OPTIMIZATION OF COAL GASIFICATION PROCESSES

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OPTIMIZATION OF COAL GASIFICATION PROCESSES

By

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SUMMARY

This project has the objective of assisting the Office of Coal Research to determine those processes which hold more promise for potential economical development for the commercial production of a high-heating-value pipeline gas.

Since the time and financial resources are limited, the studies are concentrated only on the processes which present the most attractive commercial possibilities. The mathematical optimization techniques along with the methodology of system analysis have been developed for use in optimizing various types of proposed processes and indicating the most advantageous among the available choices.

In using optimization techniques, a generalized economic standard method of comparison is established. Representative types of problems of fundamental importance to the coal gasification processes are defined and identified. Information relating to the coal gasification available in the literature and from the OCR contractors and other pertinent sources has been collected and classified. The various steps involved in a specified process are studied and the contribution of those steps to the economics of the whole process has been evaluated. This study identifies those steps having a significant effect so that a more precise and detailed evaluation can be made of those problem areas which are critical to the success of the alternative processes under consideration. This study also identifies all steps having negligible effect on the cost of the entire process so that such steps may be eliminated from further consideration. The study has indicated areas of

serious deficiency in the technical knowledge which are necessary for the successful application of proposed coal gasification scheme.

Depending on the types and nature of the problems considered, an effective and efficient optimization technique is then selected and tested for the various processes. If the existing techniques are inadequate, new techniques are developed. Computer programs are designed to determine the optimum operating conditions for the critical steps and paths of the various processes, optimal design of various systems, and policies of supply and types of coal considered.

This information is compiled in this study and the results interpreted in practical terms specifying the characteristics of coal used, the capital and operating costs of the plants as a whole, and of sections of such plants, including the necessary benefit/cost relationships. Thus, the most attractive processes or alternatives are recommended, and those areas of coal gasification technology are identified where further research and development are likely to produce beneficial results.

Although a number of coal gasification schemes to manufacture pipeline gas have been proposed and are under different stages of investigation, any of these schemes can be represented by the five separate phases of operation; namely, coal preparation and pretreatment, coal gasification, shift conversion, gas purification, and methanation. Depending on the individual scheme, some phases of operation may dominate others in terms of its size and cost.

This report deals with each of the five phases, presenting the pertinent technical information, examining the constraints and alternate processes, and formulating models for computer simulation and optimization.

Each of the subsystems optimized is then integrated to arrive at an overall evaluation of the various gasification processes. The following conclusions and recommendations are made:

1. The gas price is most significantly affected by the amount and cost of coal or lignite required for the integrated plant. Depending on the cost of coal or lignite, approximately 40 to 60% of the gas price is attributable to the cost of coal.

2. Pretreatment of coal to prevent agglomeration in the gasifiers would result in approximately 6 to 19% weight losses of coal. Since the cost of coal is by far the largest cost item, every effort should be made in the effective utilization of coal. Any means by which raw coal or char with the least pretreatment can be fed to the gasification reactor will reduce the gas price considerably. This points to the urgent need for the development of a raw coal feeding system, or the development of the technology of recovering the volatile matters lost in the pretreatment.

3. Table S-1 compares the gas price (without by-product credit), carbon utilization, thermal efficiency, total fixed investment, and operating expenses for each alternate process studied. It is seen that the gas price is lower for the process (Alternate II-3) which is assumed to be capable of feeding raw coal to the gasification reactor. The highest gas price, shown by alternate I, is due to the inefficient use of carbon and hydrogen in coal by reacting coal with oxygen during the initial period and by extensive water-gas shift reaction and methanation required later in the process.

Since the gas prices are affected by many factors such as cost of coal, accounting procedure adopted, etc., which are subject to change depending on the economic climate, they should be considered as the estimated relative prices and only be used for comparison among the various alternatives studied.

4. Although most of the processes considered are operated at approximately 1000 psig in order to produce methane at the pipeline pressure, effects of pressure on gasification systems should be investigated. Since most of the gasification reactions are favored when the pressure is increased, high pressure operation should reduce the reactor size and improve the gas purification efficiency. The equipment costs for these two phases of operation are a significant part of the total equipment cost. The advantage of a higher pressure operation, however, is offset by the requirement of thicker reactor walls, resulting in higher reactor costs. The operation at pressures lower than 1000 psig will require compression cost to bring it to the pipeline gas condition.

5. From the thermodynamic point of view, for the production of methane, direct hydrogen coal reactions utilizing devolatilization and hydrogenolysis are more efficient than the carbon monoxide-hydrogen reaction (methanation reaction). Therefore, if the

TABLE S-1

OPERATING EXPENSE, FIXED INVESTMENT, THERMAL EFFICIENCY, CARBON UTILIZATION, AND GAS PRICE FOR DIFFERENT PROCESSES

	Alternate Process	Total Fixed Investment MM $	Operating Expense MM $/year	Overall Plant Thermal Efficiency(1) percent	Carbon Utilization(2) percent	Gas Price(3) ¢/MM Btu
Bituminous Coal	I	138.0	66.4	45.6	28.7	85.9
	II-1	127.1	53.4	62.2	37.9	70.0
	II-2	124.4	56.6	53.8	34.2	73.6
	II-3*	117.9	51.6	63.2	38.4	67.4
	III	129.5	54.6	55.6	33.7	71.7
	IV-1	141.8	64.7	48.1	29.1	84.2
Lignite	IV-2*	146.2	45.8	57.1	32.2	62.2
	V*	92.7	32.5	59.2	31.2	43.3

(1) $\text{Overall Plant Thermal Efficiency} = \dfrac{\text{Btu of product gas leaving plant}}{\text{Btu of raw coal fed to plant}}$

(2) $\text{Carbon Utilization} = \dfrac{\text{lb-mole of carbon in product gas}}{\text{lb-mole of carbon fed to the plant}}$

(3) 20-year average gas price based on Bituminous Coal at $4.0/ton and Lignite at $1.5/ton

* Raw coal (or Lignite) is fed to the gasifier for these processes, while for others coal must be pretreated prior to gasification.

water-gas shift reaction is needed in the process, the shift reaction should be carried out, if possible, before the coal gasification reaction so as to maximize the hydrogen-coal reaction in the gasifier, and minimize the methanation reaction needed to achieve pipeline quality.

6. In gasification processes requiring oxygen, the cost of the oxygen plant and the associated power generation plant is the largest portion of the total equipment cost; occupying roughly 40% of the total.

7. The equipment cost either for the gasification phase or for the gas purification phase seem to be the second largest item among the total equipment costs, depending on the alternate considered.

8. Gas prices with lignite feeds shown in Table S-1 are lower than that with bituminous coal feeds. However, more detailed study based on different ranks of coal and lignite should be made in order to draw a definite conclusion.

9. In view of the large exothermic heat of reaction produced in the methanation reactor, it is desirable to operate the methanator in a state of fluidization for rapid heat removal. Catalysts rugged enough to sustain attrition in fluidized beds and less sensitive to sulfur poisoning should be developed.

10. The technology of the solids feeding and removal systems to and from a high temperature and pressure gasifier has not been fully developed. Additional efforts are needed to devise operational and more economical solid feeders which can provide uniform distribution of coal in a large diameter gasifier without agglomeration.

The results presented above are an engineering estimate based on a number of simplifying assumptions and thus are subject to certain variations. Particularly, in view of the future development of new technology, some of the engineering problems which hinder an otherwise sound process may be solved, and could alter the economic picture of the process. However, it is believed that a measure of effectiveness of a number of coal gasification processes in relation to their costs has been established which will be useful in economic evaluation of future potential for the commercialization of the various alternates considered.

Chapter I. INTRODUCTION

TABLE OF CONTENTS

INTRODUCTION

West Virginia University, under contract to the Office of Coal Research, has been engaged in the study of Optimization of Coal Gasification Processes to determine those processes which hold more promise for potential economical development for the commercial production of a high-calorie-value pipeline gas.

Since coal gasification technology is so widely varied while time and financial resources are limited, the studies must be concentrated on the process or processes which present the most attractive commercial possibilities. Mathematical optimization techniques along with methodology of system analysis have been developed for use in optimizing various types of proposed processes and indicating the most advantageous among available choices.

The methodology of system analysis through simulation and optimization based on system models has in recent years become a key element in the programming, planning and budgeting of major governmental and industrial projects. Pipeline gas production from gasification of coal appears to require a comprehensive, long-range program which would include not only a more sophisticated energy conversion and product recovery technology than had hitherto been available, but also the integration of air and water pollution control, with land use planning and transportation system development.

In using optimization technique, a generalized economic standard method of comparison is established. Representative types of problems of fundamental importance to coal gasification processes are defined and identified. Information which relates to coal gasification available in the literature and from OCR contractors and other pertinent sources has been collected and classified. The various steps involving a specified process are studied and the contribution of that step to the economics of the process has been evaluated. The study identifies those steps having significant economic effect so that a more precise evaluation can be made of those problem areas which are most critical to the success or failure of the alternative or alternatives under consideration. This study also identifies all steps having negligible effect on the cost of the entire process so that such steps may be eliminated from further consideration. The study has indicated an area of serious deficiency in technical knowledge and information which are necessary for the sucessful application of the coal gasification schemes proposed.

Based upon the data and information collected and screened, necessary process and performance equations in terms of their restraining variables are determined or developed so that representative optimal solutions can be provided. Depending on the types and nature of the problems considered, an effective and efficient optimization technique is then selected and tested for the various processes. If existing techniques are inadequate, new techniques have been developed. Aside from the optimization techniques already developed at West Virginia University, emphasis has been made on the use of dynamic optimization methods including dynamic programming, linear programming, geometric programming and the maximum principle.

Whenever possible, the problems identified are treated from both deterministic and stochastic points of view. Computer programs are designed to determine the optimum operating conditions for the critical steps and paths of the various processes, optimal design of various systems, and policies of supply and types of coal considered.

This information is compiled in this report and the results interpreted in practical terms specifying characteristics of coal used, capital and operating costs of the plants as a whole, and of sections of such plants, including the necessary benefit/cost relationships. Thus, the most attractive alternatives or processes are recommended and those areas of coal gasification technology most likely to produce beneficial results through future experimental research and development are identified.

1. Classification of Coal Gasification Systems

The various gasification processes may be classified into the following phases:

(a) Coal Preparation and Pretreatment Phase

(b) Coal Gasification Phase

(c) Shift Conversion Phase

(d) Gas Purification Phase

(e) Methanation Phase

A general flow diagram of the coal gasification processes is presented in Figure 1-1. Although a number of coal gasification

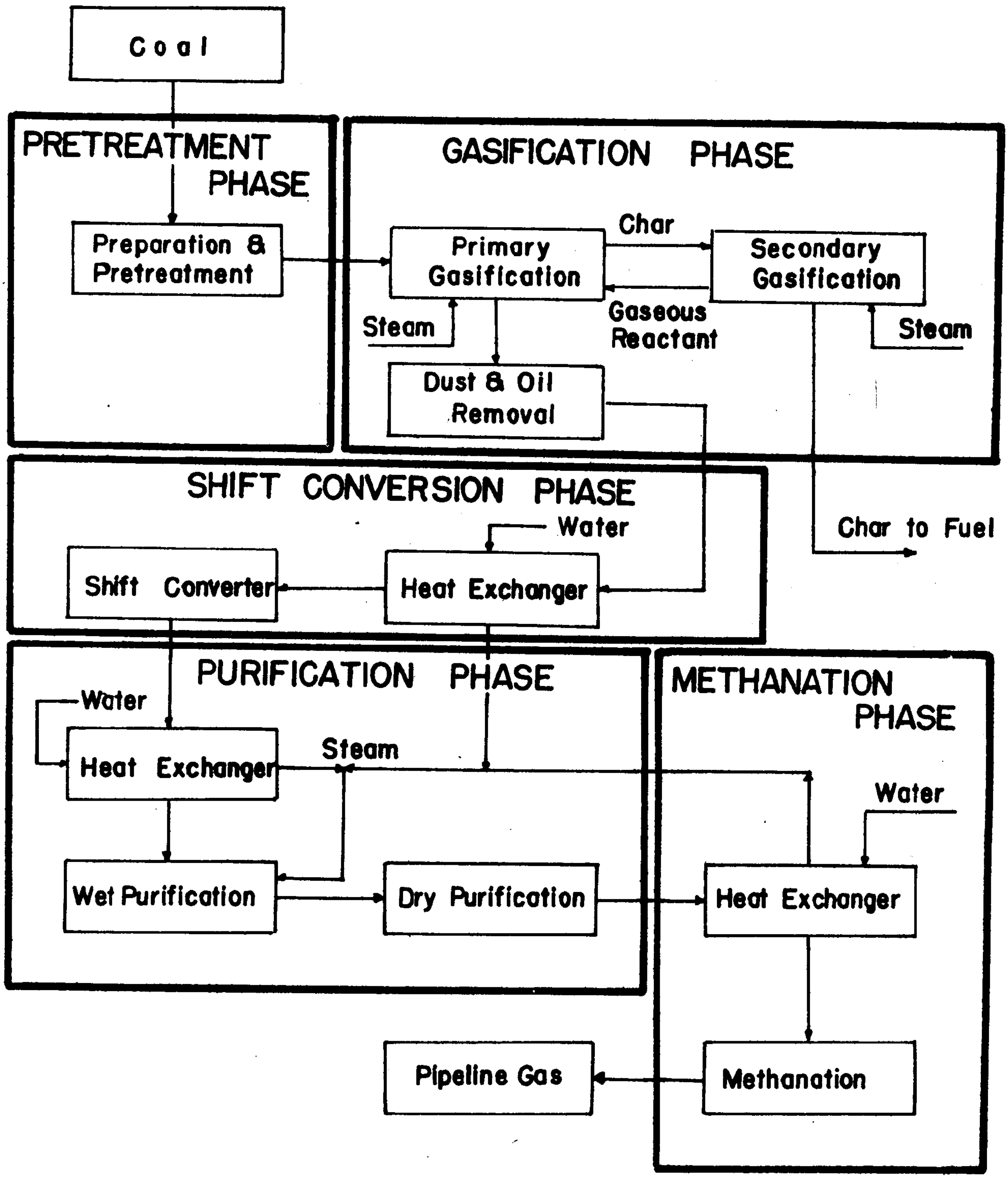

Figure I-1 General Flow Diagram of Coal Gasification Processes

processes to manufacture pipeline gas have been proposed and are under investigation either on a pilot plant scale or on a bench scale, it is believed that practically any of these schemes can be represented by the five phases shown in the diagram. Depending on the type of each individual process, naturally some phases may dominate others in terms of its size and cost, and will differ in detail; these five phases all involve similar process steps which are the essential and major subsystems of an overall pipeline gas plant from coal gasification.

This report will deal with each of the five phases presenting the pertinent technical information, examining the constraints and alternate processes, and formulating models for computer simulation and optimization. Each of the subsystems optimized is then integrated to arrive at an overall evaluation of the various gasification processes from which conclusions and specific recommendations regarding future research and development will be made. To achieve this goal, a methodology of systems analysis and optimization as described below is followed.[2]

2. Methodology of Systems Analysis and Optimization

A logic diagram illustrating the strategy of methodology to perform systems analysis and optimization is shown in Figure I-2. This methodology is applied to selected problems of coal gasification processes.

There are a number of alternative ways to gasify coal which are confronted with many problems of different magnitudes and scopes. Often the resources or

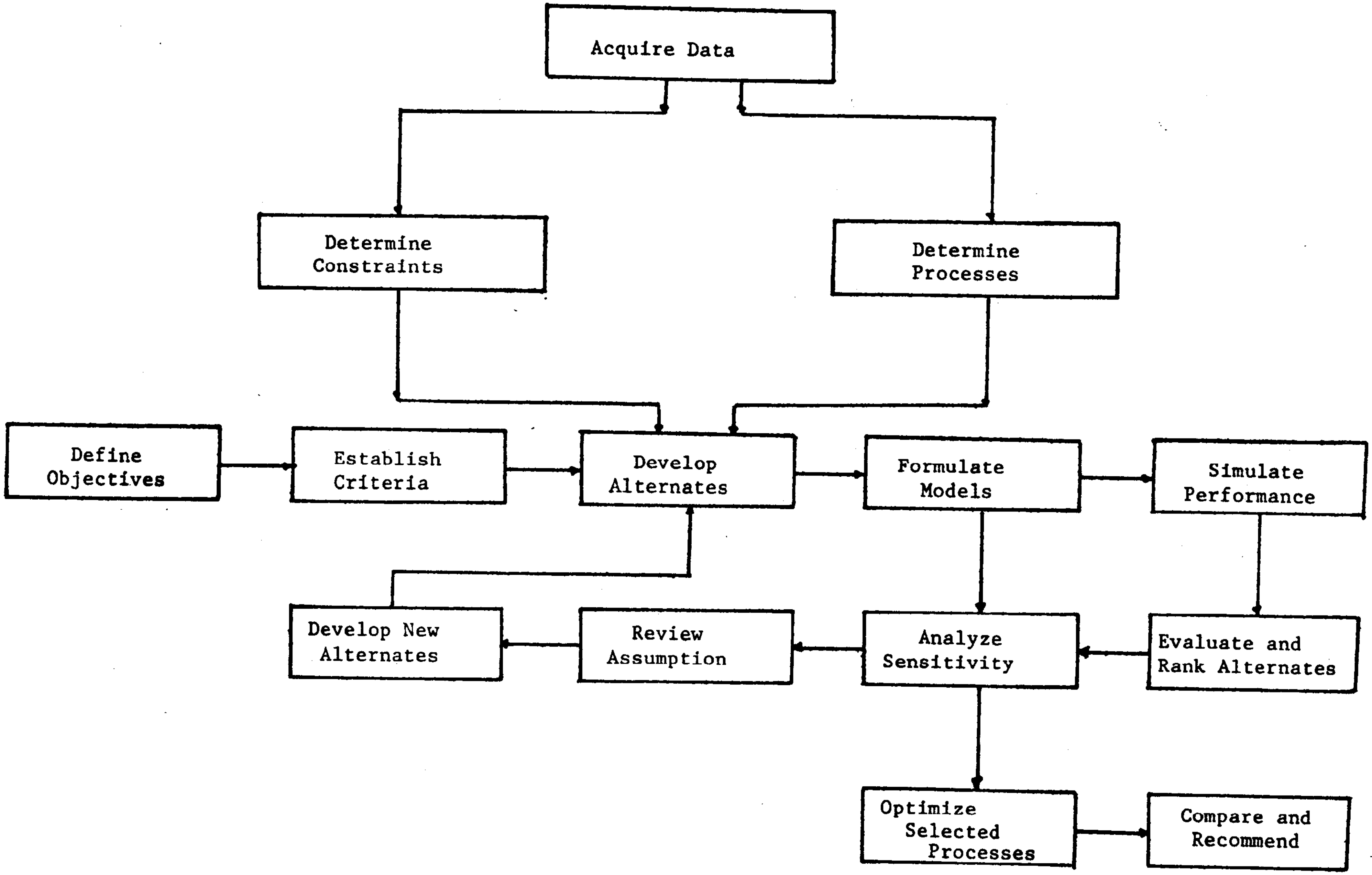

Figure I-2. Block Diagram of Methodology of System Analysis