphidine Process (Xylidine + Water)	Metallgesellschaft, A.G.		X			X
31,U,2	Improvement on Sulphidine Process (Using Dimethylaniline)	American Smelting & Refining		X			X

FUNCTIONAL MODULE # 32

Definition: High Temperature Flue Gas Thermal Energy Recovery and Partial Clean-Up

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	
						<u>State of Art</u>	<u>Out of Date</u>
32,A,1	Tubular Air Heater	Recycling of Heat from Flue Gas to Furnace Inlet Air		X		X	
32,A,2	Rotary Regenerative Air Heater	Recycling of Heat from Flue Gas to Furnace Inlet Air		X		X	
32,B,1	Steam Generator with Superheater and Reheater	Energy Recovery from MHD Exhaust	X	X	X		

FUNCTIONAL MODULE # 33

Definition: Low-BTU Gas Thermal Energy Recovery and Clean-Up Process - Removal of particulates and sulfurous gases from output of Low BTU gasifiers (Module # 1).

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	<u>Out of Date</u>
						<u>State of Art</u>	
33,A,1	Inertial Separation	Cyclone Separator		X		X	
33,B,1	Spray Chamber	Scrubber				X	
33,C,1	Closed Circuit of Dowtherm A	Heat Exchanger				X	
33,D,1	Electric Field Particulate Removal	Electrostatic Precipitator	X	X		X	

FUNCTIONAL MODULE # 34

Definition: Mineral recovery and waste treatment processes - Treatment of effluent streams to produce wastes suitable for discharge, production of by-products, and recovery of minerals/chemicals for reuse in coal conversion processes.

	<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowsheet</u>	<u>Process Schematic</u>	<u>Advanced</u>	PRIORITY	<u>Out of Date</u>
							State of Art	
B-39	34,A,1	Mechanical separation by density	Dissolved Air flotation				X	
	34,A,2	Mechanical separation by density	Clarification				X	
	34,B,1	Control of PH	Equalization				X	
	34,C,1	Biological System	Activated Sludge				X	
	34,D,1	Ammonia Stripping	Ammonia Still	X			X	
	34,E,1	Adsorption	Activated Carbon				X	
	34,F,1	Dephenolization	Vapor Recirculation				X	
	34,F,2	Dephenolization	Liquid/Liquid Extraction				X	
	34,G,1	Evaporation	Evaporation Ponds				X	
	34,H,1	Oxidation	Oxidation Using Ozone			X		
	34,H,2	Oxidation	Distillation and Incineration			X ²		

²Used by byproduct coke plant technology but apparently not yet in coal plant designs.

FUNCTIONAL MODULE # 34 (Continued)

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Process Schematic</u>	<u>Advanced</u>	PRIORITY <u>State of Art</u>	<u>Out of Date</u>
34,A,A,1	Hydrated Ferric Oxide	Iron Oxide	X	X			X
34,B,B,1	Carbon	Activated Carbon	X				X
34,C,C,1	Combustion Followed by Catalytic Reaction	Claus	X			X	
34,C,C,2	Claus Process at Lower Temperature	Sulfreen	X			X	
34,D,D,1	Sodium Carbonate and Ferric Hydroxide Solution	Ferrox	X				X
34,E,E,1	Sodium Thioarsenate	Thylox	X				X
34,F,F,1	Alkali Vanadate Additive	Stretford	X			X	

FUNCTIONAL MODULE # 35

Definition: Turbo-Electric Power Converters - Devices Used to Convert the Thermal Energy of Steam into Electrical Energy

	<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	<u>Out of Date</u>
							State of Art	
B-47	35,A,1	Stationary Nozzles	Impulse Turbine		X		X	
	35,B,1	Moving Nozzles	Reaction Turbine		X		X	

FUNCTIONAL MODULE # 36

Definition: Devices Used to Condense the Steam that Exhausts from the Steam Turbine, and to Dispose of Waste Heat

	<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	<u>Out of Date</u>
							<u>State of Art</u>	
	36,A,1	Water Filled Pipes Condense Steam	Surface Condenser		X		X	
	36,B,1	Cooling Water Mixed with the Steam	Direct Contact Condenser		X		X	
		Heat Disposal Methods						
B-42	36,C,1	Use of a Natural Body of Water as a Heat Sink						X
	36,D,1	Water Evaporation Cooling Tower	Forced Draft	X			X	
	36,D,2	Water Evaporation Cooling Tower	Crossflow Induced Draft	X			X	
	36,D,3	Water Evaporation Cooling Tower	Hyperbolic	X			X	
	36,E,1	Cooling by Contact of Spray & Air	Spray Pond				X	
	36,F,1	Finned Hot Surface in a Dry Air Flow	Dry Cooling Tower	X		X		

FUNCTIONAL MODULE # 37

Definition: Gas Turbine Electric Power Generation - Gas Turbine as a Prime Mover to Operate an Electrical Generator

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	
						<u>State of Art</u>	<u>Out of Date</u>
37,A,1	Brayton Cycle (Basic)	Basic Gas Turbine	X	X		X	
37,A,2	Exhaust Heat Returned to Combustion Chamber	Gas Turbine with Regeneration	X			X	
37,A,3	Two Compressor Stages with Cooling of Air Between Them	Gas Turbine with Intercooling	X			X	
37,A,4	Two Expanders with a Secondary Combustion Chamber Between Them	Gas Turbine with Reheating	X			X	

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FUNCTIONAL MODULE # 38

Definition: Waste Disposal - Discharge of waste material to environment.

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Process Schematic</u>	<u>Advanced</u>	PRIORITY	<u>Out of Date</u>
						<u>State of Art</u>	
38,I,1	Disposal in the mine	Mine Fill			X		
38,I,2	Land Fill	Land Fill				X	
38,J,1	Bio-Treating Sludges Used as Fuels	Boiler Fuel			X		
38,K,1	Stack	Stack				X	
38,L,1	Lagoon	Lagoon				X	

FUNCTIONAL MODULE # 39

Definition: Demethanators - Convert methane in a gas stream to CO and H₂

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	
						<u>State of Art</u>	<u>Out of Date</u>
39,A,1	Endothermic Steam-Methane Reaction	Methane Reformer				X	

FUNCTIONAL MODULE # 40

Definition: Coal/Chemical Slurry Separators - Separation of Ash and Sulfur from coal in a chemical slurry.

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<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	<u>Out of Date</u>
						<u>State of Art</u>	
40,A,1	Filter	Centrifugal Filter				X	
40,A,2	Filter	Filter Press				X	
40,B,1	Separator	Solvent-Water Separator				X	
40,B,2	Separator	Solvent-Solids Separator				X	
40,C,1	Tank with Impeller	Solvent Mixing				X	
40,C,2	Tank with Impeller	Repulping Tank				X	
40,D,1	Cooler	Cooler				X	
40,E,1	Dryer	Dryer				X	

FUNCTIONAL MODULE # 41

Definition: Char Preparation Processes

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	
						<u>State of Art</u>	<u>Out of Date</u>
41,A,1	Ball Mill	Pulverizer		X		X	

FUNCTIONAL MODULE # 42

Definition: Nuclear Dissociation of Water for Production of Oxygen and Hydrogen

<u>Sub-Group</u>	<u>Configuration</u>	<u>Process Name</u>	<u>Process Flowchart</u>	<u>Equipment Schematic</u>	<u>Advanced</u>	PRIORITY	<u>Out of Date</u>
						<u>State of Art</u>	
42,A,1	Dissociation at Extreme Temperature	Thermal Dissociation			X		

APPENDIX C

CAPITAL COST ESTIMATES FOR METHANATOR MODULE CONFIGURATIONS

In Chapter 3 we outlined the MPPM requirements for configuration data files or configuration "models", and presented, as an example of how such models would be obtained, the development of data files for three competing configurations listed under the "Methanol Synthesis" Module (No. 9). These were

- 9,A,1 Tubewall Methanator with Product-Gas Recycle
- 9,A,2 Tubewall Methanator without Product-Gas Recycle
- 9,B,1 Multiple-Fixed-Bed Methanator with Product-Gas Recycle

Flowsheets for these configurations are shown in Figures 3.2, 3.3, and 3.4. In this appendix we present the investment cost "point design" data referred to in Chapter 3, which is required for the development of configuration models.

A review of the available design documents* rather quickly reveals that the major cost items in the tubewall methanation module configurations are (a) the compressors, (b) the gas-to-gas heat exchangers that serve as feed preheaters, (c) the methanator vessel, and (d) the heat recovery system. For the multiple-fixed-bed methanator, the list is the same except that the feed gas preheater is of lesser importance. From this list and the nature of the methanation reactions described in Chapter 3, it is easy to see that the dominant external parameters in costing the configurations will be:

- Output quantity Q°
- Input gas pressure P'
- Effective input gas CO concentration, $X_c'(CO)$,

$$X_c'(CO) = (X'(CO) + f x'(CO_2)) \quad (C.1.)$$

The first, Q° , clearly sizes the module, while the second, P' , determines the output compressor cost but also affects the recycle compressor costs, heat exchanger costs, and amount of catalyst needed. The last, $X_e'(CO)$, determines the degree of methanation required and hence the level of recycle dilution, the amount of catalyst required, and the amount of thermal power generated.

In order to develop point design data, we subdivided the module configurations into ten cost elements and evaluated the material and installation labor cost for each. These cost elements are listed in Table C.1. The initial catalyst cost refers to the cost of a beginning material inventory, and initial installation cost is included in the cost of the methanation vessel. Replacement of catalyst inventory, including the replacement installation cost, is charged to direct operating expenses. The total investment is obtained by multiplying the sum of material and installation labor costs, for all cost elements except catalyst cost, by a constant factor, and then adding in the initial catalyst cost. The multiplying factor was taken at 3.3., based on the average of similar ratios taken from the available design documents. In fact, this factor is fairly close to the so-called "Lang" factor for fluid processing plants, when allowance is made for the fact that the Lang factor is based on material cost rather than material plus installation costs.*

The equations used for the individual cost elements are given in Table C.1. The compressor costs were evaluated from an equation obtained from applying some approximations to the commercial costing code generously provided by the Ingersoll-Rand Company. We assume other companies' compressors are similarly priced. Steam turbine drive costs were included in the compressor costs at a price of \$50 per brake horsepower. This is about 10% above the average of several steam turbine drives priced for us by the Terry Corporation. (The extra 10% was included because the correlation between cost and horsepower is somewhat ragged. The cost estimates could probably be improved in this area, although the effect on the overall module costs would be slight). The compressor cost function we used is:

$$\begin{aligned}
 C_C &= C_C (Q, p^a, p^b; n, MW) \\
 &= 2.25 \mu(Q) \mu(p^b - p^a) \left\{ \left(60 + 130 \frac{Q}{p^a} \right) \times 10^3 + 23 \times 10^3 \right. \\
 &\quad \left. + \left[\left(0.3 + 14 \frac{Q}{p^a} \right) \frac{8.7 \times 10^5}{MW} + 3H_2O^3 Q \right] \beta \left\{ \left[1 + 0.5 \mu(p^b - p^a) \right] \right\} \right. \\
 &\quad \left. + 94 \times 10^3 Q \beta \right.
 \end{aligned} \quad (3.6)$$

* As quoted by Bauman, reference 9 of Chapter 3, the Lang factor based on material costs for fluid process plants is 4.74. Adjusting this for an average installation cost of 40% of material costs gives an equivalent factor of 3.4 based on material plus installation labor costs.

$$\text{where } \mu(x) = \begin{cases} 1 & x > 0 \\ 0 & x \leq 0 \end{cases}$$

$$p_o^b = \begin{cases} 850 & 263 \frac{Q}{p_a} \leq 10 \\ 800 & 10 < 263 \frac{Q}{p_a} \leq 20 \\ 650 & 20 < 263 \frac{Q}{p_a} \leq 40 \\ 500 & 40 < 263 \frac{Q}{p_a} \leq 65 \\ 300 & 65 < 263 \frac{Q}{p_a} \end{cases}$$

MW = average molecular weight of gas

$$\beta = \frac{1}{n} \left[\left(\frac{p_o^b}{p_a} \right)^n - 1 \right]$$

$$n = \text{polytropic coefficient} = \frac{1}{0.78} \cdot \frac{k-1}{k}$$

k = ratio of specific heats of gas

p_a = Input pressure, psia

p_o^b = Output pressure, psia

Q = Flow rate, MMSCFH

The unit step function adds a 50% increment to compressor cost at high outlet pressures, since it is necessary to use a so-called vertically split construction in place of the normal horizontally split construction.

For those cost elements where a non-linear relationship between throughput and cost appeared appropriate, a parallel unit redundancy factor, n, was used. In general, this was taken as three, although at the higher output levels ($Q^o > 20$ MMSCFH) a higher value of n might be considered.

The weight of the shell of a spherical or cylindrical (with a fixed length-to-diameter ratio) vessel of given material and design stress level can be shown to be approximately proportional to the product of its volume and the designed-for internal pressure. The volume required in the vessel will vary with pressure, higher pressures tending to reduce volume requirements. For instance, the required volume of a multiple-

fixed-bed methanator vessel for a given gas flow rate will depend on the catalyst activity factor. Information from the Girdler Co.* indicates that catalyst activity increases almost linearly with pressure (for pressures above 100 psia), and hence the required volume of the methanation vessel should vary inversely with pressure. Then the weight of a fixed-bed methanator vessel, for a given gas flow (in SCFH) will be invariant with pressure, to a first order approximation. Cost is usually proportional to weight, so methanation vessel cost (without catalyst cost) should be roughly invariant with pressure. We suspect that various secondary costs--of flanges, nozzles, fittings, etc.--would actually cause the vessel cost to increase with pressure. In our cost model for fixed-bed methanators we have, however, used the first order approximation and normalized costs to an average point value taken from the available design documents. Similar reasoning and results hold for the tubewall methanator. Although quantitative data on tubewall catalyst activity factor as a function of pressure is not presently available, we have assumed a linear increase with pressure, the same as for the fixed-bed methanator.

The gas-to-gas heat exchanger used for the feed preheater will have a shell which must hold the same internal pressure as the methanation vessel, but pressure differentials across the internal heat exchange surfaces will be relatively small. Heat transfer coefficients for gases are roughly proportional to mass flow rates.** Therefore, we expect the feed preheater cost to increase roughly in proportion to pressure. Using some examples from the design documents, correcting for some differences in temperatures conditions, and guided by the above relationship, we obtained the cost vs. pressure and flow quantity relationships shown in Table C.1.

Similar rationales explain the other functional relationships in Table C.1. For example, the cooler and knock-out drum costs are made proportional to gas cooling load and amount of condensate generated. The

* Mr. Orville Gross, Girdler Co., Louisville, Kentucky.

** See Reference 11 of Chapter 3.

entire set of equations was programmed and evaluated for a range of throughputs, Q^o , input pressures, P' , and effective input CO concentration, $X'_e(CO)$. The results are illustrated in Figures C.1 to C.16 for the tubewall methanator with product gas recycle, Figures C.17 to C.32 for the tubewall methanator without product gas recycle, and Figures C.33 to C.48 for the multiple fixed-bed methanator. In the graphs which show cost vs. inlet pressure, the point at the highest pressure is singular, in that the cost of the product gas compressor becomes zero at that inlet pressure, and a discontinuity in the cost function results.

Some general cost comparisons between configurations show that:

- At low inlet pressures, the multiple-fixed-bed methanator is most expensive. This results from the relatively large pressure drop across the methanator vessel.
- The tubewall methanator with product gas recycle is the most expensive at medium and high inlet pressures, the differential being largely attributable to the cost of the feed preheater.
- The tubewall methanator without product gas recycle is only slightly more expensive than the multiple fixed-bed configuration. Eliminating product gas recycle saves substantial costs for the feed preheater, the recycle gas compressor, and the coolers.

The data given in Figures C.1 through C.48 are equivalent to the "point design" data referred to in Chapter 3. During Phase II of the current project, equivalent data must be obtained on the other modules and competing configurations which are to be modeled. We will depend primarily on outside sources, e.g., ERDA, its contractors, and independent process developers, to provide this data.

TABLE C.1

Methanator Module Cost Element Equations

Cost Element	Form of Equation	Parameters		
		Tube Wall With Product Gas Recycle	Multiple Fixed-Bed With Prod. Gas Recycle	Tube Wall Without PGR
Product Gas Compressor	$C_{co} = nC_c(\frac{Q^0}{n}, P' - \Delta P, P^0; 0.26, 16)$	$\Delta P = 15 \text{ psia}$	$\Delta P = 50 \text{ psia}$	$\Delta P = 15 \text{ psia}$
Recycle Gas Compressor	$C_{cr} = nC_c(\frac{Q^r}{n}, P - \Delta P, P'; 0.26, 16)$	$Q^r = Q'(\frac{X'(CO)}{0.07} - 1), \Delta P = 15$	$Q^r = Q'(\frac{X'(CO)}{0.07} - 1), \Delta P = 50$	$Q^r = 0$
Methanator Vessel	$C_m = C_{mo}(\frac{Q^0}{50})(\frac{X'(CO)}{0.07})$	$C_{mo} = \$3.4 \times 10^6$	$C_{mo} = \$1.1 \times 10^6$	$C_{mo} = \$3.4 \times 10^6$
Heat Recovery and Steam Generation	$C_h = nC_{ho}(\frac{T_e/n}{100})^{0.36}$	$C_{ho} = \$0.27 \times 10^6$	$C_{ho} = \$0.52 \times 10^6$	$C_{ho} = \$0.27 \times 10^6$
Feed Preheater (Gas-to Gas Heat X)	$C_x = C_{xo}(\frac{Q^0}{50})(\frac{X'(CO)}{0.07})^a(\frac{P'}{1000})^{0.9}$	$C_{xo} = \$5.5 \times 10^6, a = 1$	$C_{xo} = \$0.28 \times 10^6, a = 1$	$C_{xo} = \$5.5 \times 10^6, a=0$
Sulfur Guard Reactor	$C_g = C_{go}(\frac{Q^0}{50})$	$C_{go} = \$1.4 \times 10^6$	same	same
Dehydration Unit	$C_d = nC_{do}(\frac{Q^0/n}{10.4})^{0.76}$	$C_{do} = \$0.27 \times 10^6$	same	same
Start-up Heater	$C_s = C_{so}(\frac{Q^0}{50})(\frac{X'(CO)}{0.07})^a$	$C_{so} = \$0.6 \times 10^6, a = 1$	$C_{so} = \$0.1 \times 10^6, a = 1$	$C_{so} = \$0.6 \times 10^6, a=0$
Coolers and K.O. Drums	$C_z = C_{zo}[\frac{Q^0}{50a}(\frac{X'(CO)}{0.07} - b) + \frac{Q^0}{50}]$	$C_{zo} = \$2.6 \times 10^6, a=1, b=0.76$	$C_{zo} = \$2.6 \times 10^6, a = 1, b = 0.76$	$C_{zo} = \$2.6 \times 10^6, a=4.8, b=0$
Initial Catalyst	$C_a = C_{ao}(\frac{Q^0}{50})(\frac{X'(CO)}{0.07})(\frac{1000}{P'})$	$C_{ao} = \$0.1 \times 10^6$	$C_{ao} = \$0.7 \times 10^6$	$C_{ao} = \$0.1 \times 10^6$

E_m = Total Fixed Capital Cost = $3.3 (C_{co} + C_{cr} + C_m + C_h + C_x + C_g + C_d + C_s + C_z) + C_a$

n = Number of units operating in parallel

$2.6 \text{ MMSCFH} \leq Q^0 \leq 26 \text{ MMSCFH}; 0.10 \leq X'(CO) \leq 0.2466$

FIGURE C.1

Tubewall Methanator with Product Gas Recycle

Fixed Investment vs. Throughput
Input Co Fraction, $X'(CO) = 0.1$

FIGURE C.2

Tubewall Methanator with Product Gas Recycle

Fixed Investment vs. Throughput
Input Co Fraction, $X'(CO) = 0.15$

FIGURE C.3

Tubewall Methanator with Product Gas Recycle

Fixed Investment vs. Throughput
Input Co Fraction, $X'(CO) = 0.20$

A $\rightarrow P' = 100 \text{ psia}$
 B $\rightarrow P' = 300 \text{ psia}$
 C $\rightarrow P' = 600 \text{ psia}$
 D $\rightarrow P' = 900 \text{ psia}$
 E $\rightarrow P' = 1030 \text{ psia}$

FIGURE C.4

Tubewall Methanator with Product Gas Recycle

Fixed Investment vs. Throughput
Input Co Fraction, $X'(CO) = 0.2466$

A $\rightarrow P' = 100$ psia
 B $\rightarrow P' = 300$ psia
 C $\rightarrow P' = 600$ psia
 D $\rightarrow P' = 900$ psia
 E $\rightarrow P' = 1030$ psia

FIGURE C.5

Tubewall Methanator with Product Gas Recycle

Fixed Investment vs. Inlet Pressure
Throughput, $Q^o = 2.6$ MMSCFH

FIGURE C.6

Tubewall Methanator with Product Gas Recycle

Fixed Investment vs. Inlet Pressure
Throughput, $Q^o = 5.2$ MMSCFH

FIGURE C.7

Tubewall Methanator with Product Gas Recycle

Fixed Investment vs. Inlet Pressure
Throughput, $Q^o = 10.4$ MMSCFH

FIGURE C.8

Tubewall Methanator with Product Gas Recycle

Fixed Investment vs. Inlet Pressure
Throughput, $Q^o = 15.6$ MMSCFH

FIGURE C.9

Tubewall Methanator with Product Gas Recycle

Fixed Investment vs. Inlet Pressure
Throughput, $Q^o = 20.8$ MMSCFH

FIGURE C.10

Tubewall Methanator with Product Gas Recycle

Fixed Investment vs. Inlet Pressure
Throughput, $Q^o = 26.0$ MMSCFH

FIGURE C.11

Tubewall Methanator with Product Gas Recycle

Fixed Investment vs. Input CO Fraction
Throughput, $Q^o = 2.6$ MMSCFH

FIGURE C.12

Tubewall Methanator with Product Gas Recycle

Fixed Investment vs. Input CO Fraction
Throughput, $Q^o = 5.2$ MMSCFH

FIGURE C.13

Tubewall Methanator with Product Gas Recycle

Fixed Investment vs. Input CO Fraction
Throughput, $Q^o = 10.4$ MMSCFH

FIGURE C.14

Tubewall Methanator with Product Gas Recycle

Fixed Investment vs. Input CO Fraction
Throughput, $Q^o = 15.6$ MMSCFH

FIGURE C.15

Tubewall Methanator with Product Gas Recycle

Fixed Investment vs. Input CO Fraction
Throughput, $Q^o = 20.8$ MMSCFH

FIGURE C.16

Tubewall Methanator with Product Gas Recycle

Fixed Investment vs. Input CO Fraction
Throughput, $Q^o = 26.0$ MMSCFH

FIGURE C.17

Tubewall Methanator without Product Gas Recycle

Fixed Investment vs. Throughput
Input Co Fraction, $X'(CO) = 0.1$

FIGURE C.18

Tubewall Methanator without Product Gas Recycle

Fixed Investment vs. Throughput
Input Co Fraction, $X'(CO) = 0.15$

FIGURE C.19

Tubewall Methanator without Product Gas Recycle

Fixed Investment vs. Throughput
Input Co Fraction, $X'(CO) = 0.20$

FIGURE C.20

Tubewall Methanator without Product Gas Recycle

Fixed Investment vs. Throughput
Input Co Fraction, $X'(CO) = 0.2466$

FIGURE C.21

Tubewall Methanator Without Product Gas Recycle

Fixed Investment vs. Inlet Pressure
Throughput, $Q^o = 2.6$ MMSCFH

FIGURE C.22

Tubewall Methanator Without Product Gas Recycle

Fixed Investment vs. Inlet Pressure
Throughput, $Q^o = 5.2$ MMSCFH

FIGURE C.23

Tubewall Methanator Without Product Gas Recycle

Fixed Investment vs. Inlet Pressure
Throughput, $Q^o = 10.4 \text{ MMSCFH}$

FIGURE C.24

Tubewall Methanator Without Product Gas Recycle

Fixed Investment vs. Inlet Pressure
Throughput, $Q^o = 15.6 \text{ MMSCFH}$

FIGURE C.25

Tubewall Methanator Without Product Gas Recycle

Fixed Investment vs. Inlet Pressure
Throughput, $Q^o = 20.8 \text{ MMSCFH}$

$A \rightarrow X'(CO) = 0.1$
 $B \rightarrow X'(CO) = 0.15$
 $C \rightarrow X'(CO) = 0.20$
 $D \rightarrow X'(CO) = 0.2466$

FIGURE C.26

Tubewall Methanator Without Product Gas Recycle

Fixed Investment vs. Inlet Pressure
Throughput, $Q^o = 26.0$ MMSCFH

FIGURE C.27

Tubewall Methanator without Product Gas Recycle

Fixed Investment vs. Input CO Fraction
Throughput, $Q^o = 2.6$ MMSCFH

FIGURE C.28

Tubewall Methanator without Product Gas Recycle

Fixed Investment vs. Input CO Fraction
Throughput, $Q^o = 5.2$ MMSCFH

FIGURE C.29

Tubewall Methanator without Product Gas Recycle

Fixed Investment vs. Input CO Fraction
Throughput, $Q^o = 10.4$ MMSCFH

FIGURE C.30

Tubewall Methanator without Product Gas Recycle

Fixed Investment vs. Input CO Fraction
Throughput, $Q^o = 15.6$ MMSCFH

FIGURE C.31

Tubewall Methanator without Product Gas Recycle

Fixed Investment vs. Input CO Fraction
Throughput, $Q^o = 20.8$ MMSCFH

FIGURE C.32

Tubewall Methanator without Product Gas Recycle

Fixed Investment vs. Input CO Fraction
Throughput, $Q^o = 26.0$ MMSCFH

FIGURE C.33

Multiple-Fixed-Bed Methanator with Product Gas Recycle

Fixed Investment vs. Throughput.
Input CO Fraction, $X'(CO) = 0.1$

FIGURE C.34

Multiple-Fixed-Bed Methanator with Product Gas Recycle

Fixed Investment vs. Throughput
Input CO Fraction, $X'(CO) = 0.15$

FIGURE C.35

Multiple-Fixed-Bed Methanator with Product Gas Recycle

Fixed Investment vs. Throughput
Input CO Fraction, $X'(CO) = 0.20$

FIGURE C.36

Multiple-Fixed-Bed Methanator with Product Gas Recycle

Fixed Investment vs. Throughput
Input CO Fraction, $X'(CO) = 0.2466$

FIGURE C.37

Multiple-Fixed-Bed Methanator with Product Gas Recycle

Fixed Investment vs. Inlet Pressure
Throughput, $Q^o = 2.6$ MMSCFH

FIGURE C.38

Multiple-Fixed-Bed Methanator with Product Gas Recycle

Fixed Investment vs. Inlet Pressure
Throughput, $Q^o = 5.2$ MMSCFH

$A \rightarrow X'(CO) = 0.1$
 $B \rightarrow X'(CO) = 0.15$
 $C \rightarrow X'(CO) = 0.20$
 $D \rightarrow X'(CO) = 0.2466$

FIGURE C.39

Multiple-Fixed-Bed Methanator with Product Gas Recycle

Fixed Investment vs. Inlet Pressure
Throughput, $Q^o = 10.4$ MMSCFH

A $\rightarrow$ $X'(CO) = 0.1$
 B $\rightarrow$ $X'(CO) = 0.15$
 C $\rightarrow$ $X'(CO) = 0.20$
 D $\rightarrow$ $X'(CO) = 0.2466$

FIGURE C.40

Multiple-Fixed-Bed Methanator with Product Gas Recycle

Fixed Investment vs. Inlet Pressure
Throughput, $Q^o = 15.6$ MMSCFH

A $\rightarrow X'(CO) = 0.1$
 B $\rightarrow X'(CO) = 0.15$
 C $\rightarrow X'(CO) = 0.20$
 D $\rightarrow X'(CO) = 0.2466$

FIGURE C.41

Multiple-Fixed-Bed Methanator with Product Gas Recycle

Fixed Investment vs. Inlet Pressure
Throughput, $Q^o = 20.8$ MMSCFH

FIGURE C.42

Multiple-Fixed-Bed Methanator with Product Gas Recycle

Fixed Investment vs. Inlet Pressure
Throughput, $Q^o = 26.0$ MMSCFH

A $\rightarrow X'(CO) = 0.1$
 B $\rightarrow X'(CO) = 0.15$
 C $\rightarrow X'(CO) = 0.20$
 D $\rightarrow X'(CO) = 0.2466$

FIGURE C.43

Multiple-Fixed-Bed Methanator with Product Gas Recycle

Fixed Investment vs. Input CO Fraction
Throughput, $Q^o = 2.6$ MMSCFH

FIGURE C.44

Multiple-Fixed-Bed Methanator with Product Gas Recycle

Fixed Investment vs. Input CO Fraction
Throughput, $Q^o = 5.2$ MMSCFH

FIGURE C.45

Multiple-Fixed-Bed Methanator with Product Gas Recycle

Fixed Investment vs. Input CO Fraction
Throughput, $Q^o = 10.4$ MMSCFH

FIGURE C.46

Multiple-Fixed-Bed Methanator with Product Gas Recycle

Fixed Investment vs. Input CO Fraction
Throughput, $Q^o = 15.6$ MMSCFH

FIGURE C.47

Multiple-Fixed-Bed Methanator with Product Gas Recycle

Fixed Investment vs. Input CO Fraction
Throughput, $Q^o = 20.8$ MMSCFH

FIGURE C.48

Multiple-Fixed-Bed Methanator with Product Gas Recycle

Fixed Investment vs. Input CO Fraction
Throughput, $Q^o = 26.0$ MMSCFH

Models' Participation Within Energy Supply and Demand System

ROAD MAP FOR COAL PROCESSES TO END PRODUCTS