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FORMULATION OF A HEURISTIC EVOLUTIONARY PROCEDURE FOR PRELIMINARY SELECTION OF ALTERNATIVE PROCESS STRUCTURES

by

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A THESIS

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FORMULATION OF A HEURISTIC EVOLUTIONARY PROCEDURE FOR PRELIMINARY SELECTION OF ALTERNATIVE PROCESS STRUCTURES

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University of Nebraska, 1986

Adviser: Luther D. Clements

This work formulates a heuristic-evolutionary procedure for the preliminary selection of competitive process structures from a set of initial structural alternatives. The selection procedure is organized as an optimization problem, with the single objective to maximize the profit generated by the process structure.

In order to approach optimum profit, topological modifications are performed to some of the initial process structures. These topological modifications are based on parametric analysis in terms of the independent variables of the material balance equations. In this way, a final set of improved process structures is obtained.

Two major assumptions are used in the proposed procedure: (1) in the initial design stage, structural changes have more impact on the optimization function than do parametric modifications of the design variables; and (2) the analysis of one process structure provides criteria to perform topological modifications on that structure in order to approach the optimun value for the objective function.

The optimization involved in the proposed procedure presents two main characteristics: (1) the search space is reduced by identifying bounds and constraints; and (2) the search of the optimum is guided by three targets: the net value of products (value of products minus cost of raw materials) (NVP), the energy cost (EC) and the capital cost (CC).

The proposed procedure has been applied to the production of benzene by hydrodealkylation of toluene. The application of this procedure shows that it is consistent and in fact leads to the selection of competitive alternative process structures for a given process system.

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CHAPTER ONE

INTRODUCTION

The design of a chemical or physical process system involves the selection of a basic design from a number of alternative process structures. This activity is known as the synthesis of processes. As a result of the synthesis activity, typically an enormous number of alternative process structures are generated. Each process structure is characterized by : (1) the type of operational units involved, (2) the interconnection between them, and, (3) the values of the design variables unique to a particular process structure for each one of the operational units.

A potentially overwhelming task is the selection among the set of alternative process structures to find the "best" process configuration. "Best" is usually associated with a set of optimum values for the design variables in order to achieve any of several objectives, such as: profitability, reliability, resiliency, safety and controllability. A preliminary selection or screening of the process structures should be made as early as possible in the design, in order to significantly reduce the number of candidates under consideration. As a consequence of this screening, only the most promising alternatives will undergo detailed examination.

Westerberg [1980], states that one of the major problems in process synthesis research is the lack of reliable methods to perform the selection of the most promising alternatives among a set of process structures. Currently, there are no publications available that explicitly address this problem.

The preliminary selection of alternative process structures can not be performed by rigorous algorithmic methods, since the restrictions in the available codes reduce the scope of these methods to only relatively small problems.

This work is devoted to the formulation of a procedure that makes use of some of the existing heuristic rules, organizing them into a hierarchical and evolutionary procedure. The proposed method provides preliminary selection of the most promising alternative process structures for a given process system. Also, it may be used to improve a single process structure. This new procedure is not intended to substitute for algorithmic methods in the final optimization of a given process structure, but instead it is to be used as a tool to provide good initial estimates for the application of the algorithms.

A bibliographical survey, presented in Chapter Two, reviews the main contributions to the synthesis of entire processes. Based upon analysis of the approaches taken in the literature, the principles underlying the procedure proposed in this work are established. Chapter Three presents the principles, characteristics, and the detailed formulation of the new

heuristic-evolutionary procedure. Chapter Four introduces an example problem which is used to demonstrate the application of the methodology proposed.

This thesis constitutes an initial step towards the development of a reliable method for preliminary selection among alternative process structures. The proposed procedure should be further checked and improved by its application to several more process systems.

CHAPTER TWO

LITERATURE REVIEW

2.1 INTRODUCTION

This chapter reviews the main contributions to the process synthesis area in the last ten years. The emphasis is on the use of synthesis in process systems engineering and development of problem-solving logic for the synthesis activity. Particular emphasis is given to works related to the evaluation and selection of alternative process structures in whole process synthesis.

There are several different methods in the literature for dealing with the synthesis of processes. However, these methods have not been evaluated relative to one another in order to determine their potential in the process synthesis procedure. Mostly, the methods represent isolated approaches to synthesis, rather than an overall, systematic methodological framework for the process synthesis activity. In this literature review, the author: (1) identifies fundamental concepts for the methodological decomposition of the synthesis procedure, (2) evaluates the methods grouped into two levels of strategy: general and specific, and (3) points out several of the main problems in the process synthesis procedure and, (4) formulates an approach to future research.

2.2 PROCESS SYNTHESIS AND PROCESS SYSTEMS ENGINEERING

Process synthesis is a relatively new area of study in process systems engineering. It is convenient to note the nature and content of process systems engineering in order to put process synthesis into context.

Process systems engineering is "an academic and technological field related to methodologies for Chemical Engineering decisions. Such methodologies should be responsible for indicating (1) how to plan, (2) how to design, (3) how to operate, and (4) how to control any kind of unit operation, chemical and other production processes and chemical industries themselves." [Takamatsu, 1983]. Consequently, the content of process systems engineering has been expanded from the design of unit operations to the design of chemical processes and the planning of large process systems, as well as from design problems to operation or manipulation problems. This expansion of mission, in turn, implies the treatment of much more complex problems.

In process systems engineering we may distinguish the following activities in time sequence: process development, process planning, basic design, detailed design and process improvements. Currently, process synthesis deals mainly with the basic design activity. [Umeda, 1983]

It is very difficult to state a definition for process synthesis, since there is a wide range of approaches to the subject. Different authors use the term "process synthesis" to

refer to different but complementary stages in the process of design. In the author's opinion, it is convenient to conceive of process synthesis as the discipline that systematically integrates the different stages in the development of a design, towards the goal of an optimum state for a given process system.

2.3 PROBLEM-SOLVING LOGIC DIMENSION FOR PROCESS SYNTHESIS

Process synthesis, as well as each of the mentioned time-sequenced activities in process systems engineering, can be defined in terms of steps in the problem-solving logical pathway: a) problem definition; b) selection of the value system; c) system synthesis; d) system analysis; e) optimization, and f) evaluation. [Umeda, 1983]

a) Problem definition is the study of the needs met by the system and the environment of the system. Complete problem definition requires that a process system be modeled. Mathematical models are commonly used to simulate or replicate a given process system. (For a review on mathematical models formulation, see Seider [1984])

b) The value system consists of a set of objectives to be accomplished and their relationship to each other. The value system provides the criteria to select the best possible solution. The most common objectives employed are:

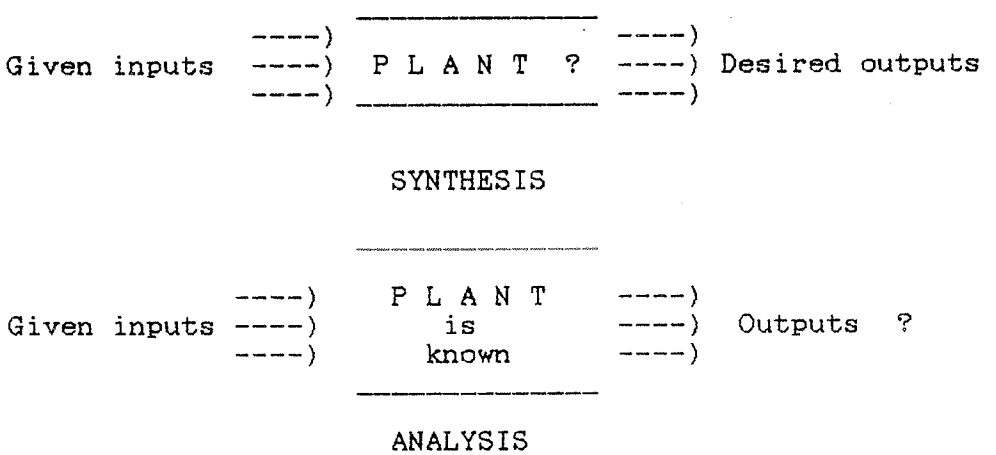
- maintainability and reliability, i.e., the ability to keep a specified production level for a certain period of operation;
- controllability and resiliency, or the adaptability to changes in internal and external or environmental conditions; and,
- economics, most typically referring to the minimization of operating and investment costs.

To achieve these multiple objectives, including the possible conflict between them, it is necessary to make decisions based upon multiple criteria. Therefore, the structural relationship of these objectives as they are related to the sequence of decision making must be determined. [Umeda, 1983]

c) The synthesis of processes is the inventive step: the outputs and inputs of the system are specified and the designer is called upon to identify the "black box" needed so that certain objectives are achieved. Consequently, a set of alternative process structures may be invented, all of which satisfy the process objectives to some degree.

d) The analysis of processes checks the performance of each of the structures generated by setting inputs and determining the corresponding outputs. (See Figure 2.1).

FIGURE 2.1: SYNTHESIS AND ANALYSIS OF PROCESSES



The analysis step is applied after the synthesis step to reduce the number of process structures evaluated.

e) Optimization consists of finding an optimum value for a given function. Process optimization will determine the "best" design and operating conditions for a given process system and value system. Before an optimum can be estimated, an optimization criterion has to be selected. For example, the yield of a product per unit volume of a reactor, or the minimum cost of product for a specified output, constitute optimization criteria. The objective function relates the optimization criterion to the dominant process parameters. The goal of the optimization, then, is to maximize or minimize the objective function by varying process parameters. [Kafarov, p.135] The problem of optimization occurs when a compromise is necessary between two or more process characteristics. The process variables must be balanced one against the other(s). (For example, the process efficiency may be balanced against throughput).

There are two general types of optimization problems: (1) dynamic optimization, that seeks to develop an optimum control system for the process; (2) static optimization, that tries to develop an optimum model for a process at steady state conditions. Currently, process synthesis deals mainly with steady state models.

Depending on the nature of the mathematical models chosen, different methods of mathematical optimization may be used. (For a comprehensive review of optimization methods in process systems engineering see Beveridge and Schechter [1970].

f) The evaluation step of the problem-solving procedure analyzes the consequences of the optimization procedure and

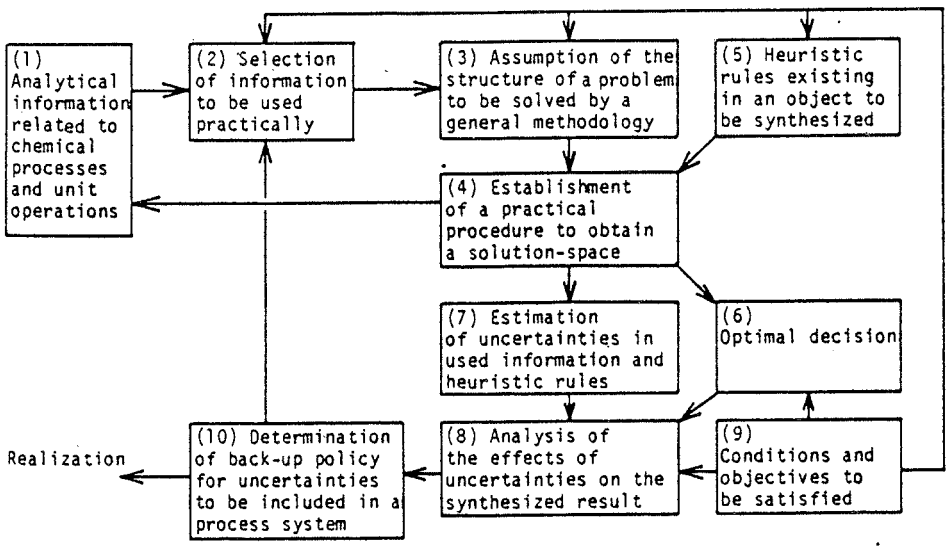
combines those results according to the decision rules prescribed by the value system.

2.4 FUNDAMENTAL CONCEPTS FOR THE METHODOLOGICAL DECOMPOSITION IN THE PROCESS SYNTHESIS PROCEDURE

2.4.1 INTERACTION BETWEEN DIFFERENT STEPS OF THE PROBLEM-SOLVING LOGIC DIMENSION IN PROCESS SYNTHESIS

Takamatsu [1983], conceives the process synthesis procedure not as a simple sequence of logical steps, but as a set of elements in interaction. Figure 2.2 describes this approach. It is clear from the figure, that in order to reach an optimum design, different aspects have to be considered simultaneously and/or in relation to each other. In particular, it is important to recognize the interrelationship between systems synthesis, systems analysis, and optimization. On the other hand, it is necessary to consider the role of heuristic methods and the evaluation of uncertainties introduced by heuristics, thermodynamic models, mathematical models and other factors. This interactive relationship between all these elements, is a fundamental characteristic of the synthesis procedure that many authors ignore.

FIGURE 2.2: PROBLEM-SOLVING LOGIC DIMENSION OF PROCESS SYNTHESIS (Takamatsu, 1983)



2.4.2 OPERATIONAL SPACES IN SYSTEMS SYNTHESIS

As mentioned before, process synthesis compiles or invents a set of alternative process structures. It is desirable to select the "best" process structure or configuration that satisfies the given value system. The synthesis of an optimum operational system involves decisions in two different spaces:

(1) The space of distinct structural alternatives defined by the topology and the nature of the interacting units.

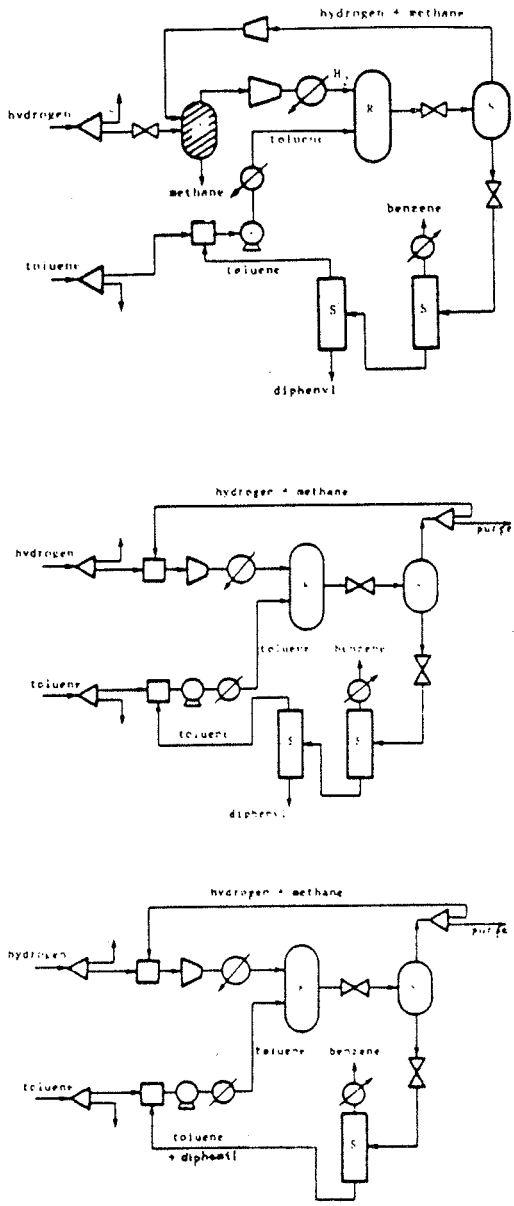
(2) The space of alternative designs for the operating modules or units composing the system.

The term topology refers to the interconnection between particular units so as to configure a structural alternative. The topology does not necessarily include design calculations for individual units or detailed material and energy balances.

As an example, Figure 2.3 presents three different structural alternatives for the production of benzene by hydro-dealkylation of toluene. During the basic design stage, it is common practice to generate an enormous number of structural alternatives by using all the possible combinations between the main units in the process. This leads to a combinatorial problem. Westerberg [1980], states that the appropriate formulation of the synthesis problem should be rich enough to include all of the interesting alternatives, but lean enough to exclude all of the unattractive ones. It is a major challenge to the designer to use appropriate methods to reduce the number of structural alternatives without excluding attractive solutions.

In the optimum process structure the corresponding units have to be optimally designed. The feasible set of allowable designs is usually continuous and relatively "easy" to determine by checking against equality and inequality constraints. [Stephanopoulos, 1981] In general, algorithmic optimization methods have been succesfully used in the optimization of single units, but no comprehensive study is available that provides

FIGURE 2.3 : DIFFERENT STRUCTURAL ALTERNATIVES FOR THE PRODUCTION OF BENZENE BY HYDRODEALKYLATION OF TOLUENE (Lu and Motard, 1985)



criteria to better select algorithmic methods for a given problem. Some important criteria for the selection of algorithms are: ease of representing the problem, accuracy of results, stability of the method and computing time.
(Details about the methodology used in both spaces is presented in Section 2.6)

2.4.3 PROCESS SYNTHESIS DESCRIBED AS A "MAPPING PROBLEM"

Stephanopoulos [1981], made an important contribution by formalizing process synthesis as a mapping problem. This conception provides, in the author's opinion, the best basis for the systematization of process synthesis procedures, since it provides criteria to decompose the synthesis problem into several sub-problems without compromising the validity of the results for the whole process synthesis.

Given a set of input conditions (such as flow rate, composition, pressure, temperature and other state indicators), by means of a transformation function the input set can be mapped into a desired output set. The successive mappings which define the complete process should go only through permissible states defined by the set of allowable operating units (reactors, separators, etc), and the valid interactions among them. Evidently, the final transformation function is going to be the process structure that produces the expected output set from the given input set.

Consider the mapping M, i.e.:

M i : S input --> S output

where "S input" and "S output" are the spaces of the available inputs (raw materials, energy, etc.) and of desired outputs, respectively. Each mapping is characterized by:

M i = { U i , T i }

where: U i is the set of operating units, and
T i represents the topology of the units' interconnections.

A given map attempts to reconcile the differences between the available inputs (sources) and the desired outputs (sinks) by introducing feasible operators. In Table 2.1 these differences are listed with the corresponding unit process operators that eliminate them.

TABLE 2.1: MAPPING DIFFERENCES AND CORRESPONDING OPERATORS

DIFFERENCES	OPERATORS
In the chemical species	reactor
In the compositions	separator
In the quantities	mixer/splitter
In the pressures	pump (compr.)/valve
In the temperatures	heat exchanger
In the enthalpies	phase indicator

Each of the operators in the table belongs to a different discrete space. Therefore, since the conformal mapping is given by the relations among a particular set of operators, the following "decomposition principle" may be stated:

"The inductive construction of a conformal mapping using operators from disjoint spaces, may proceed at various distinct levels independently of the order they are considered." This is true, provided that the intercon-

nection structure T i, which acts as the interface between two succesive levels is allowed to change completely. [Stephanopoulos, 1981]

Based on this principle, the synthesis problem has been decomposed by several authors [Mahalec & Motard, 1977; Rudd, Powers & Siirola,1971; Umeda, Shindo & Ichikawa, 1974; etc], into a series of synthesis subproblems, such as:

. synthesis of reaction paths,
. synthesis of reactor networks,
. synthesis of species allocation,
. synthesis of separation sequences, and
. synthesis of energy exchange networks.

For a dynamic process, additional sub-problems to be considered are:

. synthesis of process control structures, and
. synthesis of safety systems.

2.5 THE SYNTHESIS SUB-PROBLEMS

In this section each of the synthesis sub-problems is briefly defined. For more detailed information see the reviews by Westerberg [1980], Nishida, Stephanopoulos and Westerberg [1981], and Stephanopoulos [1981].

2.5.1 ALLOCATION OF SPECIES

The synthesis of processes proceeds through different levels of complexity, progressing towards more elaborate alternatives at each level. It is important to state that the allocation of species is one of the first steps in that procedure, since the resolution of the species allocation will

determine, to a large extent, the configuration of the process structure. The mapping concept has been extensively applied to this synthesis subproblem.

The synthesis of species allocation attempts to coordinate the "sources" and the "sinks" of the species so as to minimize the cost of the resulting process structure. Pioneering works in this field are the AIDES system [Siirola, Powers and Rudd,-1971], and the BALTAZAR system [Mahalec and Motard,1977]. Johns and Romero [1979], developed a flowsheet generator which combined the elements of dynamic programming and branch and bound techniques. By applying algebraic mappings Friedler, Blicke, Gyenis and Tarjan [1981], reported the generation of technological structures represented by petrigraphs.

Recently, Lu and Motard [1985] published a procedure for "computer-aided total flowsheet synthesis", using an heuristic--evolutionary approach, claiming the rapid generation of good process alternatives. Lu and Motard, justify the use of the heuristic-evolutionary procedure as a means of coping with the large dimensionality and the discrete structural characteristics of the total flowsheet synthesis problem. In the Lu and Motard method the matches between sources and goals are made using linear programming. Additionally, artificial intelligence principles have been applied: hierarchical planning, ruled-based production system and backtracking control.

The work in the species allocation synthesis is just starting. A main restriction in the published research works is the relatively small size of the problems that can be

synthetized. All of the systems noted above are interactive and require arbitrary assignments to orient the search. None of the approaches consider equipment sizing nor energy integration. The main objection to the available species allocation procedures is that there are no clear ways to reduce the space of structural alternatives without risking the elimination of good process structures.

2.5.2 SYNTHESIS OF REACTION PATHS

The synthesis of reaction paths attempts to find a sequence of reactions which can be used to reach a given target molecule from available raw materials. Typical objectives in reactor path synthesis are to minimize the cost of the resulting processing system, to minimize the number of required reaction steps, to maximize the conversion yields and to maximize the use of starting raw materials.

Westerberg [1980], noted that the reaction path synthesis has problems with the representation and evaluation of alternative reaction paths. The evaluation procedure is most difficult since comparison of reaction rates should be added to the thermodynamic analysis. Calusaru and Volanski [1986] address the representation of reaction paths by expressing chemical structures and reactions in matrix form. Such representation offers the advantage of performing the synthesis with the aid of computer.

Rotstein, Resasco and Stephanopoulos [1982], propose a procedure for the creation and evaluation of alternative

reaction paths guiding the search by the analysis of the Gibbs free energy and temperature space. Stephanopoulos and Townsend [1985] suggest that the search space for the reaction synthesis is conformed by: the standard Gibbs free energy change, the heat of reaction, the stoichiometry, the temperature, the pressure, the kinetics and the cost of the chemicals involved. Furthermore, they analyze the methodologies used in reaction path synthesis, i.e.: topology of the search space and pattern recognition, targeting and evolutionary procedures, and knowledge-based expert systems.

2.5.3 SYNTHESIS OF REACTOR NETWORKS

The synthesis of reactor networks pursues the optimal reactor configuration. This involves the definition of the types of reactors to be used (batch, CSTR's, tubular, fluidized bed, etc), the number of them and their connections. The main objectives are to minimize the venture cost and maximize the yield. Nishida et al. [1981], point out that very little has been done in the area of reactor network synthesis, and that it is necessary to develop the theory and heuristic rules for the synthesis of reactors with recycle and heat integration considering various reaction schemes. Conti and Paterson [1985] propose a heuristic procedure to synthetize reactor networks coupled with separation systems. Nevertheless, more work is needed in the synthesis of reactor networks.

2.5.4 SYNTHESIS OF SEPARATION SEQUENCES

The synthesis of separation sequences determines the minimum cost process to isolate the specified products from feed stream(s) of known composition, flow rate(s), temperature and pressure. The separation system synthesis results to date have dealt primarily with systems of simple, sharp separators. Still to be studied is the transformation of several source mixtures into a different set of product mixtures. [Nishida et al, 1981]

An area of increasing interest is the synthesis of distillation sequences with heat integration. The goal is to find thermally coupled distillation sequences which incorporate maximum energy conservation. It is necessary to match the heat sinks (reboilers) and the heat sources (condensers), while selecting a distillation sequence to accomplish the separation task. Andrecovich and Westerberg [1985], used a mixed integer linear programming formulation for this problem. Shankar [1985] developed a heuristic strategy to synthetize heat integrated distillation sequences. More work, though, is still needed.

2.5.5 SYNTHESIS OF ENERGY TRANSFER NETWORKS

In the synthesis of energy transfer networks, the problem is to find the minimum cost energy recovery network within a process using operations such as heat exchange, expansion, compression and/or use of refrigerants for cooling. Linhoff and Townsend [1982] and Papoulis and Grossmann [1983 a,b] made important contributions. But the research is just starting.

The synthesis of heat exchanger networks has its objective the invention of a network of heat exchangers that minimizes the energy consumption and the capital cost of the installation. Since this synthesis task deals only with heat exchangers, it is a sub-problem of the synthesis of energy transfer networks. The techniques for the synthesis of heat exchanger networks have reached a mature stage and a number of publications are available. The successful applications of heat exchanger network synthesis are due to a profound understanding of the problem.

The heat exchanger network synthesis problem has been decomposed in three major steps: (1) Pre-analysis to set targets and limitations; (2) network invention; and (3) evolution [Stephanopoulos, 1981]. Typical targets are the minimum utility consumption (energy target), the minimum number of units to be used and the minimum heat transfer area (capital targets). The network invention techniques have an appropriate representation (grid diagram) and design rules to use as a basis for this development. The design rules are: problem decomposition (about the pinch point), heat interchange options and design constraints, ticking off streams and utility placement. [Linhoff and Turner, 1981]

Step (1) restricts the search space. The evaluation of the network developed in Step (2) provides an indicator for identifying the remaining potential for improvements. Any further evolution performed in Step (3), will depend on that potential.

The thermodynamic analysis principles, upon which the heat integration techniques are based, are being extended to further applications, such as distillation trains. [Linhoff & Vredeveld, 1984; Boland & Hindmarsh, 1984]

2.5.6 SYNTHESIS OF CONTROL AND SAFETY SYSTEMS

The synthesis of control systems develops a control structure by selecting controlled and manipulated variables and pairing them, so as to satisfy control objectives. The objective of this synthesis problem is to minimize some static or dynamic performance indices by the controlled system. Among the possible performance indices there are: steady state errors, speed of transient response, smoothness of response, degree of interactions among the loops, and range of operability.

The synthesis of safety systems is intended to define a structure of measuring elements and of manipulated variables such that the likelihood that the state of the process is in a prohibited space is smaller than a predefined lower bound.

2.6 STRATEGIES FOR THE SYNTHESIS OF PROCESSES

There are a variety of methods or strategies which have been attempted to achieve the general objective of process synthesis, which is an optimum process design. However, as Takamatsu mentions [1983], the characteristics of the optimally synthetized results have not yet been summarized conveniently so that the synthesis methods may be used easily and practically.

In fact, throughout this literature survey, it can be observed that each approach remains as an isolated opinion, since the different proposed methods have not been evaluated in relation to each other in order to determine their relative effectiveness as process synthesis procedures.

This section presents only what the author considers the most important contributions in the area of whole process synthesis. The strategies are grouped into two categories: general and specific. Under general strategies a rigorous statement of the process synthesis problem is presented, the most commonly used simplifying assumptions in the synthesis procedure are reviewed, followed by a description of the search strategies employed in process synthesis. The most important approaches to process synthesis are presented as specific strategies.

2.6.1 GENERAL STRATEGIES

2.6.1.1 PROCESS SYNTHESIS AS A MULTI-OBJECTIVE MIXED-INTEGER NON-LINEAR OPTIMIZATION PROBLEM

The synthesis of complete processes is an overwhelming task that seeks to develop an entire process configuration for converting available raw materials into desired products. Several objectives must be satisfied in order to obtain a realistic solution for the synthesis. Consequently, a multi-objective value system has to be defined.

Since several structural alternatives are generated during the synthesis procedure, an optimization procedure has to be implemented to reduce the number of structures considered in

detail. The topology of the units' interconnections may be handled by integer programming. The optimization of the operating units can be treated by non-linear programming techniques. Therefore, this approach to the synthesis of processes leads to a multiobjective, mixed-integer, non-linear optimization problem. [Grossmann and Santibanez, 1980]. However, the solution of such a problem formulation is still not possible with the available techniques. It is necessary to introduce some simplifying assumptions.

2.6.1.2 COMMON SIMPLIFYING ASSUMPTIONS FOR THE OPTIMIZATION PROCEDURE

1) Assume a simple value system.
2) Use only the most significant design variables.
3) Estimate the range of variation for each design variable.
4) Work only with a few discrete values within the chosen intervals of the continuous design variables.

1) The value system, usually is simplified in one of the following ways:

- Consider a dominant objective as the only one and express the remaining objectives as inequality constraints.
- Construct a composite scalar objective function, assigning appropriate weighting factors to the different objectives.
- Decompose the process design into a series of sub-problems.

Each sub-problem should be solved so that a corresponding objective is achieved. Then, the relationship among the objectives has to be determined and the possible contradictions resolved.

2) A general methodology to define the most significant variables for a given design task is not available. Fisher, Doherty and Douglas [1985], classify the design variables as "process flow optimization variables" and "unit optimization variables". A process flow optimization is defined as the optimization of a variable that has a significant impact on the input and output flowrates or the recycle flowrates. In general, these variables will also affect the capital and operating costs of each piece of equipment. On the other hand, the unit optimizations affect the design only of single pieces of equipment.

For example, for petrochemical processes the common design variables corresponding to each category are:

- Process flow optimization variables: reactor conversion, reactor temperature, reactor pressure, molar ratio of reactants at reactor inlet and purge composition.
- Unit optimization variables: reflux ratio in distillation columns, solvent flowrate in gas absorbers, fractional recovery in distillation columns or gas absorbers, approach temperature in heat exchanger networks, flash drum temperature, flash drum pressure and distillation column pressure.

There are no reliable heuristic rules to initialize the process flow optimization variables. On the other hand, the unit optimization variables can be specified using well-known rules of thumb. Fisher et al. [1985], developed an economic analysis procedure using simplified cost models to specify which of these variables has a significant effect on the economic optimization of the given process structure.

2) Degree of completeness:
   . Work only with completely synthetized systems.
   . Allow for partially developed configurations with variable degrees of detail.
3) Methodology used:
   . Algorithmic methods.
   . Heuristic methods.
   . Hybrid methods. [Stephanopoulos, 1981]

What follows is a brief analysis of each of these search strategies.

1) At the first level it is usually better to work only with the attractive alternatives. There are three ways to reduce the space of structural alternatives: (a) using branch and bound techniques; (b) using heuristics; and (c) using an evolutionary approach combined with either of the remaining two. The branch and bound algorithm is the most widely used method for solving both integer and mixed integer programming problems in practice. (For more details about this method, see Phillips, Ravindran and Solberg [1976]).

The term heuristics refers to empirical rules or prescriptions. "Inductive" heuristics are those resulting from past experience. For example, the optimum ratio of the actual reflux ratio to the minimum one in a distillation column is aproximately 1.2. On the other hand, "analytical" heuristics are the ones developed from simplifying analysis of physico-chemical phenomena; for example, the heuristics applied in the synthesis of heat exchanger networks are derived from a "second law" analysis.

2) At the second level, to work with partially developed configurations requires fewer computations, but the decisions made early may lead to conflicts later as the process structure

is being completed. It might be more apropriate to use the so called "evolutionary method", which works initially with simple process structures and proceeds through several stages, progressively more complex, in order to configure a detailed process structure.

3) At the third level, the rigorousness that the algorithmic methods offer has to be evaluated against the simplicity of the heuristics. Many times a hybrid approach is more convenient, if it appropriately combines the advantages of algorithms and heuristics.

The algorithmic methods most often used in process synthesis are: mathematical programming techniques, non-linear search techniques and multilevel optimization techniques. The most commonly used mathematical programming techniques are: linear programming, non-linear programming (quadratic programming, geometric programming, etc), dynamic programming and mixed-integer linear programming. The main non-linear optimization techniques are: direct search methods (Powell's method), gradient search methods (steepest descent, Newton's, Davidson's, etc.), and constrained optimization methods (Rosenbrock's method) [Box, Davies, and Swann, 1969]. The multi-level optimization technique requires the construction of a unified network which includes all imaginable process structures. Evidently, this procedure is restricted to relatively small problems. (The MILP method presented in the following section is a multi-level technique.)

2.6.2 SPECIFIC STRATEGIES

2.6.2.1 SYSTEMS SYNTHESIS AS A SINGLE OBJECTIVE OPTIMIZATION PROBLEM

Grossmann [1985], states the synthesis of integrated process structures (conformed by utility systems, heat recovery networks and processing system), as a single-objective, mixed integer linear programming (MILP) optimization problem, thus simplifying the multi-objective, mixed integer, non-linear programming model. As a multi-level technique, MILP has the ability to evaluate several structural alternatives at the same time. However, with MILP the optimality of the solutions can only be guaranteed with respect to the alternatives that have been considered in the problem representation. There may be other, better process structures which were not included in the set of alternatives considered. The major features of this formulation are:

- Structure and parameter optimization can be performed simultaneously.
- Discrete and logical constraints can be handled explicitly.
- A variety of different synthesis problems can be formulated with the same mathematical tool.

The main restriction on the MILP formulation is the relatively small size problems that the existing computer codes can handle. Therefore, it is essential to efficiently represent process systems while using the MILP technique. An interesting conclusion of Grossmann's work is that a mathemati-

cally valid decomposition of the integrated MILP model might also lead to near optimal solutions. Representation, as used here, is an image in which a set of variables are correlated against another set of variable(s) in order to find specific trends between them.

2.6.2.2 USE OF HEURISTICS AND THERMODYNAMIC TARGETS TO COMPLEMENT ALGORITHMIC METHODS

Grossmann [1985], proposes to combine heuristics, thermodynamic targets and algorithmic methods in order to cope with the synthesis problem. Heuristics can be used to eliminate alternatives that are not promising and to generate good initial estimates for the application of algorithmic models. Thermodynamic targets can be used to develop bounds or representations, that will eliminate from consideration, energy inefficient alternatives. Algorithmic methods can be used to automatically generate integrated flowsheets in which the interactions and finer modelling points are taken fully into account.

Umeda [1983], also recommends the use of an exergy analysis in the synthesis procedure to determine energy bounds for particular units. Previously, material and energy balances have had to be developed.

This author, Takamatsu [1983], and Stephanopoulos [1981], recognize the evolutionary methods as the most useful for the synthesis of processes. Umeda, recommends developing allocation procedures which focus on the material recycle streams. For that purpose he developed the following heuristic rules:

1) Direct recycling should be at the earliest possible step in a process.
2) Wastes should be taken out at the earliest possible step in a process.
3) When a solvent is used, it should be recovered at the earliest possible step in a process.

This set of rules is based on the principle that the value of a stream increases every time it passes through a unit because energy is invested at the unit. In addition, recycling streams is often justified economically.

Takamatsu [1983], points out a number of problems in using heuristic rules for the screening of process alternatives. These problems include: 1) how to develop a method in which some heuristics may be easily introducible; 2) what kind of heuristic rules should be effectively extracted to combine with a general methodology, and (3) how to optimally combine a general methodology and its set of heuristic rules.

2.6.2.3 USE OF HEURISTICS AND HIERARCHICAL PLANNING

Lu and Motard [1985], and Douglas [1985], addressed Takamatsu's questions by using an evolutionary procedure based on the application of heuristics and oriented by hierarchical planning. The first work is devoted to the species allocation problem, while the second proposes a methodology to synthetize and preliminarily optimize a given base-case process structure.

Lu and Motard's approach suggests the designer first develop the material balance and then the energy balance. Lu and Motard then rank the stream descriptors in the following hierarchy: species, composition, quantity, enthalpy and pres-

sure. Only the first three properties will be considered initially.

Douglas' procedure is restricted to single product plants that handle fluids under continuous operation. He approaches the synthesis of processes by decomposing the design problem into the following hierarchy of decisions:

Level 1: Batch vs. continuous.
Level 2: Input-output structure of the flowsheet.
Level 3: Recycle structure of the flowsheet and reactor considerations.
Level 4: Separation system specification
a: Vapor recovery system
b: Liquid recovery system
Level 5: Heat exchanger network.

Actually, Level 1 assumes only continuous operation. Level 2 is defined by the assignment of the feed streams, product and by-products streams, and waste streams. In Level 2 the "economic potential" is equivalent to the net value of the streams. That is, the economic potential is the value of the product and by-product streams minus the cost of raw materials. The economic potential, which is evaluated in terms of gas recycle and purge stream rates, is used to define a region of profitable operating conditions. In Level 3, the economic potential includes the reactor and compressor (if any) costs, and their corresponding operating costs. The compressor is used when a gas recycle stream exists. Additionally, in Level 4a, the economic potential includes the cost of the gas separation system (if any) and/or the cost of valuable material lost in the purge. Level 4b subtracts from the economic potential the capital and operating costs of the liquid separation system. Finally, in Level 5 heat integration is performed to reduce the

energy consumption. Douglas [1985], claims that the above hierarchical decision procedure should lead to a reasonable process flowsheet and a base-case design.

The disadvantage of the hierarchical procedure proposed by Douglas is that it just leads to a single base case, but it does not explore alternative structures. Douglas and Woodcock [1985], propose the use of "cost diagrams" to infer structural modifications of a given process system and also to identify the significant design variables. In the cost diagram each equipment item is represented by a box in which the annualized installed cost is listed; and, the annual operating costs are attached to the stream lines.

But, the use of cost diagrams, according to Douglas and Woodcock, is useful just for getting some "feeling" for the economic incentive for evaluating various alternatives in more detail. Consequently, the cost diagram technique does not provide a reliable procedure to explore several structural alternatives for a given process system.

2.6.2.4 CONSIDER SEPARATION AND REACTOR STRUCTURE IN CONTEXT

Douglas, Malone and Doherty [1985], state that the selection of the separation system for a process is coupled to the determination of the optimum process flow rates. In addition, Conti and Paterson [1985], state that reactors must be designed along with the flowsheet and not as isolated units. They show that designing the reactor for maximizing the product yield does not necessarily lead to an optimum solution because of the

important effect of the separation system on the objective function that contradicts the trend followed by the reactor units.

Conti and Paterson use a "procedural approach" to generate a near optimal process structure. This approach allows us to take the decisions for design in a sequential fashion; instead of simultaneously.

The procedural approach can be described as follows:

1. Develop a base case design using the following heuristics sequentially:
1.1 Minimize process complexity in order to reduce the capital costs for the whole flowsheet. Target: minimum number of units.
1.2 Maximize process yield. The target is the reactor configuration and the conversion which leads to the maximum reactor system selectivity. This is justified because the raw material costs typically dominate the economics.
1.3 Minimize the separation cost. Use the separation sequence which minimizes the total heat load.
2. Evolution from the base case. The heuristics are relaxed in reverse order.
2.1 Find the lowest cost distillation sequence for a range of reactor conversions near that of the base case.
2.2 Keep the reactor structure found in step (1.2) and optimize the conversion.
2.3 Increase process complexity by changing the reactor structure and/or allowing recycle of waste product(s).

2.6.2.5 USE OF THERMODYNAMIC ANALYSIS

Alternatively, the use of thermodynamic analysis has been extended to the optimization of entire processes. Linhoff and Vredeveld [1984], propose the use of the pinch point concept to design process systems having as their objective the minimization of energy consumption. For this purpose, Linhoff and Vredeveld represent independently the hot process streams (to be

cooled) and the cold process streams (to be heated) in a temperature-enthalpy diagram corresponding to a given process structure and operating conditions. These curves are called the hot and cold composite, respectively. From the temperature-enthalpy diagram, a "pinch point" is identifiable. The "pinch point" or simply "pinch" is the temperature at which the heat flow in the system is zero. [Linhoff and Turner, 1981] The changes in the material and energy balances of the process that would benefit the energy target are:

. To increase the hot stream duty above the pinch.
. To decrease the cold stream duty above the pinch.
. To decrease the hot stream duty below the pinch.
. To increase the cold stream duty below the pinch.

Changing temperatures rather than duties about the pinch would also benefit the energy target. Therefore, it is recommended:

. To shift hot streams from below the pinch to above.
. To shift cold streams from above the pinch to below.

Boland and Hindmarsh [1984], claim to have a structural procedure to cope with total energy synthesis. They divide the process system in three sub-systems: power system, distillation system and background process. Each of these sub-systems has a pinch point and characteristic composite curves that are represented on the temperature-enthalpy diagram.

The power system heat acceptance and heat rejection profiles can be altered either by changes in operating conditions or by choice of thermodynamic cycle. The shape of the distillation system heat acceptance and heat rejection profiles can be manipulated by changes in individual column pressures. The background process consists of all streams not considered

in the power or distillation sub-systems. The thermodynamic analysis establishes the pinch location and the utility requirements above and below the pinch. To perform an overall energy integration, the pinch point and composite curves for each sub-system have to be identified. Then, the sub-systems are matched together (modifying their composite curves for that purpose), so as to reduce the utility demand.

2.6.2.6 DEVELOPMENT OF ANALYTICAL INSIGHTS AND EXPERT SYSTEMS

Stephanopoulos [1985], indicates that due to the high complexity of the synthesis problem and because of the lack of useful general theoretical results, the synthesis of processes issues have been addressed and resolved through empirical, unsystematic procedures. Stephanopoulos proposes to proceed through two complementary directions: (1) to generate new analytical tools that would guide the screening of large sets of unattractive process alternatives and establish achievable targets for the process being developed; and, (2) to systematize the existing knowledge. The thermodynamic analysis of processes constitutes one step in the first direction and the development of expert systems points in the complementary direction.

The expert systems are conformed by a set of "production rules", called the "knowledge base", and an "inference engine" that executes the rules. It is very important to find appropriate methods for representing expert knowledge.

A first expert system in process design could be aimed at minimizing design errors by checking inconsistencies in the

assumptions and constraints governing each step. The next step could be a "constraint-satisfying" expert system that manipulates the process parameters in an attempt to satisfy constraints. A more ambitious system might be able to investigate structured as well as parametric modifications. An improved system should be able to consider optimization tasks. [Hart, 1984]

The major disadvantage of expert systems is that they are expensive and therefore their use is most easily justified for tasks that are performed repeatedly. Westerberg [1984], states that the synthesis problems are combinatorial and if they are precisely defined, they should be attacked by other means.

Umeda [1983], characterizes the fifth generation computers' configuration as a knowledge base management system, a problem solving and inference system, and an intelligent interface system. Such computers would face appropriately the multi-objective synthesis problem. In fact, the first generation of expert systems are in the developing stage. [Chowdbury, 1985]

2.7 PERSPECTIVES FOR FUTURE RESEARCH IN PROCESS SYNTHESIS

From the above literature survey it is clear that the synthesis of entire processes is in a very early stage of development. Whole process synthesis can be stated formally as a multi-objective, mixed-integer, non-linear programming problem, but most of the research done so far reduces the synthesis to a single-objective problem.

There have been several proposed procedures to automatically generate structural alternatives. Most of them screen the structural alternatives based on heuristic rules, but these rules have not been sufficiently proved to be used with confidence. Therefore, the major problem in process synthesis is to find appropriate methods to screen among a set of structural alternatives and reduce the number of alternatives to get only the most promising ones.

Most of the authors agree that the generation of structural alternatives can be treated as an evolutionary procedure, oriented by heuristics, in which a hierarchy of decisions is solved. The general hierarchy is synthesis of the reaction path, followed by the species allocation. Then the reactor(s) configuration and the separation sequencing have to be defined. Later, finer details should be added to the topological structure. A serious problem is how to detect when a decision at a certain level in the evolutionary procedure is going to negatively affect decisions at a later stage.

Once a set of structural alternatives has been identified, the analysis of processes is suggested as the tool that can lead to a better understanding of the phenomena involved and, hopefully, to validate heuristics for the evaluation of these alternatives. This expectation is motivated by the success of the thermodynamic analysis in heat integration and distillation sequencing.

The optimization of an entire process mainly involves the topology of the given process, particularly if energy integra-

tion is considered. The individual optimizations of the equipment items often provide only a marginal improvement within a given process.

Once some topological structures have been optimized with respect to an economic objective function, considering also safety bounds as constraints, other objectives such as operability, reliability, or controllability should be incorporated in order to end up with a "workable" system. However, there is no agreement on how to implement the multi-objective formulation.

Two basic elements of process synthesis applied to entire processes have not been treated sufficiently in the existing literature. They are:

. The only representation available for the synthesis of entire processes traditionally is the "flow diagram". In the author's opinion, such a representation is not sufficient for the ambitious task of synthetizing entire processes. For the systematization of the enormous amount of information generated in the synthesis procedure, it is necessary to develop substitute or complementary forms of representation.

. The thermodynamic analysis has been used to set boundaries that allow the identification of energy inefficient process structures. However, other type of bounds should be incorporated to the synthesis procedure, to reduce the searching space of the structural alternatives, for example, the maximum net value of products.

CHAPTER THREE

PROBLEM FORMULATION: THE SCREENING OF STRUCTURAL ALTERNATIVES

3.1 INTRODUCTION

This chapter is devoted to the formulation of a heuristic evolutionary procedure that selects promising alternative process structures for a given process system.

First, the need to develop such a procedure is justified, and the principles and assumptions upon which this formulation relies are established. Then, the characteristics of the proposed methodology are pointed out, and finally the method is formulated.

This work applies available optimization techniques in the context of the proposed heuristic procedure, but it is not devoted to the improvement of optimization techniques.

3.2 JUSTIFICATION FOR THE DEVELOPMENT OF A HEURISTIC METHODOLOGY TO SELECT AMONG ALTERNATIVE PROCESS STRUCTURES

As was stated in the literature review, algorithmic methods are the most reliable for addressing most synthesis problems. However, due to the restrictions in the available computer codes, the algorithms presently available can handle only relatively small problems. The number of structural

alternatives that can be considered in the multi-level techniques also is very small. Therefore, a heuristic procedure is needed to perform a preliminary selection or screening among several process structures that represent the same process system.

Douglas [1985] has proposed a heuristic-hierarchical procedure to generate a base-case design. Conti and Paterson [1985] propose a procedural approach based on heuristics to evaluate reactor configurations linked to their corresponding separation systems. These appear to be the only two systematic heuristic procedures existent for the generation and improvement of a base case design for a given process system. However, neither work addresses the problem of the preliminary screening of alternative process structures.

This work is devoted to the development of a heuristic procedure that provides preliminary selection of competitive alternatives among a given set of process structures. This procedure is not intended to substitute for the algorithmic methods, but is to be used as a tool to provide good initial estimates for the application of such algorithms.

3.3 PRINCIPLES UNDERLYING THE PROPOSED HEURISTIC PROCEDURE

The heuristic procedure proposed for the selection of competitive process structures is based on the following principles:

. The screening procedure among several process structures is conceived of as an optimization problem. This optimization

has a single objective: to maximize the profit of the process structure. The profit is defined as the net value of products (NVP) minus the energy cost (EC) and minus the capital cost (CC).

$$PROFIT = NVP - EC - CC \qquad (3.1)$$

The net value of products is equal to the value of the products and by-products minus the cost of raw materials.

. The optimization to select alternative process structures is performed in terms of the independent variables of the material balance equations. These independent variables determine the flow rates in the entire process structure. For a given set of bounds and constraints inherent to the process system, the flow rates determine to a great extent the size of the major operational units and the enthalpic condition of the streams. In addition, the independent variables of the material balance equation fix the net value of products (NVP), which constitutes an upper bound for the profit.

The studies of Conti and Paterson [1985], Fisher, Doherty and Douglas [1985] and Floquet, Pibouleau and Domenech [1985], and the results obtained in Chapter Four of this thesis show that the most important variables in optimizing a given process are the independent variables of the material balance equations (conversion, selectivity which may be a function of the reactor temperature, and the composition of recycle streams).

. The optimum search space is bounded by the maximum net value of products (max NVP), the minimum energy cost (min EC),

and the minimum capital cost (min CC). This principle is derived from the analysis of Equation (3.1). According to this equation, the maximum profit for a linear system would be:

$$\max \text{PROFIT} = \max \text{NVP} - \min \text{EC} - \min \text{CC} \qquad (3.2)$$

For a non-linear system, which is the case encountered in process design, the objective function appears to be bounded by the maximum net value of products, the minimum energy cost and the minimum capital cost.

. The procedure is evolutionary. The evolution principle can be understood in two different ways: (1) initially only the main elements of the process alternatives are considered in the evaluation; later, more detail may be added to the competitive process structures in order to refine the evaluation; (2) the decisions taken in the course of the screening procedure gradually become more complex. The evolutionary character of the method allows the decisions to be made sequentially.

. This procedure satisfies the synthesis "decomposition principle", performing structural modifications on a given process in several stages allowing changes in the topology, if necessary, at each stage of the evolution.

. This procedure uses the hierarchical planning principle, which states that the decisions pertaining to evaluation are categorized in different levels of importance.

. This procedure assigns higher precedence to the development of the material balance and the definition of the values for the independent variables that define it, rather than to the

definition of the variables that exclusively affect the energy consumption.

. This procedure uses the back-tracking principle, which means that decisions made earlier in the evolution are reviewed at a later stage to check their continued validity.

3.4 ASSUMPTIONS USED IN THE PROPOSED HEURISTIC PROCEDURE

Two major assumptions are used in the proposed heuristic--evolutionary procedure. These are:

1) This procedure assumes that, in the initial design stage, structural changes have more impact on the optimization function than do parametric modifications of the design variables. Therefore, structural modifications have higher precedence than the tuning of design variables.

Stephanopoulos [1981] points out that structural modifications have more impact than parametric changes. Douglas and Woodcock [1985], state that "experience seems to indicate that greater savings normally are possible by evaluating a new process alternative rather than optimizing a process". Design procedures proposed by Seider [1985], Westerberg [1980] and Takamatsu [1983] also state the importance of topological modifications. The results of the example process system developed in Chapter Four validate this assumption.

2) This procedure assumes that the analysis of one process structure (called "reference structure"), belonging to a set of alternative process structures, provides criteria to perform topological modifications on that structure in order to approach

the optimum value for the objective function. The characteristics of the reference structure and the procedure for its selection are detailed in Step 1 of the proposed heuristic procedure.

3.5 GENERAL CHARACTERISTICS OF THE PROPOSED HEURISTIC PROCEDURE

The proposed heuristic procedure incorporates the following general characteristics:

1. The method integrates some of the existent heuristic rules, organizing them into a more comprehensive heuristic-evolutionary procedure. The use of available techniques for the major synthesis sub-problems: heat integration [Linhoff and Hindmarsh, 1983], distillation sequencing [Shankar, 1985], and exergy analysis [Kaiser, 1981] is recommended.

2. Each of the steps involved in this evolutionary procedure has its own specific target(s). Therefore, at each step only part of the overall search space is covered.

3. It is not a method to initially generate process structures. **The method requires as a basis, at least one process structure developed by other means.** To generate an initial set of process structures the technique proposed by Lu and Motard [1985] or the one proposed by Johns and Romero (1979) is recommended.

4. The procedure could be applied to the evaluation of: (1) only one process structure; (2) a set of alternative process structures.

5. Reaction schemes and kinetic information should be provided as initial information.

6. The initial reduction of the search space is made by identifying bounds and/or constraints inherent to the problem. (Safety, restrictions in the services available, materials characteristics, production capacity, etc.)

7. This procedure requires the selection of one process structure, among the available alternatives, which will be used to study the influence of the main variables in the process system in order to guide the search for better structures.

8. This procedure uses simplified economic models for each one of the operating units in the given process structure. Shortcut methods can be used initially for the unit operations. The models can be refined in later stages of the evolution.

9. This procedure evaluates alternative operational units to perform a given goal. For example, absorption can be used instead of distillation to perform the same separation.

3.6 PROPOSED HEURISTIC PROCEDURE

The following heuristic-evolutionary procedure is proposed for the preliminary screening of alternative process structures:

Step 1: Selection of a "Reference Structure". This method is intended to evaluate competitive process structures, but not to generate them. To generate process structures, the work of Lu and Motard [1985] or the work of Johns and Romero [1979] are recommended. Among the initial set of available process structures (at least one), generated by other means, select one

process structure. This first process structure is called "reference structure".

To select the reference structure use the following procedure:

1.a) represent the initial set of process structures only by "material operators", eliminating from the representation units such as pumps, compressors and heat exchangers. Material operators are: reactors, separators, mixers and splitters.

1.b) Group the available alternatives using the material equivalence concept. Two or more process structures are called "material equivalent", if their respective material operators perform the same tasks, regardless of their number.

1.c) Select within each group of "material equivalent" process structures, one alternative using the following criteria:

(1) Simplicity of operational units. An operational unit is "simpler" than a competitive one if it achieves a lower number of goals. The operational units should be as simple as possible for the selection procedure (for example, if four components are going to be separated by distillation, the structure that has three distillation columns is considered the simplest one in this context because each column performs only one goal, ie, the separation of two components).

(2) Degree of development of the process structure. The degree of development of a process structure refers to the number of goals achieved by that structure. For the selection

procedure, the structure should be as developed as possible, i.e., it should include the maximum number of goals (for example, a structure that does not recuperate a by-product, but recirculates it, is not fully developed since this structure does not consider the goal of separating a component, and therefore it does not allow the evaluation of the unit that performs the recuperation).

(3) Degree of interaction between operational units. The interaction between material operators is given by the material recycled or by-passed from one operator to another, constituting a material loop. For the selection procedure it is desirable to have a highly interactive process structure in order to evaluate the effect of loops on the behavior of the system.

The above criteria respond to the need of understanding the behavior and relative importance of the operational units involved.

The best process structure should be selected according to the following "selection procedure": (a) evaluate the candidate process structures by their degree of development (criterion (2)), (b) if necessary, evaluate the remaining alternatives by the simplicity of the operational units (criterion (1)), and (c) if still there is more than one candidate alternative, select the most integrated structure (criterion (3)).

1.d) Rank the alternatives selected in the previous step, using the same "selection procedure". If there is doubt involved in the selection of the reference structure, select the

structure that offers the maximum net value of products (NVP). The computation of the maximum NVP is detailed in Steps 4 and 5. If the "selection procedure" finishes with more than one process structure, then perform steps 2 through 5 with all the selected alternatives, until the determination of the maximum NVP.

1.e) Choose the first process structure from the ranked alternatives. This one will be considered the "reference structure".

Use this reference structure to develop the following steps:

Step 2: Determination of bounds and/or constraints inherent to the problem. This step determines safety and other specific bounds and/or constraints inherent to the given problem. For example, explosive conditions for hazardous materials, corrosivity and other properties of materials, temperature and pressure limits for operational units, restrictions in the services available, and production and storage limits constitute bounds to the problem.

Step 3: Definition of "core variables". This section formulates the material balance equations in terms of the "core variables" and identifies the "core operators". For the selected "reference structure", the corresponding material balance equations are stated in terms of the minimum number of independent variables that fix the material balance. These independent variables are called "core variables", since they determine the material flow in the whole process structure.

The material operators to which the core variables are primarily related, are, then, called "core operators". For example, in a chemical process the conversion is a core variable, since it determines the flow rates of products and reactants. Therefore, the reactor would be a core operator.

A process structure can be identified by the number of material loops that it has. At least one independent variable is related to each material loop. The number of loops will determine the minimum number of independent variables.

Step 4: Determination of bounds and/or constraints for the "core variables". In order to set bounds for the "core variables" it is necessary to evaluate the net value of products. The net value of products (NVP) is defined previously as the value of products and by-products minus the cost of raw materials. The flow rates of products, by-products and raw materials are described by material balance equations, developed in Step 3. Since the material balance equations are formulated in terms of the core variables, by changing the values assigned to these core variables the corresponding NVP values can be computed. For certain values of the core variables the NVP may become small or even negative. Those undesirable values for NVP will determine bounds for the core variables.

Step 5: Maximization of the NVP. The maximum net value of products can be determined by search techniques which are applied to the material balance equations. The maximum NVP is very easy to find by using interactive search, when only two core variables are considered. For a higher number of core

variables, Powell's method is recommended [Beveridge and Schechter, 1980].

Step 6: Development of simulation model. Up to this point, only material balance equations and material operators were considered. To further evaluate the reference structure it is necessary to consider the effects of the core variables on the capital cost and energy cost, which are components of the objective function. Consequently, the formulation of a simulation model is required.

To develop the mathematical model for the reference structure, consider material operators (reactors, separators, mixers and splitters), as well as non-material operators (compressors, pumps, heat exchangers, etc.). This model should include material and energy balances, equipment sizing and economical models for each one of the major operational units involved.

To establish the values for the design variables of the operational units, useful heuristics are provided by Happel and Jordan [1976, Appendix C] and Douglas [1985]. To set the operating pressure of distillation columns, the procedure proposed by Henley and Seader [1981, p.432] is recommended. To set up distillation trains, Shankar's heuristic procedure [1985] is recommended. The initial estimation for the reactor conversion can be set to achieve maximum selectivity [Conti and Paterson, 1985].

Step 7: Execution of parametric studies. In order to determine the potential for structural changes in the reference

process structure, parametric studies are performed using the simulation model. For that purpose, use the following procedure:

7.a) Perform a few parametric changes in the values of the core variables to evaluate the corresponding effect in the following factors: (1) net value of products (NVP), (2) capital cost (CC), (3) energy cost (EC), and (4) profit. The core variables may assume just three values: upper and lower bounds (determined in Step 4), and an average value between these bounds. These initial parametric changes will reveal the relative impact of each of the economic targets (i.e.,NVP, EC and CC) on the profit, and their sensitivity with respect to the core variables (except for NVP, since its sensitivity has been determined with more detail in Step 5).

7.b) With the information provided in 7.a), extend the parametric modifications of the core variables to determine the sensitivity of the major operational units with respect to the variations in the core variables. In this step the following aspects have to be analyzed: (1) range of stability of the unit (i.e., convergence of the model under various conditions), and degree of difficulty to achieve specifications, (2) violation of bounds (for example, under certain values of the core variables the temperature of a reactor might overcome a specified limit), (3) changes in the net value of products (NVP), (4) changes in the energy cost (EC), (5) changes in the capital cost (CC), and (6) changes in the profit.

It is important to register the effect of the core variables on each one of the targets (NVP, EC and CC), and not only on the profit, because the analysis of these records provide additional criteria to decide what type of structural changes are needed to better affect each one of the targets. Observe that in a previous step the maximum NVP has been determined for the reference structure. Therefore, this value constitutes a target for the parametric evaluation.

This parametric analysis also helps to tune up the values of the core variables improving the initial estimates.

7.c) List all the major operational units in the reference structure, recording the following information: (1) the operational bounds and/or constraints, (2) the behavior in the simulation (from Step 7.b record if the unit is unstable or difficult to simulate); (3) If goal of a unit is stricly necessary for the process (for example, a separation unit that recuperates a by-product might not be strictly necessary if that by-product could be recirculated); (4) if unit could be lumped to another operational unit (for example, two simple distillation columns can be transformed into one that has a side-draw); (5) if the goal of the unit can be better achieved by decomposing it into two or more operational units (for example, in a process that intends to recuperate a valuable by-product, probably the introduction of a new reactor with different operational conditions would improve the formation of the desired by-product); and, (6) the ratio of change in the NVP, EC, CC and profit with respect to changes in the core varia-

bles (sensitivity of targets and objective function with respect to core variables).

The analysis of the information accumulated will provide criteria for guiding structural modifications of the process structure.

Step 8: Determination of minimum utility requirements. Using the pinch point analysis, determine the minimum utility requirements using the value of the core variables that show a higher profit [Linhoff and Hindmarsh, 1983]. This result will be later compared with the one obtained in Step 10.

Step 9: Topological modifications in the process structure From the results obtained in Step 7, modifications of the topology of the reference structure may be convenient to better satisfy the objective function. The decision procedure to introduce topological changes is as follows:

9.a) List the units that do not perform a strictly necessary task. These units might be: (1) eliminated, (2) lumped into other operational units, or (3) replaced by a competitive unit (if possible). The topological changes should be performed in the sequence established, unless the information from Step 7.c) shows a clear option. If undesirable effects result from the elimination of the unit, lump it with another operational unit. If that is not possible, replace the unit with a competitive one. In any case, evaluate the effects of the structural changes.

9.b) List the units that might be conveniently replaced, even though they perform a necessary task. The reasons that

justify a change are: (a) narrow operational range, (b) violation of bounds and/or constraints, or (c) high sensitivity to core variables. Replace operational units only if all of the following conditions are satisfied: (1) the specifications stated for that unit are fulfilled, (2) the technology is reliable, (3) the cost of the new unit is competitive; and, (4) the operational cost is approximately equal to or less than the corresponding for the old unit. Besides, it is desirable to avoid the inclusion of new services, such as refrigerants, hot process fluids, etc. that are not used by other units. For example, azeotropic distillation might be evaluated against vacuum distillation or solvent extraction. [Dec, 1983]

9.c) List the units that perform a necessary task which can be lumped to other operational units, without compromising the economic targets. Execute the lumping of units (if it is possible) and simulate in order to evaluate the effects.

9.d) Add to the structure a new operational unit if that benefits the objective function. Evaluate the effects of introducing the new unit by means of simulation.

Careful evaluation should be exercised if topological changes affect characteristics of a given loop in the process structure. Therefore, each time that a unit is eliminated or replaced by another operational unit that introduces new services (refrigeration, hot process fluid or additional compression), go to Step 10. Otherwise, perform additional structural modifications (if possible).

Step 10: Evaluation of energy benefits introduced by topological modifications. Determine the heat integration potential for the new topology, establishing the minimum utility consumption that can be expected. Use the pinch point analysis of Linhoff and Hindmarsh [1983]. Compare the results of this step and the results for the previous process structure obtained in Step 8. If the new topology does not offer energy savings, check carefully the advantages of the new process structure.

Step 11: Performing additional topological modifications. If necessary repeat Step 9 and Step 10.

Step 12: Heat integration of process structure. Perform heat integration in order to approach the minimun energy cost target. Follow the method suggested by Linhoff and Hindmarsh [1983].

Step 13: Registration of target values. For the process structure under evaluation, register the following values: (1) actual net value of products (NVP), (2) energy cost (EC), (3) capital cost (CC), and (4) profit. Evaluation of the structure under study is finished with this step.

Step 14: Selection of another process structure from the initial set. Check the next process structure selected in Step 1. If a similar structure has been generated while performing Step 9, take the next alternative, because the former alternative has been already evaluated. Repeat this step.

Step 15: Determination of bounds and core variables for the new process structure. Repeat Steps 2 and 3 for the new process structure.

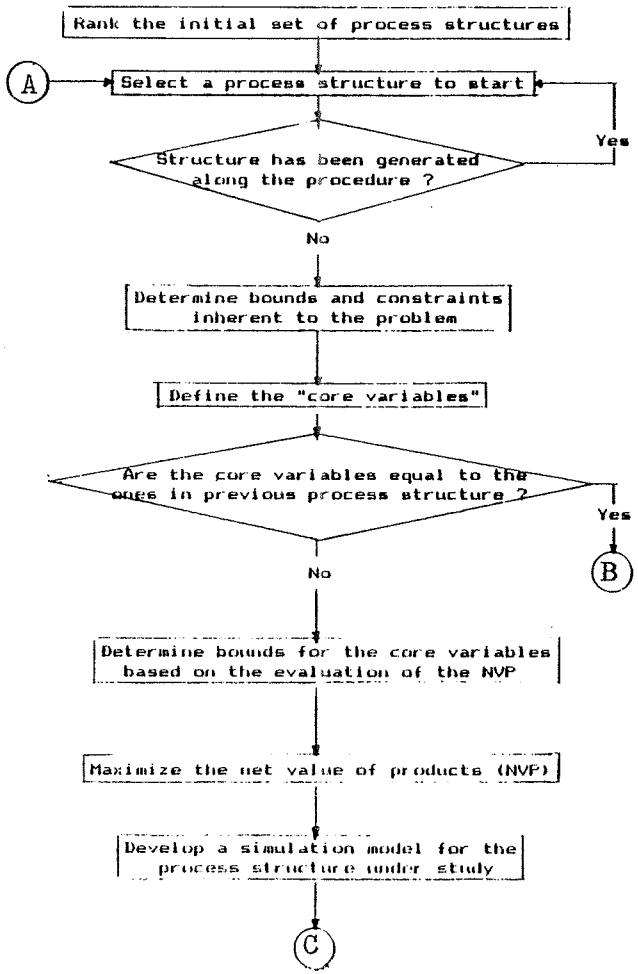
Step 16: Evaluation of the new process structure. Evaluate the new process structure using the information of Step 7.c), if the core variables of the reference structure and the new one, are the same. If not, repeat Steps 5 through 13, for the new process structure.

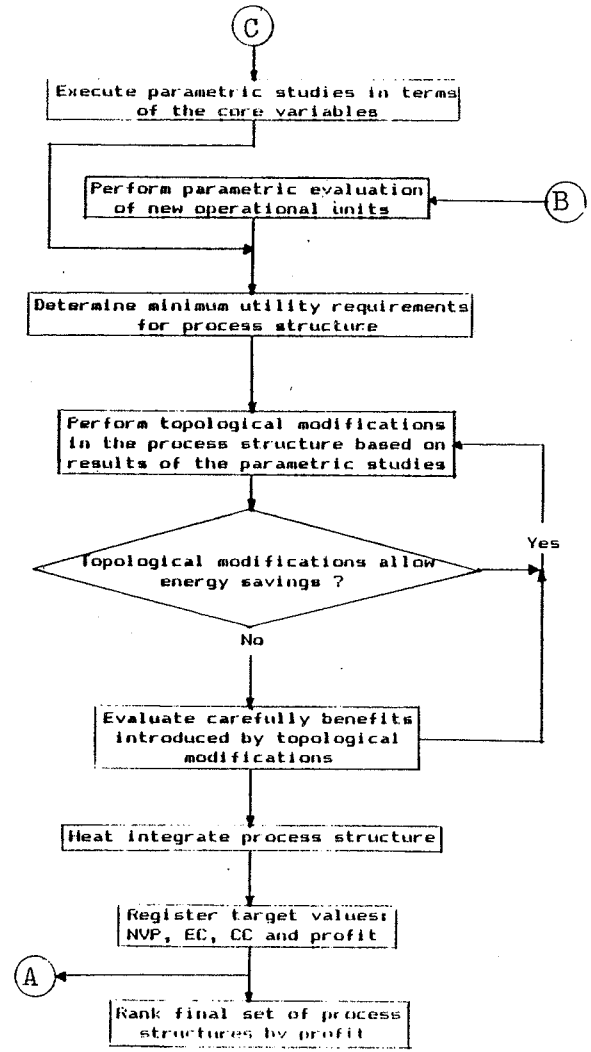
Step 17: Ranking of the final set of process structures. Rank the resultant set of screened process structures in terms of the profit. Register also the values of the targets (NVP, EC and CC).

These alternatives constitute the final set of process structures to which algorithmic methods may now be applied to find the optimum conditions for the given process system.

Figure 3.1 shows a summary of the proposed heuristic procedure.

FIGURE 3.1: HEURISTIC-EVOLUTIONARY PROCEDURE FOR THE PRELIMINARY SCREENING OF ALTERNATIVE PROCESS STRUCTURES





CHAPTER FOUR

APPLICATION OF THE PROPOSED HEURISTIC PROCEDURE TO THE EXAMPLE PROCESS SYSTEM: HYDRODEALKYLATION OF TOLUENE TO PRODUCE BENZENE

4.1 INTRODUCTION

In this chapter, the heuristic-evolutionary procedure proposed in Chapter Three is applied to an example process system. The thermal hydrodealkylation of toluene to produce benzene has been selected as the example problem because it offers several alternative process structures and it has been discussed by Douglas [1985] and Lu and Motard [1985]. The results obtained are checked against those presented by J. Douglas [1985], who used a hierarchical decision procedure.

4.2 STATEMENT OF THE EXAMPLE PROCESS SYSTEM

Select competitive process structures to produce 265 kgmoles of benzene per hour by thermal hydrodealkylation of toluene (the information used in the problem statement has been taken from the AIChE 1967 Student Contest Problem). The benzene purity has to be 99.99 %. The reactions of interest are:

$$2\ CH3(C6H6) + H2 \longrightarrow C6H6 + CH4 \qquad (4.1)$$

$$2\ C6H6 \longleftrightarrow (C6H6)2 + H2 \qquad (4.2)$$

Reaction (4.1) can be considered irreversible. Reaction (4.2) is an equilibrium secondary reaction that transforms

benzene to diphenyl. A general flowsheet for the production of benzene is shown in Figure 4.1. Additional information about the problem formulation is presented in Appendix A.

4.3 DEVELOPMENT OF THE PROPOSED HEURISTIC-EVOLUTIONARY PROCEDURE

4.3.1 SELECTION OF THE "REFERENCE STRUCTURE"

Figure 4.2 presents 5 alternative process structures for the given problem. These alternatives are given as part of the problem; they are not generated by the proposed procedure. Figure 4.2 describes the proposed alternatives only in terms of material operators (i.e., reactors, separators, mixers and splitters), satisfying Step 1.a of the heuristic. Following Step 1.b of the heuristic procedure, it is necessary to group the available process structures by the material equivalence concept. A brief analysis of the structures is presented.

The five process structures all have a reactor and a phase separator (F1). These units perform the same tasks in all the structures. Moreover, alternatives 4.2.a, 4.2.b and 4.2.c show splitter S1 that performs the same task in the three structures. The only difference between structures 4.2.a and 4.2.b is the number of distillation units; nevertheless, the distillation train of these two alternatives have common goals: namely, the elimination of volatiles (stream FUEL), and the recuperation of benzene and diphenyl. The non-reacted toluene is recirculated. In conclusion, alternatives 4.2.a and 4.2.b are "material equivalent".

FIGURE 4.1 : FLOW SHEET FOR BENZENE PROCESS

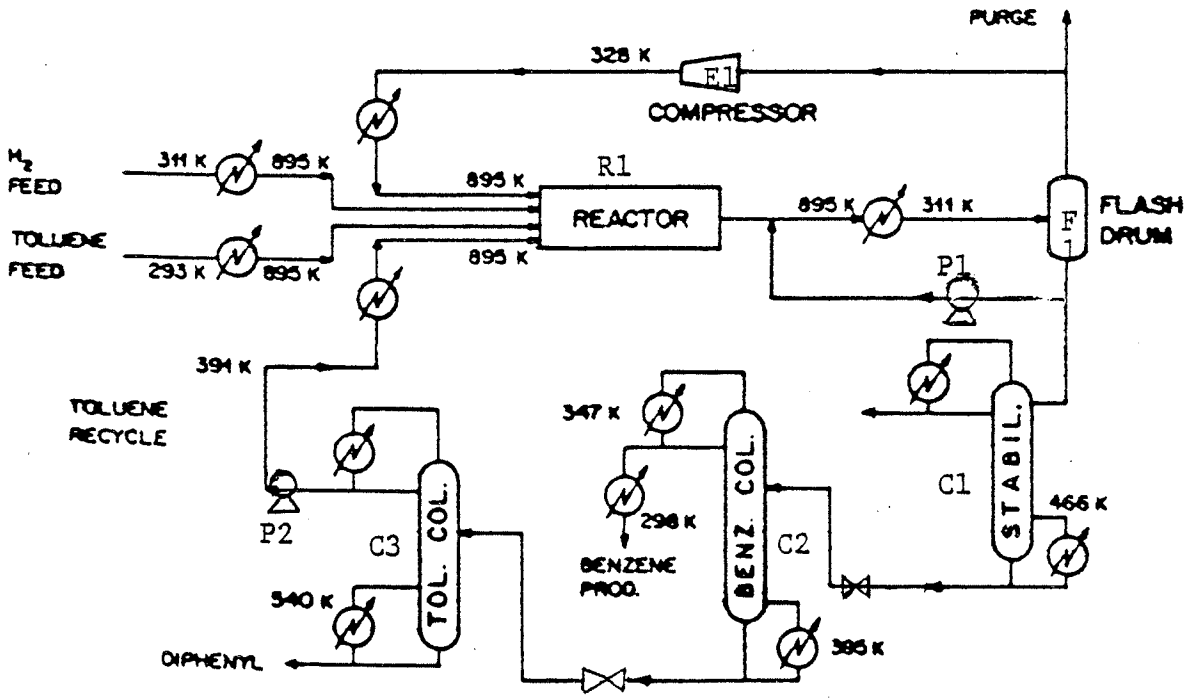
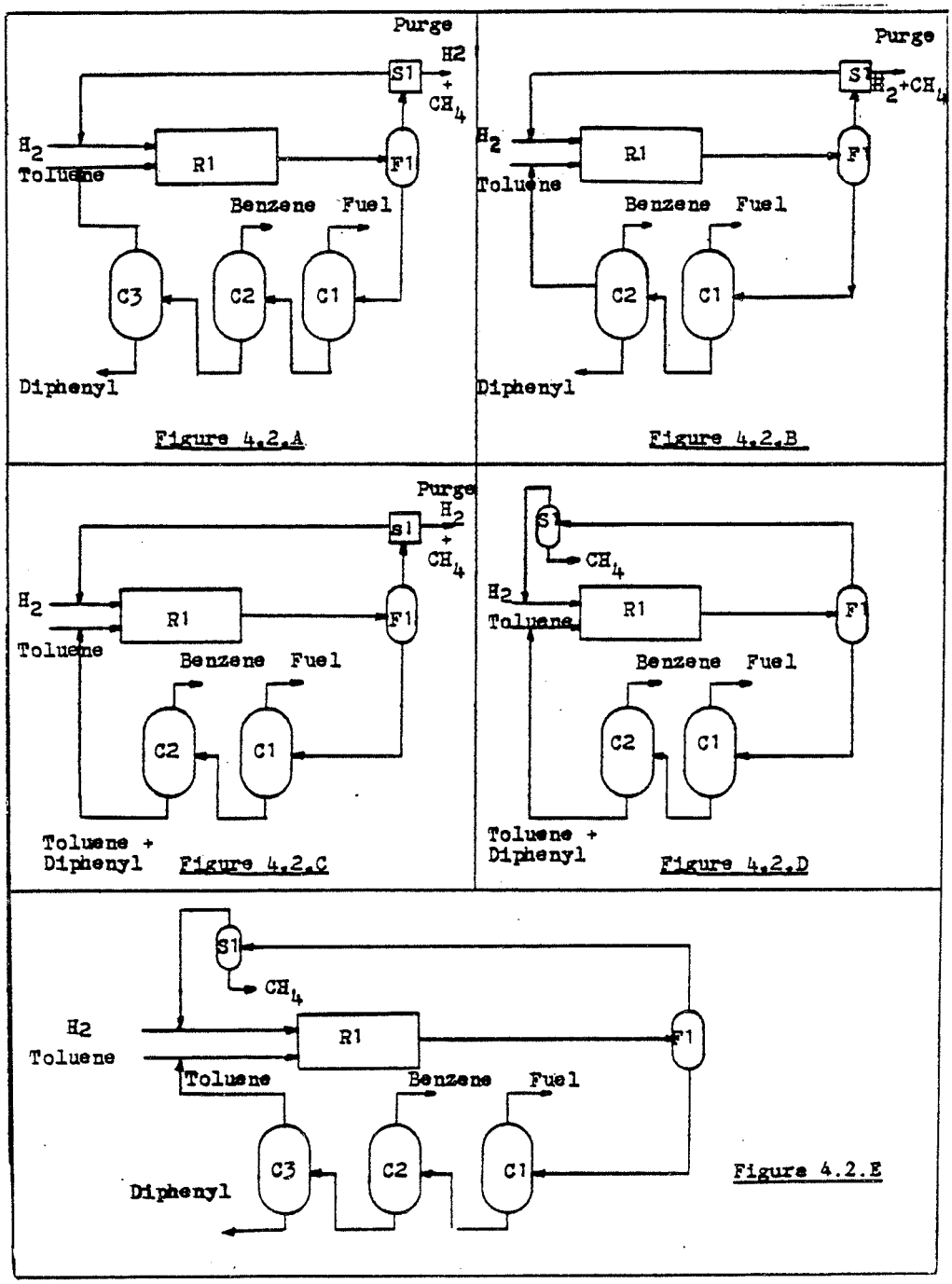


FIGURE 4.2: AVAILABLE ALTERNATIVE PROCESS STRUCTURES FOR BENZENE PROCESS



Alternative 4.2.c differs with respect to 4.2.a and 4.2.b because the diphenyl is being recirculated. Alternatives 4.2.c and 4.2.d have equivalence in the distillation train, but the gas loop is different, since no hydrogen is purged in alternative 4.2.d. Alternatives 4.2.d and 4.2.e have the same goals in the gas loop, but they differ in the goals of the liquid loop.

In summary, 4 groups of material equivalent process structures are defined:

Group 1: process structures 4.2.a and 4.2.b.

Group 2: process structure 4.2.c.

Group 3: process structure 4.2.d.

Group 4: process structure 4.2.e.

Following Step 1.c of the heuristic, it is now necessary to select one process structure for each group of material equivalent process structures. In group 1 the selected alternative is structure 4.2.a, since the second distillation column of structure 4.2.b, in the context of this work is not a simple unit (this column has a sidedraw). Therefore, the set of material non-equivalent process structures is:

Alternative 1: process structure 4.2.a

Alternative 2: process structure 4.2.c

Alternative 3: process structure 4.2.d

Alternative 4: process structure 4.2.e

To perform Step 1.d of the heuristic is necessary to rank the four alternatives listed according to the criteria of simplicity of operational units, degree of interaction between the units and degree of development of the topology.

Alternatives 4.2.c and 4.2.d recirculate the diphenyl, therefore their degree of development is not as good as that shown by alternatives 4.2.a and 4.2.e. Alternatives 4.2.a and 4.2.e fulfill all the above requirements. Alternative 4.2.e has a higher value for the maximum NVP, since it does not purge hydrogen. Therefore, the process structures are ranked in the following way:

Alternative 1: process structure 4.2.e

Alternative 2: process structure 4.2.a

Alternative 3: process structure 4.2.d

Alternative 4: process structure 4.2.c

At Step 1.e of the proposed heuristic the reference structure is selected. In spite of the ranking stated, we select alternative 4.2.a as the reference structure, for the following particular reasons: (1) the phase separator S1 shown in alternatives 4.2.d and 4.2.e can be a refrigerated flash drum or a membrane separator. Membrane separation is a relatively new technology, and no references are available as to the size and cost of these units. The energy cost associated with the separation of hydrogen from methane in a refrigerated flash drum might be extremely high, making these alternatives not attractive. But, the main reason for us to select alternative 4.2.a is that it has been studied by others [Douglas, 1985], and therefore there is the chance to compare procedures and results. Consequently the selected reference structure is 4.2.a. Alternatives 4.2.e, 4.2.c and 4.2.d are ranked next.

4.3.2 DETERMINATION OF BOUNDS AND CONSTRAINTS INHERENT TO THE PROBLEM

The following can be identified as bounds inherent to the problem.

Conditions for the operation of the reactor:

1) At the reactor inlet the mole ratio of hydrogen with respect to aromatics has to be 5:1.

2) Pressure = 3,450 kPa.

3) Temperature: greater than 895 K, and less than 980 K.

Heat exchangers conditions:

4) Maximum temperature : 895 K.

Specifications for the distillation columns:

5) Stabilizer column (C1): distillate to bottons mole ratio for methane is 50,000; and for benzene is 0.005.

6) The toluene losses have to be less than 1% of the net toluene feed.

7) Liquid recycle stream: maximum allowable benzene content is 4 mole percent. Diphenyl content has to be less than 25 mole percent of net diphenyl produced.

8) Distillation reboilers: kettle type reboilers are used with a maximum heat flux of 12,000 BTU/hr/sq.ft.

Fired-heater:

9) Overall heat transfer coefficient is 16,000 BTU/hr/sq.ft.

10) Pressure drop: 70 psi.

4.3.3 IDENTIFICATION OF "CORE VARIABLES" AND "CORE OPERATORS"

This step requires the formulation of the material balance equations in terms of the minimum number of independent variables. The material balance equations of interest are the following:

$$S = 1.0 - 0.0036/(1 - X)^{**}1.544 \quad (4.3)$$

$$FTol = Bz/S \quad (4.4)$$

$$Di = Bz(1 - S)/2S \quad (4.5)$$

$$Hyd = Bz\,[1 - (1-yH2)(1-S)/2]/[0.95-yH2] \quad (4.6)$$

$$Purg = Hyd + Bz\,[(1 - S)/2S] \quad (4.7)$$

$$Rgas = [(5\ Bz/SX) - 0.95\ Hyd]/yH2 \quad (4.8)$$

$$Tol = Ftol/X \quad (4.9)$$

where: S represents the selectivity, X the conversion and yH2 the concentration of hydrogen in the gas recycle stream; Bz, FTol, Hyd, Di, Tol, Purg and Rgas stand for the molar flow rate of the benzene produced, the fresh toluene feed, the hydrogen feed, the diphenyl produced, the toluene at the reactor inlet, the gas purge and the recycled gas, respectively. The derivation of the material balance equations is shown in Appendix B.

The conversion determines the amount of toluene and hydrogen consumed, and the amount of benzene and methane produced. Since in this problem the selectivity is defined as a function of the conversion, then the conversion will also determine the rate of diphenyl produced and the net production of benzene. Therefore, the conversion is considered to be an independent variable in the material balance equations. As can be seen in Figure 4.1 the amount of gas recycled depends on the

amount of material purged, and, of course, it also depends on the production rates of the reactor (which are a function of conversion).

By contrast, the rate of the purge stream is set to achieve a desired hydrogen concentration in the recycle gas. The whole purpose of the purge is to avoid the build up of methane in the recycle gas. Consequently, the conversion in the reactor (X) and the hydrogen concentration in the recycle gas (yH2) are the only two independent variables in the material balance equations. Therefore, the "core variables" for the reference structure are (1) the conversion (X), and (2) the hydrogen concentration in the gas recycle stream (yH2), since these are the only two independent variables in the material balance equations.

Consequently, the "core operators" (operators to which the core variables are primarily related) are: (1) the reactor, and (2) the splitter (S1).

4.3.4 BOUNDS SET FOR THE CORE VARIABLES BY THE NET VALUE OF PRODUCTS

To compute the net value of products (NVP) as a function of the core variables (X and yH2), use the material balance equations (4.3 through 4.7). To each input or output stream assign the corresponding value. The prices for benzene, toluene diphenyl, hydrogen and the purge stream are presented in Section 4.3.6. The results for the NVP as a function of X and yH2 are presented in Table D.1 (Appendix D).

FIGURE 4.3.A : INFLUENCE OF CORE VARIABLES ON THE NET VALUE OF PRODUCTS (NVP)

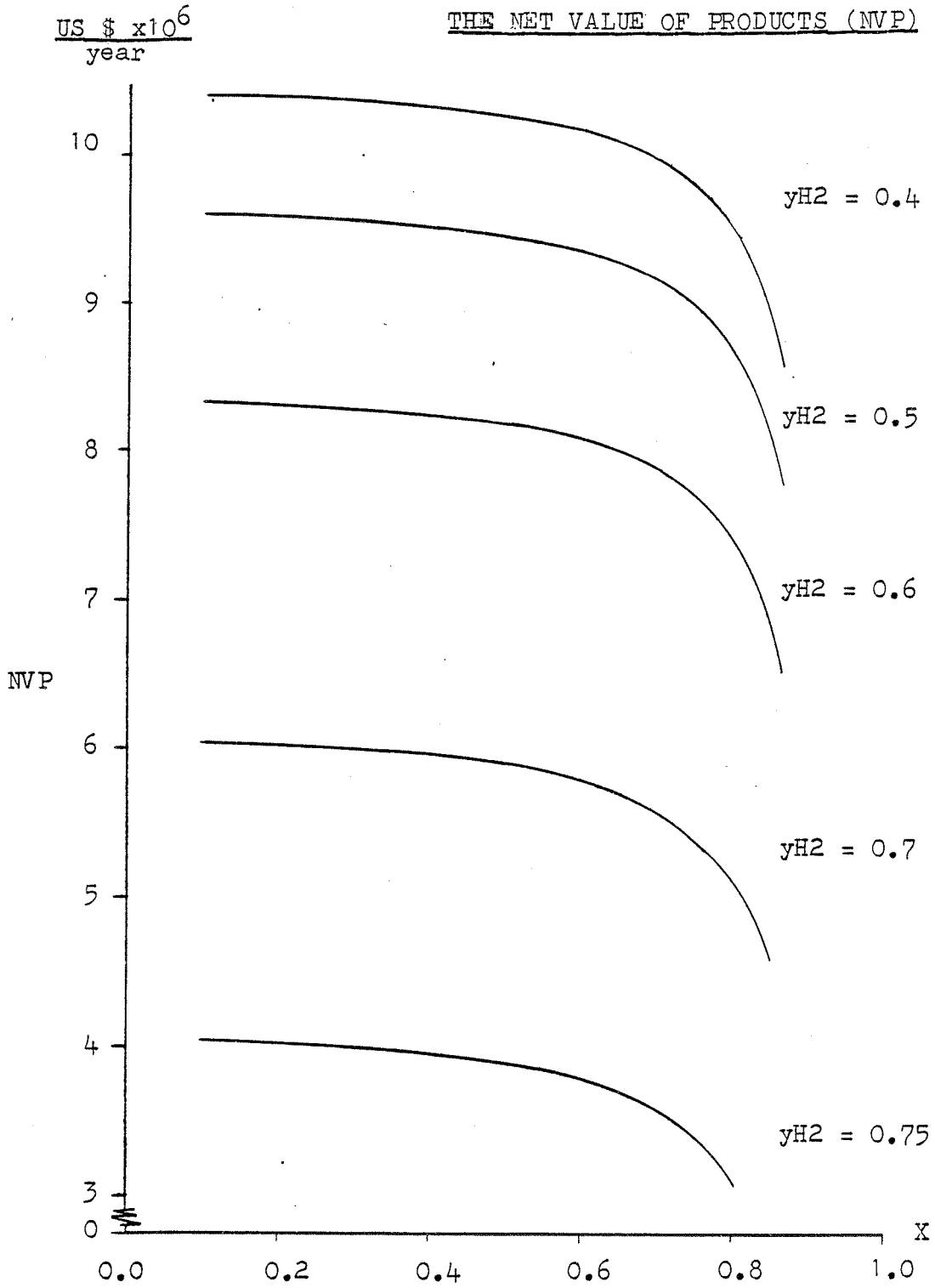


Figure 4.3.B

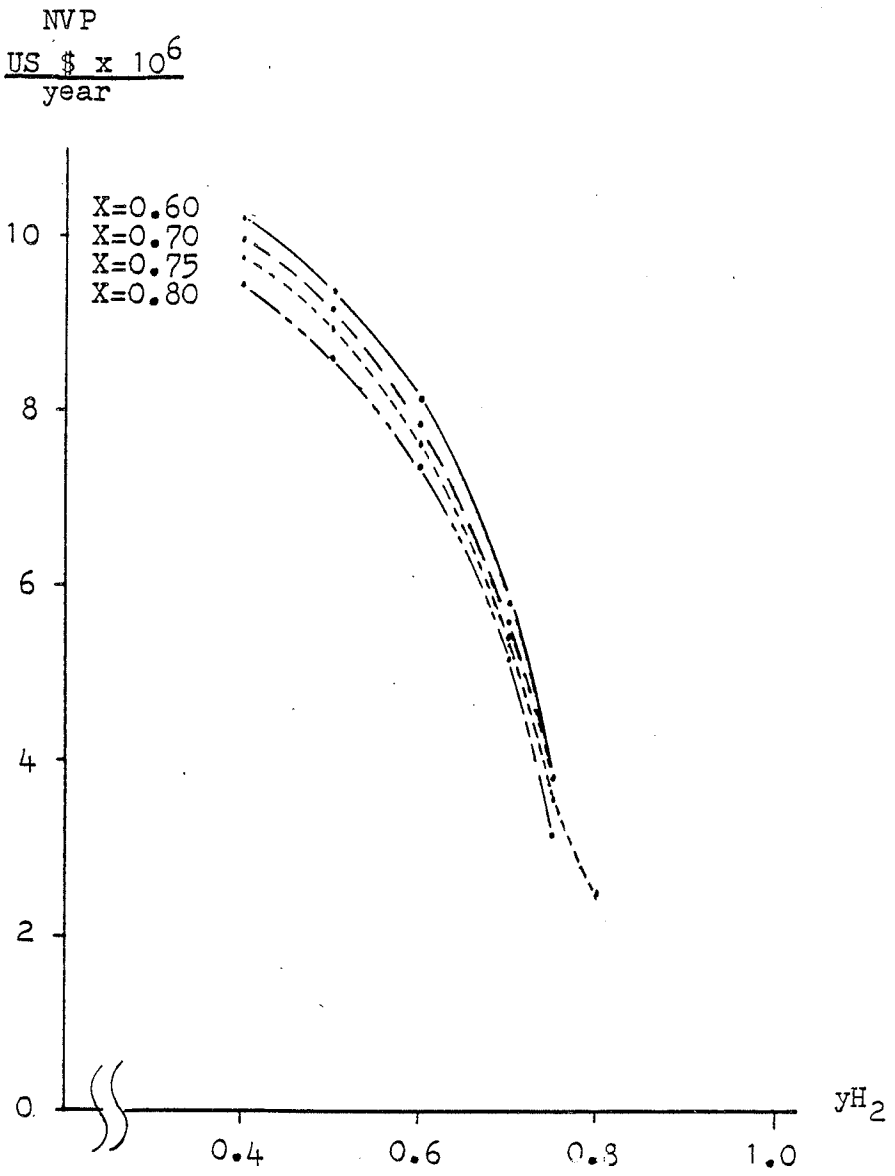


Figure 4.3.a shows the correlation of NVP with respect to the conversion (X) and the hydrogen concentration (yH2) in the gas recycle stream. It can be seen that at a conversion higher than 0.75, for any value of yH2, the NVP sharply decreases. This value constitutes an "upper bound" for the conversion.

Figure 4.3.b shows the correlation of the NVP with respect to yH2. It can be seen that the NVP decreases as yH2 increases. At a value of yH2 equal to 0.8 the NVP becomes negative. Therefore, for this process structure, yH2 equal to 0.8 is an "upper bound" for this variable.

Figure 4.3.a and Figure 4.3.b also show that for conversions less than 0.4, the NVP is not significantly affected (NVP decreases only 0.85 % in the conversion range of 0.1 to 0.4). Therefore, 0.4 may be tentatively considered the lower bound for the conversion.

On the other hand, the value of yH2 strongly influences the NVP value. However, the lowest possible value for yH2 is 0.4, since this is a bound given in the problem statement. It is important to note, that the pattern followed by the NVP as a function of conversion, corresponds to the relationship between selectivity and conversion presented in Figure 4.4.

In conclusion, the lower and upper bounds for the conversion (X) are 0.40 and 0.75, respectively. The hydrogen concentration in the recycle gas has 0.40 and 0.80 as lower and upper bounds.

4.3.5 DETERMINATION OF THE MAXIMUM NVP

As shown in Figure 4.3.b, the maximum NVP is achieved at the lowest possible value for yH2, that is, 0.4, and at a conversion of 0.1. The maximum NVP for the reference structure is then: $ 10.4 million per year.

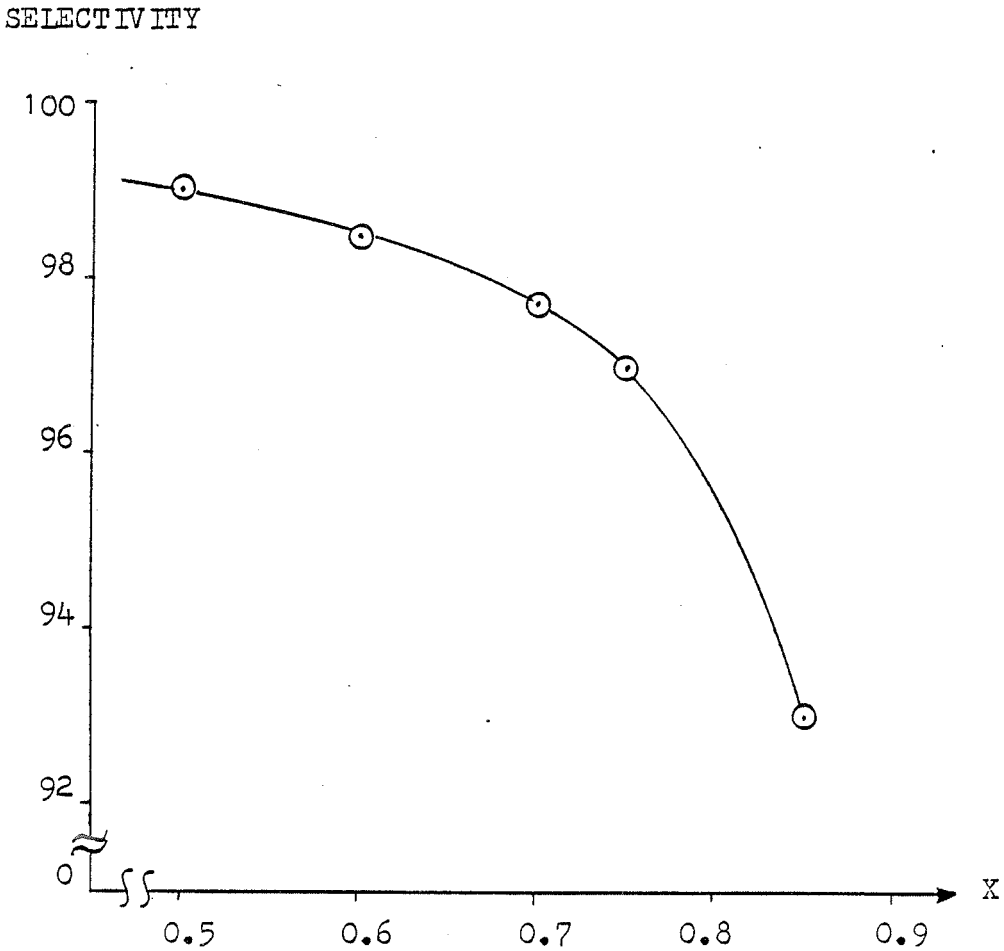
4.3.6 DEVELOPMENT OF A SIMULATION MODEL FOR THE REFERENCE STRUCTURE

The following information is required to develop the simulation model:

- prices of products, by-products and raw materials,
- prices of utilities, power and fuel,
- cost models for each of the main equipment items, and
- operational conditions for each of the major units.

The material and energy balances and the sizing of the distillation columns and some other equipment items have been done using the PROCESS simulator [Simulation Sciences, 1983]. Economic models for the operational units and profit calculation functions have been incorporated in the input file to the PROCESS simulator. A sample of that input file is presented in Appendix C.

FIGURE 4.4: RELATIONSHIP BETWEEN SELECTIVITY AND CONVERSION (X)



To provide good initial stream estimates during the case studies performed with PROCESS, the material balance equations presented in Section 4.3.3 have been applied. The prices of chemicals assumed for the modelling of this problem are the following: [Chemical Marketing Reporter: January 6 and March 17, 1986]

CHEMICAL	UNIT	VALUE
Toluene	$/m3	174.37
Benzene	$/m3	282.69
Diphenyl	$/m3	66.05
Hydrogen	$/std. m3	0.0657
Fuel	$/MM BTU	1.65

The price of hydrogen is evaluated at standard conditions, i.e., 101 kPa and 273 K. The gas effluents from the process are priced by their net heating value, because they can be used as fuels. The heating value for the gas effluent changes with the composition of the stream. The prices given are valid for January 1986. The details for their determination are shown in Appendix E.

The price of services are listed below [Monthly Energy Review, Energy Information Administration, December 1985]. For more details see Appendix F.

SERVICE	UNIT	VALUE
Residual Fuel Oil	$/GJ	3.856
Electricity	$/kWh	0.0877
Cooling Water	$/m3	0.0549
Refrigerant	$/kJ	2.327E-5
Process Steam	$/kg	0.01329

The flow diagram corresponding to the simulation for the reference structure, performed by PROCESS, is shown in Figure

4.5. This diagram is very similar to the one shown in Figure 4.1.

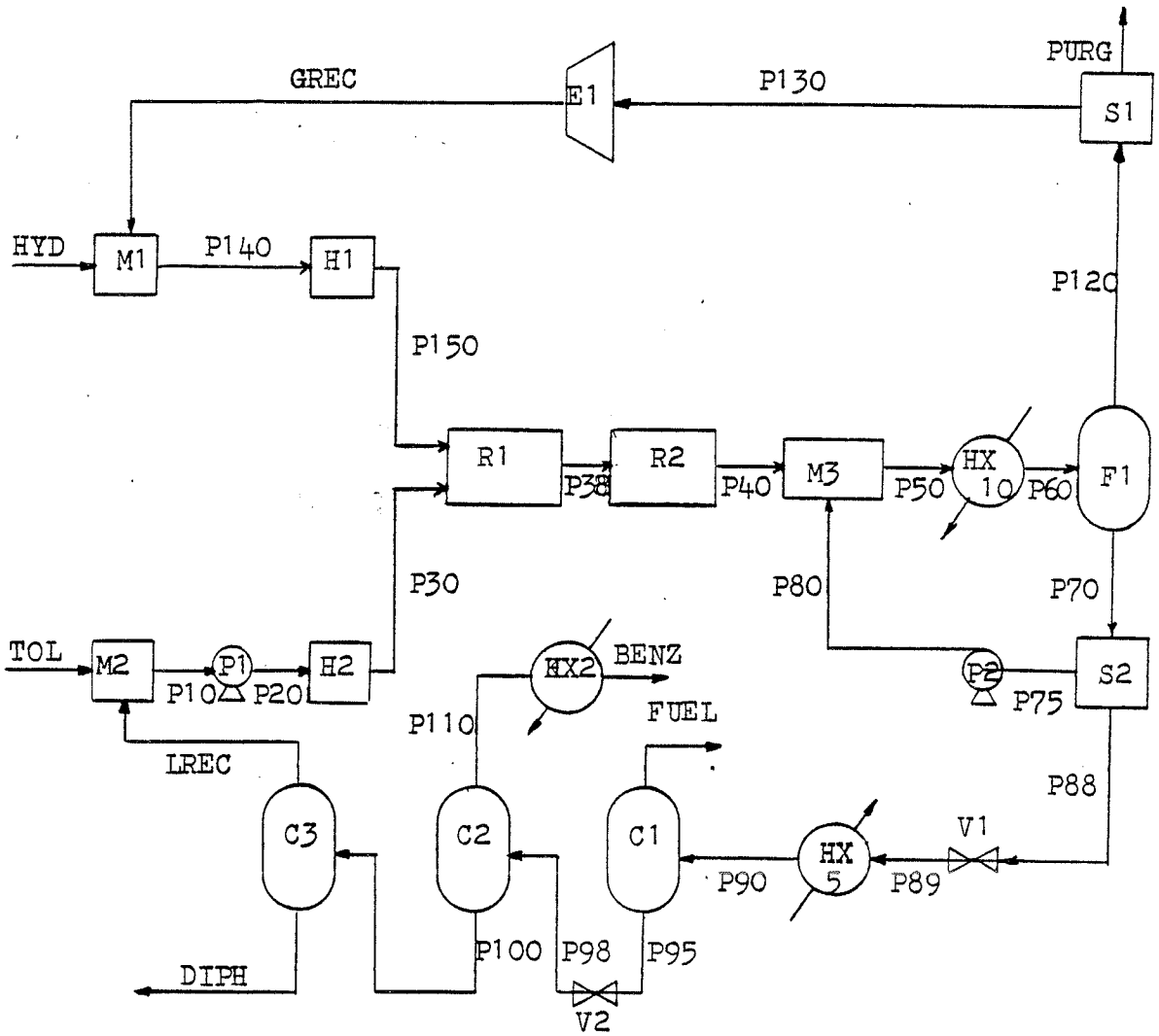
The cost models for the main equipment items are presented in Appendix G. The operational conditions for the major equipment items were set as follows: (1) the reactor inlet temperature and pressure were given in the problem statement, (2) the furnace heat transfer rate and pressure drop was also given in the problem statement, (3) the flash drum temperature was set at 311 K, according to the heuristic proposed by Douglas [1985], (4) the pressure of the distillation columns was fixed following the procedure proposed by Henley and Seider [1981, p. 432], and (5) the reflux ratios for the columns were set initially at 1.2 times the minimum reflux ratio [Douglas, 1985].

4.3.7 PARAMETRIC STUDIES USING THE SIMULATION MODEL

In this section the results obtained from the simulation of the reference structure are presented and discussed.

As stated in Step 7.a of the proposed heuristic, initially a few case studies were performed to broadly describe the behavior of the targets (NVP, EC, CC and profit), while changing the values of the core variables. Taking into account the bounds for the core variables (X: from 0.4 to 0.75; yH2:- from 0.4 to 0.8, determined in Step 4), the following case studies were performed: X=0.75, yH2=0.4; X=0.75, yH2=0.8; and,

FIGURE 4.5: SIMULATION FLOW SHEET FOR BENZENE PROCESS



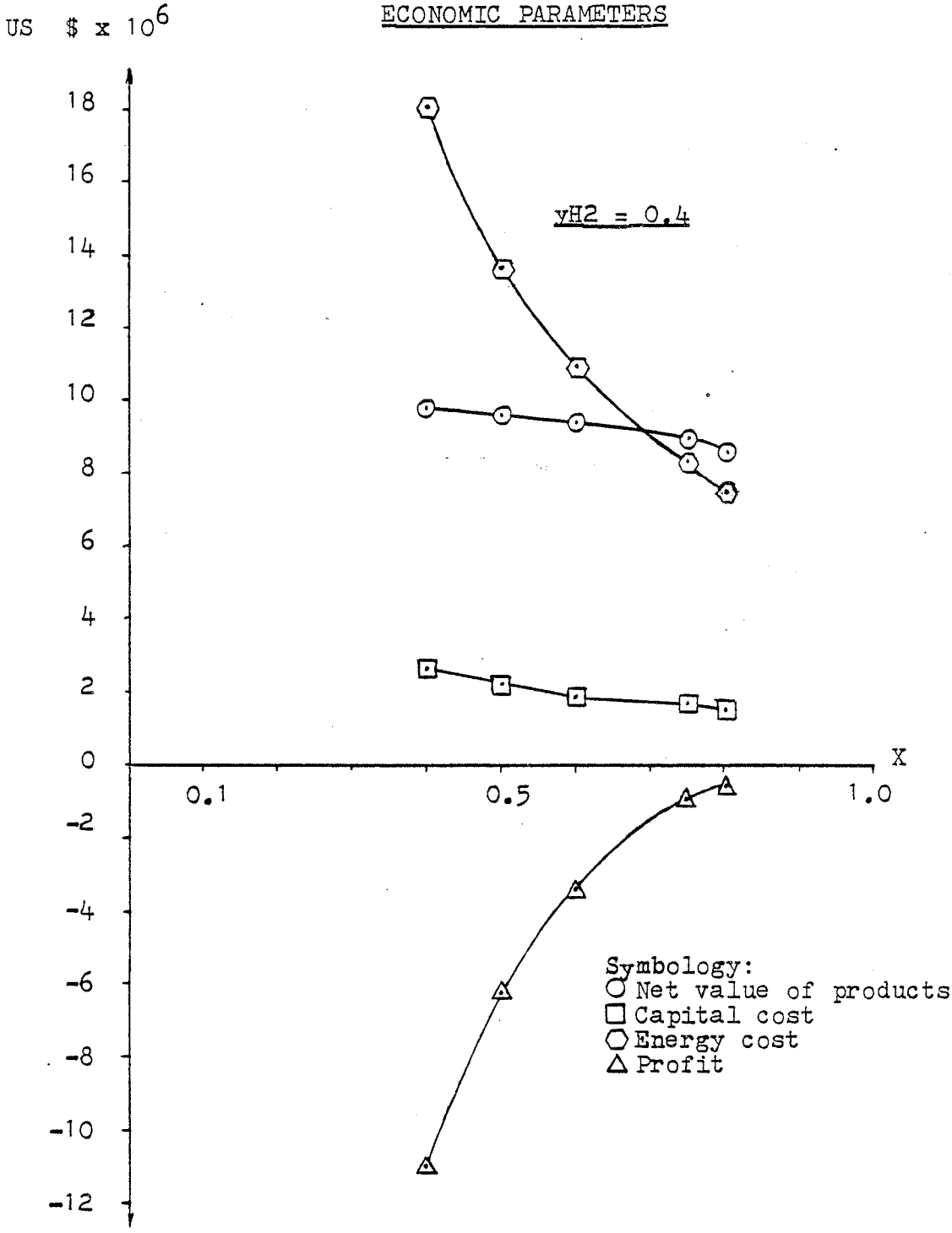
X=0.4, yH2=0.4. The results are shown in Figure 4.6, and will be discussed in the next section. With this first insight about the behavior of the system, further parametric studies were performed: the value of yH2 was kept constant at 0.4 while changing the conversion values.

4.3.7.1 INFLUENCE OF THE "CORE VARIABLES" ON THE ECONOMIC TARGETS

. Evaluation of conversion (X): Figure 4.6.a shows the relationship between "X" and each of the economic targets. The net value of products (NVP) decreases when "X" increases. However, the influence of "X" in the NVP may be considered not significant (this was also observed in Figure 4.3), since the variation of NVP while changing X from 0.4 to 0.75 is only 8.4 %. The capital cost decreases as "X" increases, but the contribution of changes in "X" to the reduction of this cost is minimal. The energy cost appears to be highly sensitive to changes in "X". For every 10 percent increment in "X", the energy cost is reduced approximately 20 % within the range defined by the bounds stated in Section 4.3.4 (X=0.4 to 0.75).

Figure 4.6.e shows the relationship between "X" , "yH2" and the parameter "level 4a" proposed by Douglas [1985]. The "level 4a" has been defined by Douglas as the NVP minus the cost of the reactor and minus the capital and operating costs for the compressor, in order to evaluate the effect of the main varia-

FIGURE 4.6.A: INFLUENCE OF CONVERSION (X) ON ECONOMIC PARAMETERS



bles on the gas recycle loop. With this definition, the parameter "Level 4a" follows a pattern parallel to the NVP, since the cost of the reactor and of the compressor are minimal with respect to the total cost of the plant. To better evaluate the effect of the gas recycle loop costs, from the level 4a should be substracted the capital and energy cost of the heater H1 (Figure 4.1), which is responsible for the heating of the gas stream fed to the reactor.

Evaluation of the hydrogen concentration in the recycle stream (yH2): Figure 4.6.b presents the influence of "yH2" on the economic targets. Figure 4.6.b indicates the strong negative effect of changes in "yH2" on the NVP. Although clear bounds cannot be defined, it can be seen that for values of "yH2" between 0.4 to 0.6, the negative effect is less severe than in the range of 0.6 to 0.8. This is a very important aspect to consider, since the NVP actually represents the profit margin of the process.

Incrementing the value of "yH2" causes a reduction in the energy cost. However, this effect is not as significant as the one caused by increasing "X" (see Figure 4.6.c). It is important to check if the negative effect of "yH2" in the NVP may be compensated by the positive effect of "yH2" in the cost of energy. The result is that for values of "yH2" greater than 0.6, the energy savings are not significant enough to compensate for the sharp reduction in the NVP. Therefore, the profit also experiences a sharp reduction.

FIGURE 4.6.B : INFLUENCE OF THE HYDROGEN CONCENTRATION IN THE GAS RECYCLE STREAM (yH2) ON ECONOMIC PARAMETERS

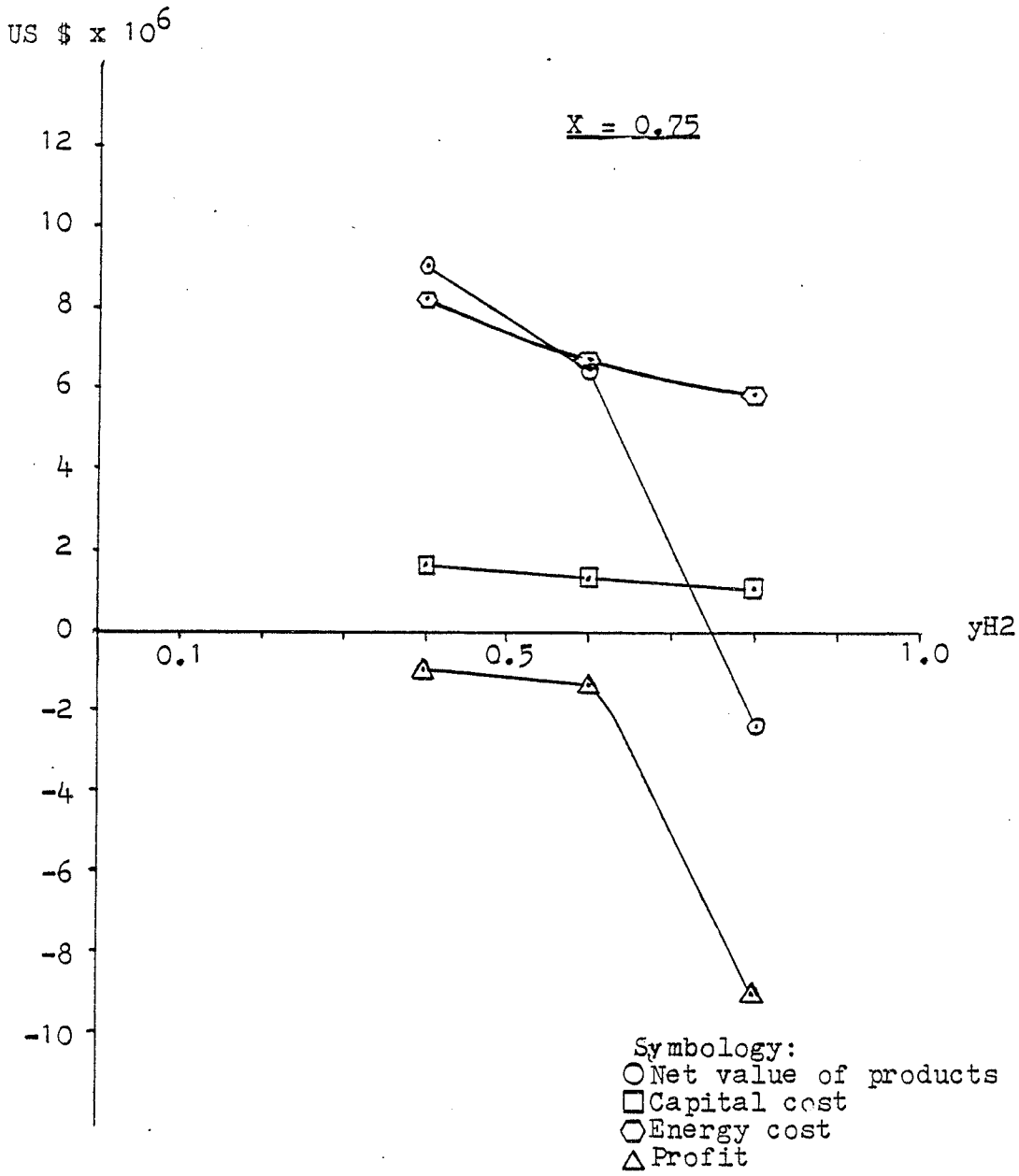


Figure 4.6.C

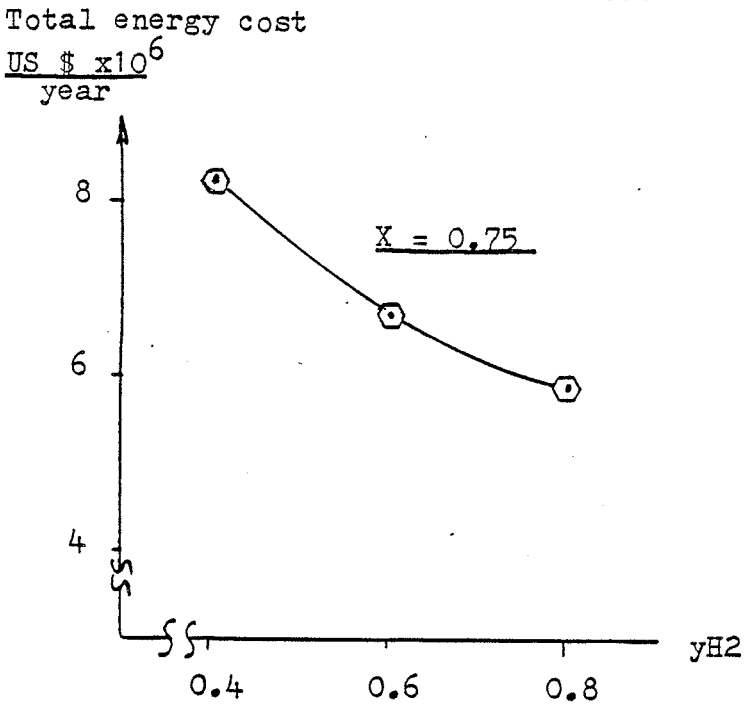


Figure 4.6.D

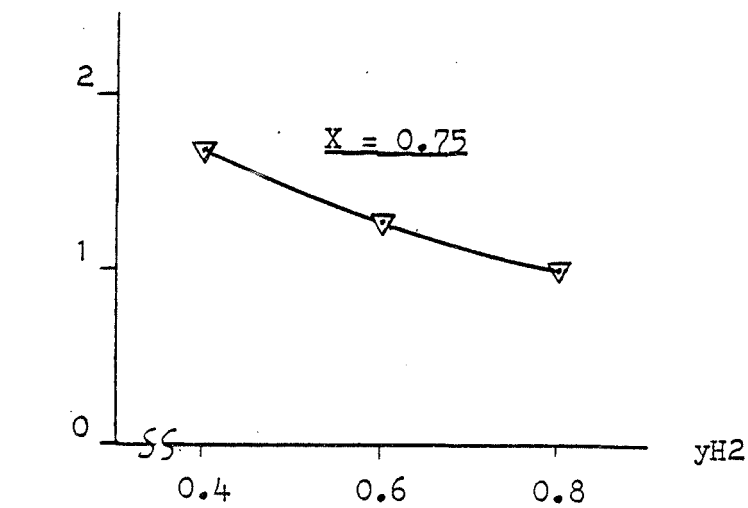
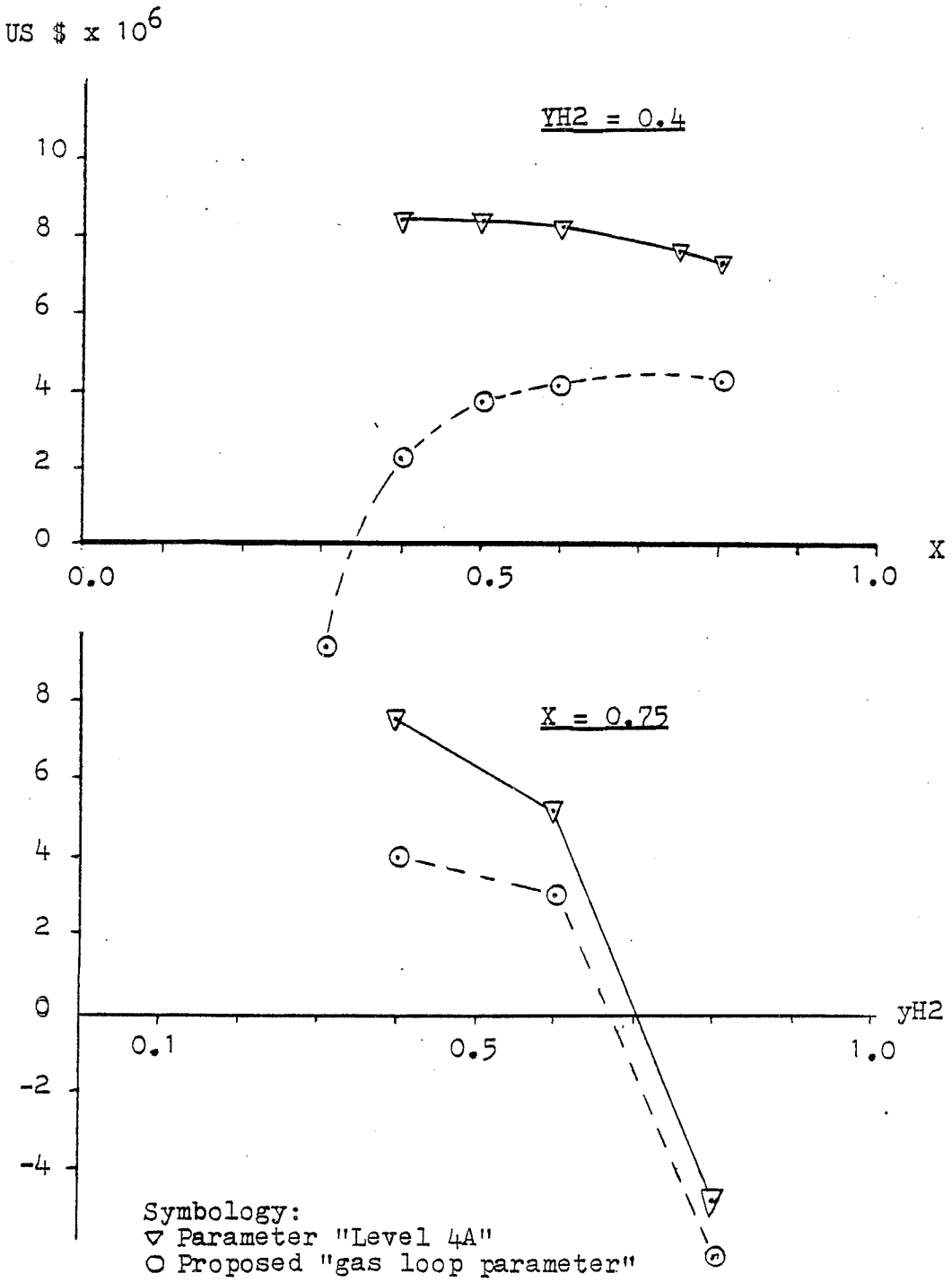


FIGURE 4.6.E: INFLUENCE OF THE CORE VARIABLES ON THE ECONOMIC PARAMETER "LEVEL 4A"



The value of "yH2" at which the highest profit is obtained is 0.4. From this analysis, a lower and upper bound for the variable "yH2" have been indirectly determined. They are 0.4 and 0.6, respectively. Figure 4.6.b also shows that the capital cost decreases when "yH2" is increased, but this effect is not significant (see Figure 4.6.d).

The above analysis leads to the following conclusions:

(1) The core variable "yH2" determines, almost totally, the NVP. (2) The core variable "X", mainly determines the cost of energy. (3) Energy costs are much more sensitive to changes in the core variables than capital costs. (4) The bounds for the conversion (X), are fixed by the NVP with "X" greater than or equal to 0.4, and less than or equal to 0.75. (5) The bounds for "yH2" are fixed by the cost of energy in relation with the NVP with "yH2" greater than or equal to 0.4, and less than or equal to 0.6.

The above conclusions are important and justify the evaluation of the effect of the core variables on the economic targets (NVP, EC and CC), and not only on the profit.

From the information obtained via simulation of the reference structure, each one of the major operational units can now be evaluated in accordance with Step 7.c of the proposed heuristic procedure.

4.3.7.2 EVALUATION OF THE REACTOR

(1) Operational bounds and constraints: Pressure= 3450 kPa, inlet temperature= 895 K, maximum outlet temperature= 980 K (adiabatic operation).

(2) Behavior in the simulation: The reactor did not present any problems while performing the simulation.

(3) Goal of the reactor: To produce benzene from toluene. This is a strictly necessary goal. The production of diphenyl also occurs in the reactor. This is not a strictly necessary goal. The production of diphenyl is increased at higher temperatures [Dasgupta et al, 1986]. If the production of diphenyl were desired, then another reactor operating at higher temperature should be included.

(4) Operating conditions of the reactor with respect to variations in the core variables: Figure 4.7.a shows the relationship between "X", "yH2" and the reactor volume. It can be seen that the volume of the reactor is significantly reduced by increasing the value of "yH2". This fact can be explained considering the reduction in the volumetric flow of inert gas (CH4). Also, at a conversion of 0.5, the reactor volume is minimum. The reactor cost is not an important factor in the overall cost of the reference structure, since the energy constitutes by far the most important cost component.

Figure 4.7.b shows that the reactor outlet temperature increases proportionally with "X" and "yH2". However, the

FIGURE 4.7: EVALUATION OF THE REACTOR OPERATION WITH RESPECT TO THE CORE VARIABLES

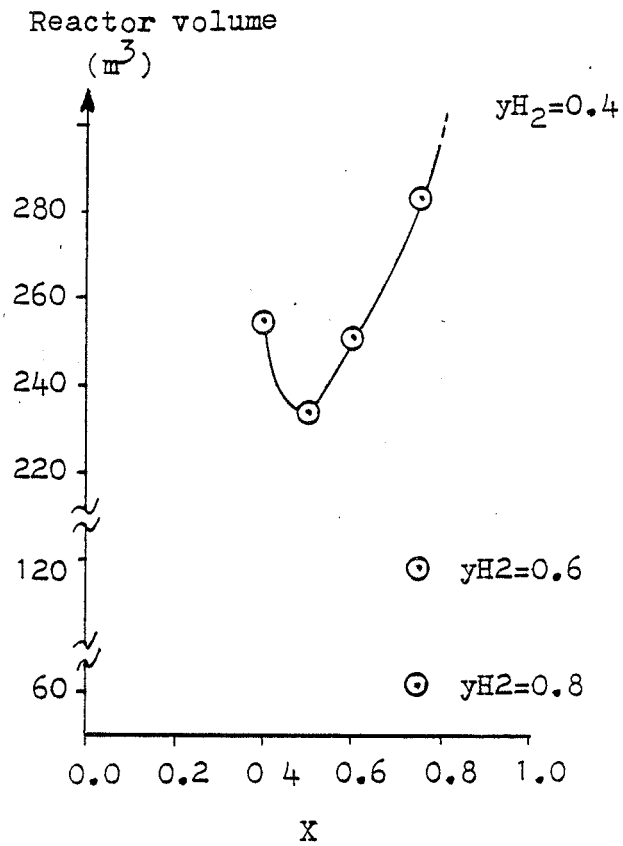


Figure 4.7.A

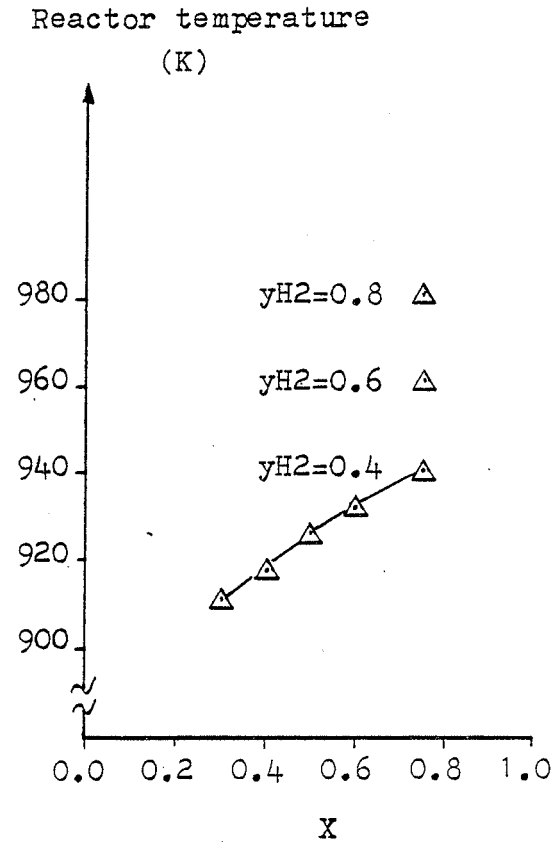


Figure 4.7.B

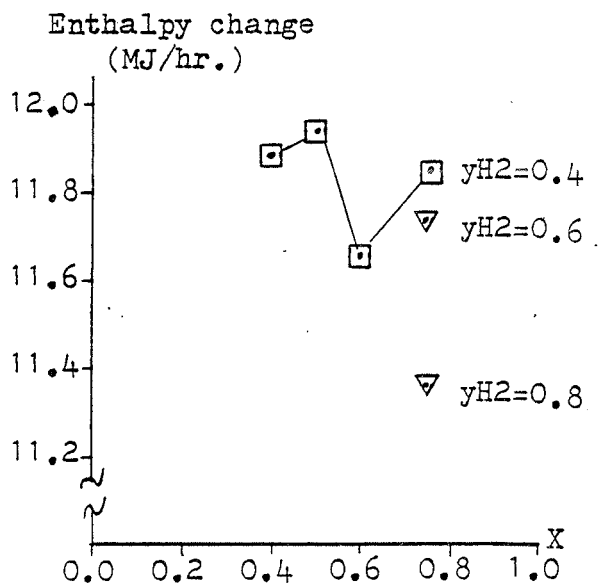


Figure 4.7.C

increment of "yH2" drives the operation of the reactor close to the maximum allowed temperature. For yH2=0.8 and X=0.75 the reactor reaches the upper outlet temperature bound of 980 K.

Figure 4.7.c correlates the enthalpy change in the reactor (enthalpy in the outlet stream minus enthalpy in the inlet streams) as a function of "X" and "yH2". Since the reaction in this case is exothermic, it provides heat to the system. As a result, between the given temperature bounds it is convenient to obtain high enthalpy changes to favor the heat integration procedure. Apparently, there is not a smooth correlation between "X" and changes in enthalpy, with the enthalpy change almost constant. On the other hand, by increasing the values of "yH2" the changes of enthalpy decrease.

The analysis of the last two figures leads to the following conclusions: (1) The reactor cost, determined by the degree of conversion, does not constitute a significant component of the total cost because the cost of energy is by far predominant. In fact, the reactor cost constitutes 10.2 % of the capital cost (for the case study where X=0.75 and yH2=0.4 in which the profit is higher). If the values of capital and energy cost are added, then the reactor cost constitutes only 1.7 %, for the same case study. However, in a heat integrated structure, cost of equipment may become more important. (2) The effects of "yH2" on the temperature of the reactor and on the change of enthalpy confirm previous conclusions that concentra-

tions higher than yH2=0.8 are not desirable in the process. However, the reactor cost (which is proportional the the reactor volume) is favored by increasing yH2.

Since the reactor does not require utility consumption, because it operates adiabatically, it follows that the energy cost target is not affected by its operation for a non-heat integrated process structure. However, the reactor operation at high values of yH2 (below 0.8) will favor the capital and energy cost targets for a heat integrated process structure. On the other hand, increasing the conversion, within the given bounds, favors the efficient operation of the reactor in terms of yield.

4.3.7.3 EVALUATION OF THE DISTILLATION TRAIN

In the liquid loop of the reference structure, three distillation columns [(C1), (C2) and (C3)] constitute the main operational units. Column C1 is a stabilizer column that eliminates the non-condensable gases from the liquid loop. Column C2 recovers the benzene product and column C3 separates diphenyl from the recycled toluene. These columns will be evaluated simultaneously.

(1) Operational bounds. In distillation it is desirable that cooling in the condenser be done using water (available at about 300 K), and the heating in the reboiler be performed using steam (maximum recommended temperature is 500 K). To satisfy these conditions, the pressures in the distillation columns have been set in the simulation model at 1100 kPa (C1),

and at 170 kPa (C2). The pressure of column C3 is set also at 170 kPa, but the reboiler temperature is 550 K. To obtain a bottoms temperature lower than 500 K in column C3 requires vacuum operation which is expensive. A heat integrated structure will avoid the need of introducing a hot process fluid for the reboiler of C3.

(2) Behavior in the simulation. Simulations of the example problem show that the stabilizer distillation column (C1), has a narrow range of stability for the given specifications. Short-cut methods using the Fenske-Underwood-Gilliland correlations failed to converge due to failure of the bubble point relations at the top part of the column. It was necessary to simulate C1 using the rigorous "sure" method available in PROCESS [SimSci, 1983]. For the specifications assigned to this column (distillate to bottoms mole ratio for methane is 50,000 and for benzene is 0.005), the computations converged (for a wide range of feed compositions) only for 15 trays and at an input temperature of 410 K.

The distillation column for the separation of diphenyl (C3), was difficult to simulate with the Fenske-Underwood-Gilliland method (failure in the Underwood calculations). This was probably due to the fact that toluene and diphenyl do not define a sharp split, [SimSci, 1983]. To overcome this problem, while satisfying the constraints inherent to the reference structure (see Section 4.3.2), the following specifications have been used: the mole fraction of diphenyl in the distillate is 0.0005,

and the mole fraction of toluene in the bottoms is 0.01, for an operating pressure of 170 kPa.

(3) Analysis of goals. Column C1 performs a strictly necessary goal which is to eliminate the non-condensable vapors. Column C2 also performs a strictly necessary task, to recuperate benzene as the main product. The goal of column C3 (recuperation of diphenyl) is not strictly necessary, since the diphenyl can be recirculated.

(4) Lumping of units. Since columns C2 and C3 operate at the same pressure (170 kPa) they can be transformed into a single column with a sidedraw. This possibility is also justified by the fact that C3 is a relatively small column (due to the small amount of diphenyl produced). Column C1 operates at much higher pressure (1100 kPa), therefore it is difficult to lump it to C2.

(5) Sensitivity of each of the columns to changes in the core variables. Figures 4.8.a and 4.8.b show the influence of the "core variables" in the flow rates of the columns. Conversion determines the flow rates of the columns, especially of column C3 (separation of diphenyl from toluene). "yH2" has no influence on the columns at all.

Figure 4.8.c presents the contribution of each one of the distillation columns to the energy cost. Column C3 for values close to the lower bound of "X" (X=0.4), contributes more than 25 % of the total energy cost. In the region near the upper bound of "X" (X=0.75), the contribution of C3 to the total

FIGURE 4.8: EVALUATION OF THE DISTILLATION COLUMNS WITH RESPECT TO THE CORE VARIABLES

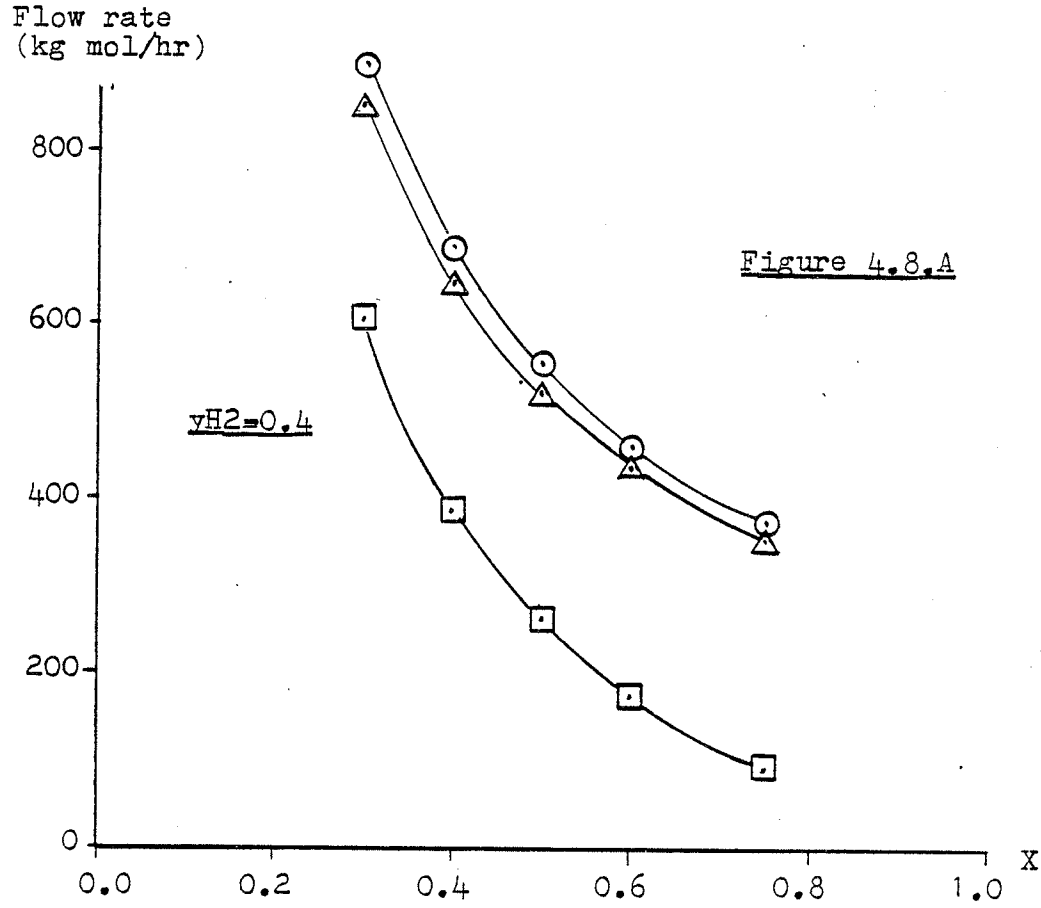


Figure 4.8.A

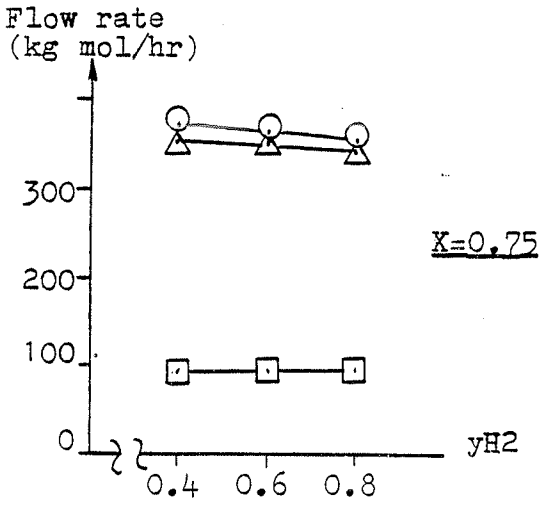


Figure 4.8.B

Symbology:
○ Column C1
△ Column C2
□ Column C3

Figure 4.8.C

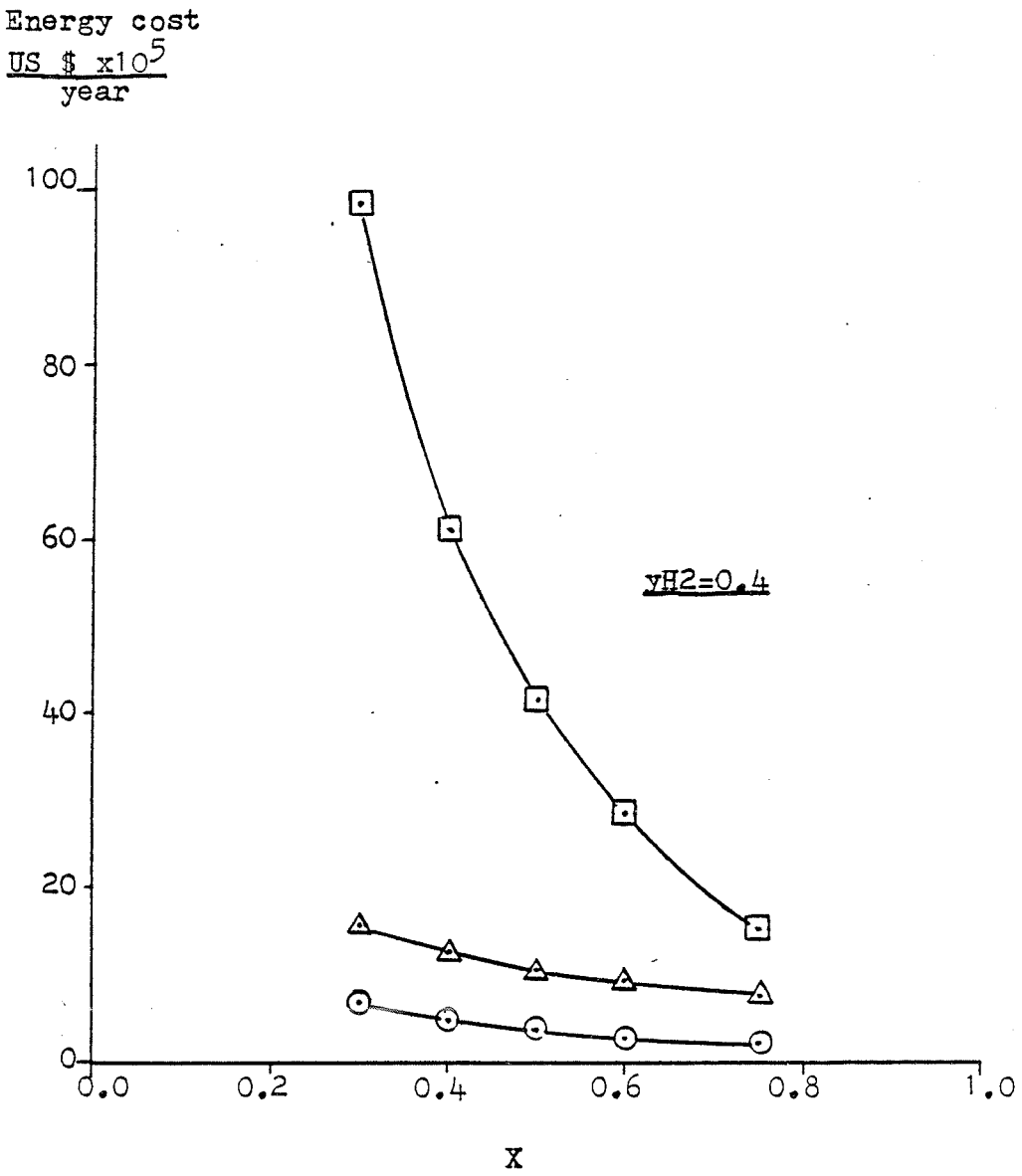
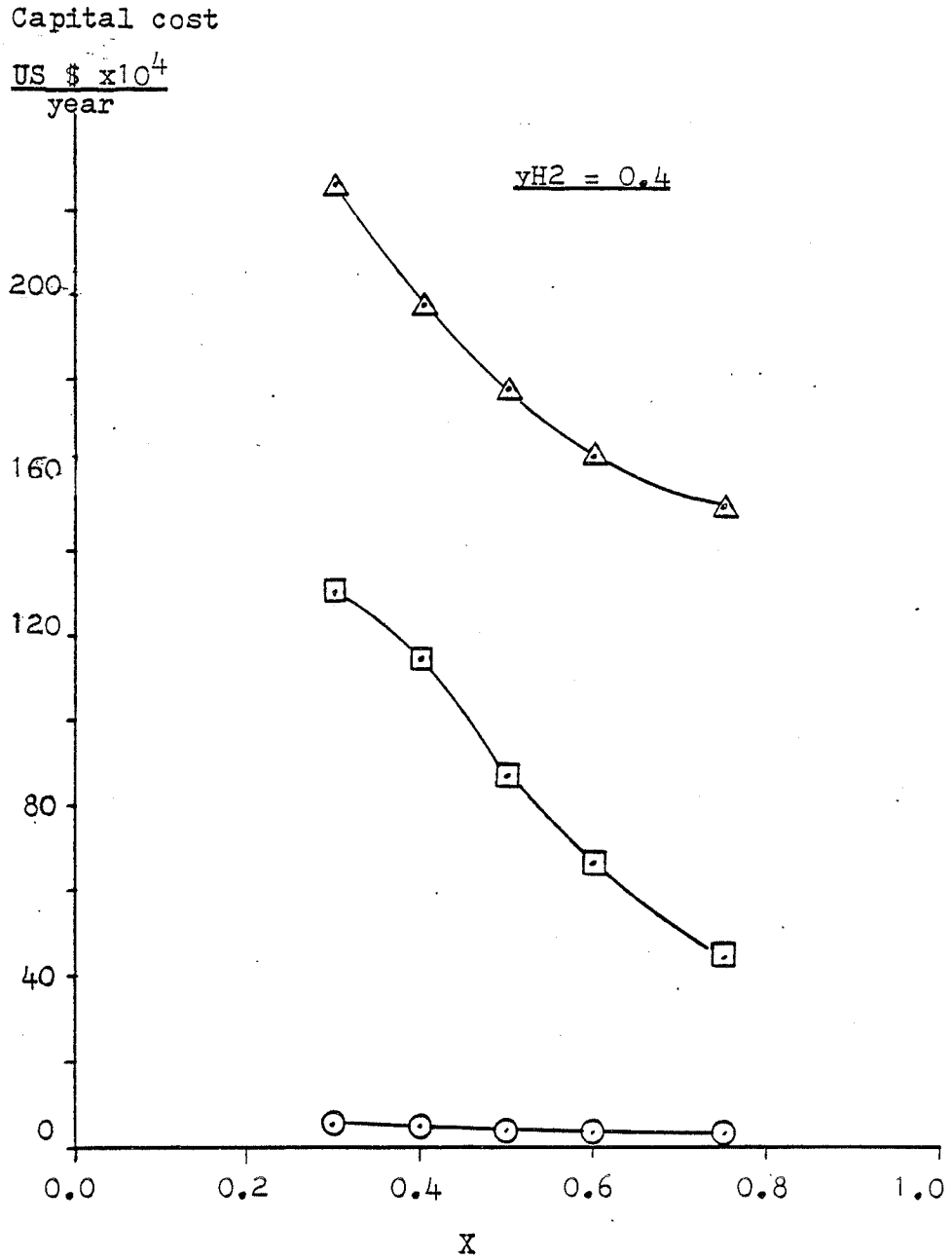

Energy cost
US $ x10^5
year
100
80
60
40
20
0
0.0
0.2
0.4
0.6
0.8
1.0
X
yH2=0.4

Figure 4.8.D


Capital cost
US $ x10^4
year
yH2 = 0.4
200
160
120
80
40
0
0.0
0.2
0.4
0.6
0.8
1.0
X

energy cost is still significant (approximately 18%). The least expensive column in terms of energy costs is column C1.

Figure 4.8.d shows the contribution of each column to the capital cost. C2 is the most expensive one, comprising approximately 9 % of the total capital cost at the upper bound of "X". Columns C1 and C3, represent 1.8 % and 2.6 % of the total capital cost at the upper bound of X (X=0.75), respectively. The low capital cost contribution by the distillation columns is due to the high cost of the furnace units H1 and H2 (refer to Figure 4.5). For a heat integrated structure, however, the capital cost of the distillation columns is more important.

From the above analysis, the following conclusions can be stated: (1) The liquid loop is mainly defined by the core variable "X". (2) Column C1 does not constitute an important unit in terms of energy consumption or capital cost. (3) Column C2 is the most expensive piece of equipment, with an operation cost of approximately 13 % of the total energy cost. (4) Column C3 is the unit with the highest sensitivity to changes in "X", representing an average of 22 % of the total energy cost in the region near the upper bound of "X". In addition, it is important to recall that the reboiler temperature for C3 is aproximately 550 K. For a non heat integrated structure C3 would require the use of a hot oil system.

4.3.7.4 EVALUATION OF THE RELATIVE IMPORTANCE OF OTHER UNITS

The units that conform the gas loop, i.e., splitter, compressor and furnace H1, are highly dependent on the flow rate

of the gas recycle stream, which, in turn, is determined by "yH2". It is important to mention that the goal of splitter S1 is not stricly necessary, since the build up of methane can be avoided by using a separator instead of a purge.

The performance of the compressor depends on the structure of the gas loop. For example, if a separator is used instead of the splitter S1, then the compressor will be located after the separator, and the amount of gas compressed will depend on the operation of the separation unit.

4.3.8 MINIMUM UTILITY REQUIREMENTS FOR THE REFERENCE STRUCTURE

Following the procedure proposed by Linhoff and Flower [1978], the minimum utility requirements have been determined for the reference structure. The minimum cold utility is equal to 7790 MJ/h. The minimum hot utility is equal to 16261. The pinch point temperature is 405 K. Refer to Appendix H for details in the computation procedure.

4.3.9 MODIFICATION OF THE TOPOLOGY OF THE REFERENCE STRUCTURE

Through the parametric analysis it has been observed that:

(1) A high concentration of hydrogen in the gas recycle stream reduces the cost of energy and equipment in the gas recycle loop. However, to obtain a high concentration of hydrogen with the given process structure it is necessary to increase the amount of material purged, leading to very low values of the NVP. Therefore, a very competitive process structure would be one that can keep the hydrogen concentration

at a relatively high value, without purging a significant amount of valuable material. Consequently, a topological modification in the gas recycle loop of the "reference structure" is desirable. Candidate alternatives are the ones shown in Figure 4.2.d and 4.2.e.

(2) The distillation column C3 has a not strictly necessary goal. C3 is highly sensitive to changes in conversion, and it represents approximately 22 % of the total energy cost for values of conversion close to the upper bound (X=0.75). Besides, the simulation shows that the reboiler of column C3 operates at a temperature greater than 550 K, which will require the use of a thermal fluid or a furnace for a non-heat integrated process structure.

In addition, the separation of diphenyl in this process system is not strictly necessary because it is formed by a reversible reaction. The complete recycling of diphenyl to the reactor will not damage the performance of the system. Moreover, the difficulty of simulating this unit and its high sensitivity to conversion changes might indicate unstable operation of C3. The above considerations, which are valid also if C3 is lumped to C2, strongly suggest the elimination of the column C3 from the system.

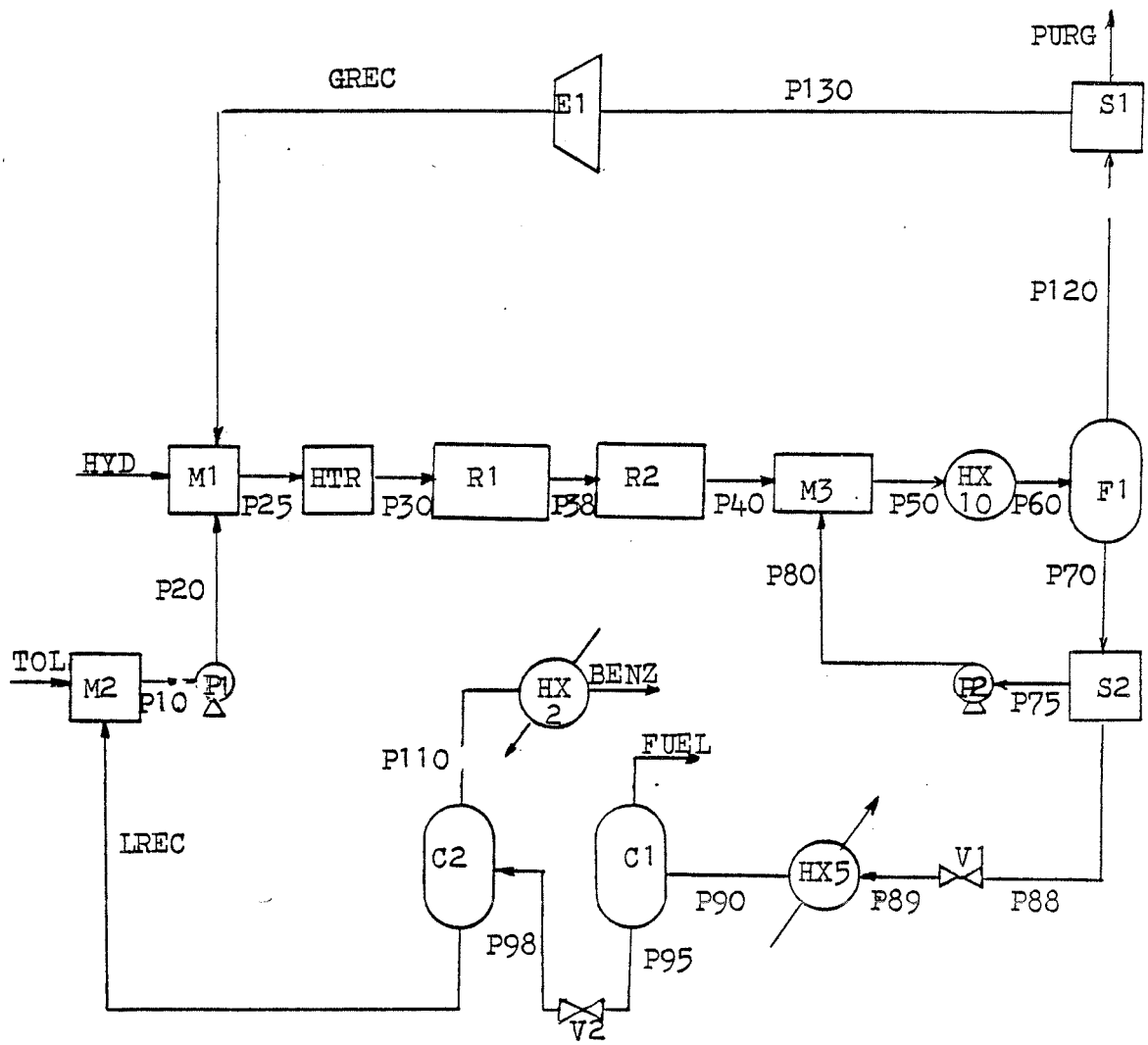
The topological modification to be introduced is the elimination of column C3. The conclusions from the parametric analysis reduce the initial set of alternative process structures to just two, which are represented by Figure 4.2.c and 4.2.d.

A diagram of the "modified" process structure is presented in Figure 4.9.a. Note also that only one furnace has been considered in this structure, reducing in this way the installation cost for this unit. Simulation of the new process structure reveals that a reduction of 12.5 % in energy cost has been achieved (with no heat integration) with respect to the reference structure. The reduction in the capital cost is only 1.2 % since the complete recirculation of diphenyl leads to an increase in the size of other units.

In order to achieve convergence in the simulation of the modified process structure, the model for the reactor R2 has been modified from a conversion model to an equilibrium one [SimSci,1983]. The expression used for the equilibrium constant ($\ln K=-1.734038 + 1.516.26/T$) is a simplified version of the one presented by Dasgupta and Malti [1986].

Simulation results show that potential parametric improvements can be obtained by relaxing some constraints stated in the problem formulation. For example, a slight reduction in the hydrogen/aromatics ratio at the reactor inlet (from 4.92 to 4.20) for the modified non-heat integrated process structure (Figure 4.9.a) significantly improves the process performance. The results for the economic targets, in millions of dollars per year, are:

FIGURE 4.9.A : MODIFIED PROCESS STRUCTURE



H2/aromatics	NVP	EC	CC	Profit
4.20	10.258	7.076	1.612	1.570
4.92	9.718	7.261	1.672	0.785

(The core variables were set at: X=0.75, yH2=0.4)

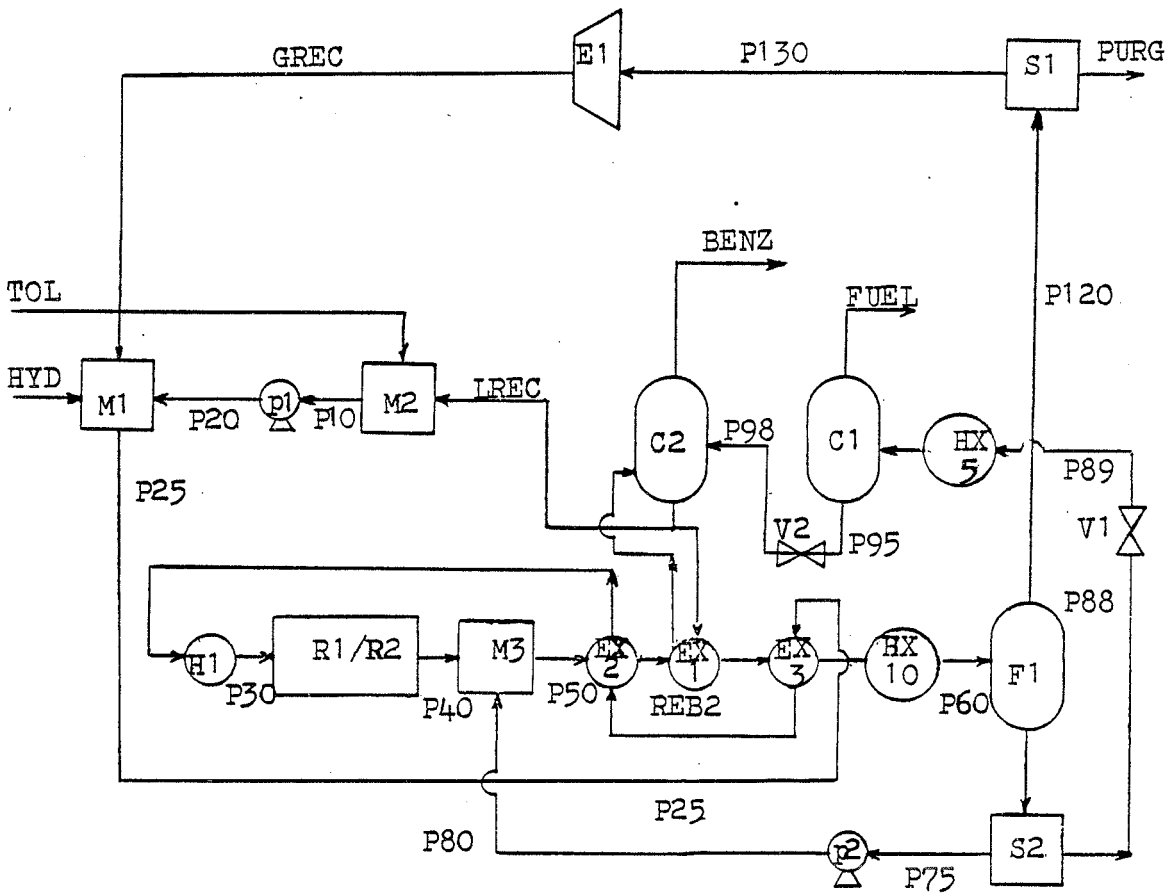
Observe that all the economic targets (NVP,EC and CC) are favored by the reduction in the hydrogen to aromatics ratio. This is due to the corresponding reduction in the flow rate of the gas recycle stream.

If the constraint that heat exchangers cannot operate at temperatures above 895 K is relaxed, then the recirculation of the liquid stream P80 (see Figure 4.9.a) to quench the reactor outlet stream might be eliminated, providing an important source of heat for the heat integration procedure.

4.3.10 EVALUATION OF ENERGY BENEFITS INTRODUCED BY TOPOLOGICAL MODIFICATIONS

The results of the heat integration potential for the modified process structure applying heat integration [Linhoff and Hindmarsh, 1983] show that the minimum cold utility requirement is equal to 9000 MJ/h and the minimum hot utility is 6686 MJ/h (refer to Appendix G for details). This implies an increment of the minimum cold utility, with respect to the reference structure, of 15.5 %; and a reduction of the minimum hot utility equivalent to 41.1 %. Therefore, the potential savings in the hot utility justify the topological modifications

FIGURE 4.9-B : HEAT INTEGRATED PROCESS STRUCTURE



performed. This result is in agreement with the energy savings reported for a non-heat integrated modified structure (refer to Table 4.1).

4.3.11 HEAT INTEGRATION OF THE MODIFIED PROCESS STRUCTURE

Applying the technique proposed by Linhoff and Hindmarsh [1983], heat integration has been performed for the modified process structure. The heat integrated modified structure is presented in Figure 4.9.b. The energy savings obtained with the heat integrated structure are enormous. Also, important savings in equipment cost are achieved due to the reduction of the furnace capacity. Results are presented in Table 4.1.

TABLE 4.1

COMPARISON OF TARGETS FOR PROCESS STRUCTURES

Values for core variables: X = 0.75, yH2 = 0.4

Results are given in millions of US Dollars per year

STRUCTURE	NVP	CC	EC	PROFIT
Reference	8.995	1.692	8.291	-0.989
Modified	9.718	1.672	7.261	0.785
Heat int. modified	9.718	1.118	1.823	6.777

The results show the advantage of eliminating column C3. The economic advantage of lumping furnaces H1 and H2 into one unit (HTR), has not been computed by the simulation model because of the simplicity of the furnace economic model (which is formulated only as a function of duty).

4.4 CONCLUSIONS OF THE APPLICATION OF THE PROPOSED HEURISTIC PROCEDURE

The following conclusions can be stated from the application of the proposed heuristic-evolutionary procedure to the hydrodealkylation of toluene to produce benzene (example problem):

1) The proposed procedure is consistent and in fact leads to the selection of competitive alternative process structures for a given process system.

2) The results of the example problem illustrate the validity of assumption (1), Section 3.4, which states that in the initial design stage structural modifications have more impact on the optimization function than do parametric modifications on the design variables. For example, tuning the values of the reflux ratios for the distillation columns results in cost savings of 2.3 %. On the other hand, the topological modifications introduced (with no heat integration) lead to energy savings of 12.5 %.

3) The parametric evaluation of the "reference structure", as proposed in Step 7 of the heuristic method, has provided important criteria to perform topological modifications on that structure approaching the maximal profit (objective function). In this way, assumption (2), Section 3.4, has been validated for the example problem.

4) The procedure leads to the reduction of the search space. In the example problem, the following bounds have been identified for the core variables: X=0.4 to 0.75, and yH2=0.4 to 0.8. The upper bound of yH2 is valid for any process structure, because its violation will cause coking in the reactor. For the modified structure shown in Figure 4.9.a and 4.9.b the upper bound of 0.6 for yH2 is recommended.

5) The evaluation of targets in the proposed procedure (i.e., NVP, CC and EC) has proven to be useful to guide the decisions for structural modifications. This is because: (1) the relative importance of these targets suggests what type of structural changes are desirable, and (2) the sensitivity of the major operational units, while modifying the core variables with respect to these targets, indicates which units may favor the desired changes.

The application of the proposed heuristic procedure to the example problem shows that the energy cost is more important than the capital cost (8.29 compared to 1.69 million dollars per year, respectively). Therefore, the desired structural modifications must reduce the energy cost. In fact, the elimination of the distillation column C3 satisfies this objective.

6) The procedure provides criteria to evaluate new process alternatives. The parametric analysis performed as part of the heuristic shows the relative importance of each of the major units in the system. This analysis also reveals the sensitivity of the major units with respect to variations in the core variables. These results are not only valid for the

"reference structure", but for other process structures that have similar operational units. For example, the conclusions about the reactor and the distillation train are valid for any process alternative.

7) The application of the proposed heuristic method shows that the evaluation of structural alternatives, and their improvement by introducing topological modifications, does not require finding optimum values for the design variables of the operational units.

8) The parametric analysis of the core variables (Step 7 of the proposed heuristic) also helps to "tune up" the values of the core variables, improving the initial estimates.

9) The hierarchical procedure proposed by Douglas [1985] to formulate a base-case design, generates the reference structure shown in Figure 4.1. Douglas' method is mainly focused on "tuning up" the core variables rather than improving the topology of the process structure. Douglas and Woodcock [1985], by means of "cost diagrams" identify potential savings, for the reference structure, by completely recirculating the diphenyl and by changing the structure of the gas loop. However, the estimation made by Douglas and Woodcock is based only on rough cost evaluations. The parameter "Level 4a" defined by Douglas [1985] in order to check the efficiency of the gas recycle loop (constituted by the reactor R1/R2, the splitter S1, the compressor E1 and the furnace H1) proved to be useful. But, Douglas' definition for Level 4a did not consider the important effect of furnace H1, leading to inaccurate conclusions: the greater the

value of the conversion, the less the amount of energy saved (refer to Figure 4.6.e).

10) The results of the procedure also suggest the importance of modifying the gas recycle loop, which shows that alternative 4.2.d of Figure 4.2 is an important candidate.

11) Simulation results show that potential parametric improvements can be obtained by relaxing some constraints stated in the problem formulation. For example, a slight reduction in the hydrogen/aromatics ratio at the reactor inlet (from 4.92 to 4.20) for the modified non-heat integrated process structure (Figure 4.9.a) improves the profit by 100 % (from $ 0.785 to $ 1.571 million per year).

If the constraint that heat exchangers cannot operate at temperatures above 895 K is relaxed, then the recirculation of the liquid stream, P80, (see Figure 4.9.a) to quench the reactor outlet stream might be eliminated, providing an important source of heat for the heat integration procedure.

CHAPTER FIVE

CONCLUSIONS

CONCLUSIONS REFERED TO THE LITERATURE REVIEW

1) The synthesis of entire processes is in a very early stage of development. Whole process synthesis can be stated formally as a multi-objective, mixed-integer, non-linear programming problem, but most of the research done so far reduces the synthesis to a single-objective problem.

2) There have been several proposed procedures to automatically generate structural alternatives. Most of them screen the structural alternatives based on heuristic rules, but these rules have not been sufficiently proved to be used with confidence. Therefore, a major problem in process synthesis is to find appropriate methods to screen among a set of structural alternatives and reduce the number of alternatives to select only the most promising ones.

3) Most of the authors agree that the generation of structural alternatives can be treated as an evolutionary procedure, oriented by heuristics, in which a hierarchy of decisions is solved. A serious problem is to detect when a decision at a certain level in the evolutionary procedure is going to negatively affect decisions at a later stage.

4) Once a set of structural alternatives has been identified, the analysis of processes is suggested as the tool that

can lead to a better understanding of the phenomena involved and, hopefully, to validate heuristics for the evaluation of these alternatives. This expectation is motivated by the success of the thermodynamic analysis in heat integration and distillation sequencing.

5) In addition to the optimization with respect to an economic objective function, other objectives such as operability, reliability, or controllability should be incorporated in order to end up with a "workable" system. However, there is no agreement on how to implement the multi-objective formulation.

6) Two basic elements of process synthesis applied to entire processes have not been treated sufficiently in the existing literature. They are:

. The only representation available for the synthesis of entire processes traditionally is the "flow diagram". In the author's opinion, such a representation is not sufficient for the ambitious task of synthetizing entire processes. For the systematization of the enormous amount of information generated in the synthesis procedure, it is necessary to develop substitute or complementary forms of representation.

. The thermodynamic analysis has been used to set boundaries that allow the identification of inefficient energy process structures. However, other type of bounds should be incorporated to the synthesis procedure, to reduce the searching space of the structural alternatives, for example, the maximum net value of products.

CONCLUSIONS REFERED TO THE PROPOSED HEURISTIC-EVOLUTIONARY PROCEDURE

7) A procedure has been proposed for the preliminary selection of competitive process structures from an initial set of process structures. This procedure is not intended to generate process structures, but to evaluate them. The proposed procedure uses heuristic rules organized in a hierarchical fashion and allows making decisions sequentially. The decisions taken during the procedure are reviewed in a later stage.

8) The screening procedure is conceived as an optimization problem. This optimization has a single objective: to maximize the profit of the process structure. It is performed in terms of the independent variables of the material balance equations.

9) The proposed heuristic procedure presents the following characteristics: (a) classifies the initial set of process structures in terms of the goals of material operators and the interaction among them (material operators are: reactors, separators, mixers and splitters); (b) identifies bounds and constraints in order to reduce the search space; (c) considers three targets to guide the decisions, i.e., the net value of products, the energy cost and the capital cost; and (d) analyses the effect in changes of the independent variables of the material balance equations in a "reference structure" in order to identify potential topological improvements.

The following conclusions are stated based on the application of the proposed heuristic evolutionary procedure to an

example problem, the hydrodealkylation of toluene to produce benzene.

10) The application of the proposed procedure shows that it is consistent and in fact leads to the selection of competitive alternative process structures for a given process system.

11) The application of the proposed procedure illustrates the validity of Assumption (1), Section 3.4, which states that in the initial design stage structural modifications have more impact on the optimization function than do parametric modifications on the design variables.

12) The parametric evaluation of the "reference structure", as proposed in Step 7 of the heuristic method, has provided important criteria to perform topological modifications on that structure approaching the maximal profit (objective function). In this way, Assumption (2), Section 3.4, has been validated for the example problem.

13) The procedure leads to the reduction of the search space. In the example problem, the following bounds have been identified for the core variables: X=0.4 to 0.75, and yH2=0.4 to 0.8. The upper bound of yH2 is valid for any process structure, because its violation will cause coking in the reactor. For the modified structure shown in Figure 4.9.a and 4.9.b the upper bound of 0.6 for yH2 is recommended.

14) The evaluation of targets in the proposed procedure (i.e., NVP, CC and EC) has proven to be useful to guide the decisions for structural modifications. This is because: (1) the relative importance of these targets suggests what type of

structural changes are desirable, and (2) the sensitivity of the major operational units, while modifying the core variables with respect to these targets, indicates which units may favor the desired changes.

The application of the proposed heuristic procedure to the example problem shows that the energy cost is more important than the capital cost (8.29 compared to 1.69 million dollars per year, respectively). Therefore, the desired structural modifications must reduce the energy cost. In fact, the elimination of the distillation column C3 satisfies this objective.

15) The procedure provides criteria to evaluate new process alternatives. The parametric analysis performed as part of the heuristic shows the relative importance of each of the major units in the system. This analysis also reveals the sensitivity of the major units with respect to variations in the core variables. These results are not only valid for the "reference structure", but for other process structures that have similar operational units. For example, the conclusions about the reactor and the distillation train are valid for any process alternative.

16) The application of the proposed heuristic method shows that the evaluation of structural alternatives, and their improvement by introducing topological modifications, does not require finding optimum values for the design variables of the operational units.

17) The parametric analysis of the core variables (Step 7 of the proposed heuristic) also helps to "tune up" the values of the core variables, improving the initial estimates.

18) The hierarchical procedure proposed by Douglas [1985] to formulate a base-case design, generates the reference structure shown in Figure 4.1. Douglas' method is mainly focused on "tuning up" the core variables rather than improving the topology of the process structure. Douglas and Woodcock [1985], by means of "cost diagrams", identify potential savings for the reference structure by completely recirculating the diphenyl and by changing the structure of the gas loop. However, the estimation made by Douglas and Woodcock is based only on rough cost evaluations. The parameter "Level 4a" defined by Douglas [1985] in order to check the efficiency of the gas recycle loop (constituted by the reactor R1/R2, the splitter S1, the compressor E1 and the furnace H1) does not consider the important effect of furnace H1, leading to inaccurate conclusions (refer to Figure 4.6.e).

19) The results of the procedure also suggest the importance of modifying the gas recycle loop, which shows that alternative 4.2.d of Figure 4.2 is an important candidate.

20) Simulation results show that potential parametric improvements can be obtained by relaxing some constraints stated in the problem formulation. For example, a slight reduction in the hydrogen/aromatics ratio at the reactor inlet (from 4.92 to 4.20) for the modified non-heat integrated process structure

(Figure 4.9.a) improves the profit by 100 % (from $ 0.785 to $ 1.571 million per year).

If the constraint that heat exchangers cannot operate at temperatures above 895 K is relaxed, then the recirculation of the liquid stream, P80, (see Figure 4.9.a) to quench the reactor outlet stream might be eliminated, providing an important source of heat for the heat integration procedure.

RECOMMENDATIONS

1) It is necessary to apply the heuristic-evolutionary procedure proposed in this thesis to the other example problems in order to validate and improve the procedure.

2) It is recommended to formulate a general methodology to identify the independent variables of the material balance equations, in particular, for complex process structures.

3) It is recommended to formulate new forms of representation to systematically organize the information generated along the selection of alternative process structures.

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APPENDIX A

EXAMPLE PROBLEM: HYDRODEALKYLATION OF TOLUENE TO PRODUCE BENZENE

This appendix presents the statement of the example problem: the hydrodealkylation of toluene to produce benzene.

The conversion (X) is defined as the fraction of toluene moles that react to produce benzene. The selectivity (S) is equal to the number of benzene moles produced for each mole of toluene converted. Selectivity and conversion are related by the following equation:

$$S = 1.0 - 0.0036/(1 - X)^{1.544} \qquad (4.3)$$

where the symbol "**" means raised to the power ...

At the reactor inlet the mole ratio of hydrogen with respect to aromatics is 5:1, where the aromatics are the sum of the benzene, toluene and biphenyl present. The reactor operates at a pressure of 3450 kPa. The inlet temperature to the reactor must be greater than 895 K and the outlet temperature must be less than 980 K to avoid coking. A tubular, adiabatic reactor is recommended. A length to diameter ratio of 6:1 is recommended for the reactor. The reactor requires 6 inches of internal insulation to maintain the wall temperature of the shell at 755 K.

The reaction rate in terms of toluene moles converted is given by:

$$rTol = - k [Tol] [H2]^{0.5} \qquad (4.4)$$

where the quantities inside the brackets represent the toluene and hydrogen molar concentration, respectively. The rate constant is:

$$k = 6.3E10\ (gmole/lt)^{-.5}\ (sec^{-1})\ EXP[-52000cal/gmole/RT] \qquad (4.5)$$

where R is the universal gas constant and T is the absolute temperature in K.

A preliminary flow diagram for the process is shown in Figure 4.1. The reactor has two feed streams: the liquid stream and the gas stream. The liquid stream contains mainly of toluene and results from mixing the fresh toluene feed with the liquid recycle. The gas stream is the fresh hydrogen, feed and the gas recycled. The recycle gas contains at least 40 % hydrogen with the rest mainly methane.

The fresh toluene is available with a purity of 100 % at 293 K and a pressure of 101 kPa. The fresh hydrogen contains 95 mole % hydrogen and the rest is methane. This stream is available at 311 K and 3790 kPa.

The reactor effluent has to be quenched to 895 K, at least, before entering a heat exchanger. The reactor effluent is

cooled down to aproximately 310 K in order to be fed to a flash separator. The gas effluent from the flash is partially purged to keep the hydrogen concentration to a defined value and the rest of it is recompressed and recirculated.

The liquid effluent from the flash is distillated: first to eliminate the non-condensable gases; second, to separate the benzene; and, finally to separate the diphenyl. The top product from the last column is recirculated.

In the first column, the distillate to bottoms mole ratio for methane is 50,000 and for benzene is 0.005. The toluene losses have to be less than 1 % of the net toluene feed. In the liquid recycle stream the maximum allowable content of benzene is 4.0 mole percent; the diphenyl content has to be less than 25 mole percent of net diphenyl make.

The three distillation towers have valve-type trays. They will use kettle type reboilers with a maximum heat flux of 12,000 BTU/hr/sq.ft.

The overall heat transfer coefficient for the process fired-heater is assumed as 16000 BTU/hr/sq.ft. The maximum permissible radiant extraction from the hot flue gas can then be 50 % of the available fired heat. The pressure drop in this unit can be assumed as 70 psi.

The compressor has an efficiency of 70 %. [AIChE, Student Contest Problem (SCP), 1967]

APPENDIX B

DERIVATION OF THE MATERIAL BALANCE EQUATIONS OF THE REFERENCE STRUCTURE

This appendix presents the derivation of the material balance equations of the reference structure corresponding to the hydrodealkylation of toluene to produce benzene.

BASES OF THE DERIVATION

In the hydrodealkylation of toluene to produce benzene the most important reactions are:

$$2\ C_6H_5CH_3 + H_2 \longrightarrow 2\ C_6H_6 + 2\ CH_4 \qquad (B.1)$$

$$2\ C_6H_6 \longrightarrow (C_6H_5)_2 + H_2 \qquad (B.2)$$

A constraint of the problem is that the ratio of hydrogen to aromatics at the reactor inlet should be 5:1. The toluene feed is 100 % pure and the gas feed is composed of 95 % hydrogen and 5 % methane.

NOMENCLATURE

Bz	moles of benzene produced
Ftol	moles of fresh toluene feed
Di	moles of diphenyl produced
Rgas	moles of gas recycled
Hyd	moles of fresh gas feed
Tol	moles of toluene at the reactor inlet
Purg	moles of gas purged from the system
X	conversion
S	selectivity

DERIVATION OF MATERIAL BALANCE EQUATIONS

By definition:

$$S = Bz/Ftol \quad or \quad Ftol = Bz/S \tag{B.3}$$

The diphenyl produced is equal to the toluene not converted to benzene:

$$Di = Ftol\ (1 - S)/2 \tag{B.4}$$

Replacing Equation (B.3) in the Equation (B.4):

$$Di = Bz\ (1-S)/2S \tag{B.5}$$

Performing a toluene balance

$$Tol = Ftol + Tol\ (1 - X)$$

The above expression is simplified to:

$$Tol = Ftol/X \tag{B.6}$$

Condition at the reactor inlet

$$0.95\ Hyd + yH2\ Rgas = 5\ Tol \tag{B.7}$$

Replacing Equation (B.3) into Equation (B.6)

$$Tol = Bz/SX \tag{B.8}$$

Replacing Equation (B.8) into Equation (B.7)

$$0.95\ Hyd + yH2\ Rgas = 5\ Bz/SX \tag{B.9}$$

Solving Equation (B.9) for Rgas

$$Rgas = (5\ Bz/SX - 0.95\ Hyd)/yH2 \tag{B.10}$$

Balance for methane

$$0.05\ Hyd + Bz/S = (1 - yH2)\ Purg \tag{B.11}$$

Balance for hydrogen

$$0.95\ Hyd = Tol\ X - Di + yH2\ Purg \tag{B.12}$$

Replacing Equations (B.8) and (B.5) into Equation (B.12)

$$0.95\ Hyd = Bz/S\ [1 - (1 - S)/2] + yH2\ Purg \tag{B.13}$$

Solving simultaneously Equations (B.11) and (B.13)

$$Hyd = Bz/(0.95 - yH2)\ [1- (1-yH2)(1-S)/2] \qquad (B.14)$$

From equation (B.13)

$$Purg = Fgas + Bz\ (1 - S)/2S \qquad (B.15)$$

APPENDIX C

INPUT FILE TO THE "PROCESS" SIMULATION

This appendix presents the input file to the PROCESS simulator corresponding to the simulation of the reference structure.

```
VERSION 0484
***********

       SM                                                              119
PROCESS   INPUT LISTING - PAGE  1

TITLE PROJECT=BENZENE3,PROBLEM=CASE 4.1,USER=L.MIRANDA,DATE=07-11-86
 $
 $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
 $                                                                       $
 $    THIS PROGRAM CACULATES THE MATERIAL AND ENERGY BALANCES FOR        $
 $    THE THERMAL HYDRODEALKYLATION OF TOLUENE TO PRODUCE BENZENE        $
 $    A SIDE REACTION IS THE EQUILIBRIUM CONVERSION OF BENZENE TO        $
 $    DIPHENYL.  A PLUG FLOW REACTOR IS ASSUMED                          $
 $                                                                       $
 $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
 $                                                                       $
 $$$$$$$$$$$$$$$$$$$$ MAIN VARIABLES: X=0.4; YH2=0.4   $$$$$$$$$$$$$$$$
 $
 DIMENSION SI
 PRINT INPUT=NONE
 EXERGY TZERO=298.15
 TOLERANCE BUBBLEPT=0.01,COMPONENT=0.01
 CALCULATION NOTRIAL=25
COMPONENT DATA
 LIBID 1,HYDROGEN/2,METHANE/3,BENZENE/4,TOLUENE/5,BIPH
THERMODYNAMIC DATA
 TYPE SYSTEM=SRK,LIQD=RACKETT,VAPD=SRK
STREAM DATA
 PROP STRM=HYD,TEMP=311,PRES=3790,PHASE=V,RATE=480.7,COMP=95/5
 PROP STRM=TOL,TEMP=293,PRES=101,PHASE=L,RATE=267.1,COMP=4,100
 PROP STRM=GREC,TEMP=328,PRES=3790,PHASE=V,RATE=7205.8,COMP=40/60
 PROP STRM=LREC,TEMP=393,PRES=350,PHASE=L,RATE=400.7,COMP=4,80/20
 PROP STRM=P150,TEMP=895,PRES=3790,PHASE=V,RATE=7686.5,COMP=65/35
 PROP STRM=P80,TEMP=311,PRES=3450,PHASE=L,RATE=110,*
      COMP=0.57/4.91/70.02/23.2/1.3
UNIT OPERATIONS
 MIXER UID=M2,NAME=LIQMIXER
  FEED TOL,LREC
  PRODUCT L=P10
 PUMP UID=P1,NAME=FEEDPUMP
  FEED P10
  PRODUCT L=P20
  OPER PRES=3930,EFF=70
 HX UID=H2,NAME=FURNACE
  COLD FEED=P20,V=P30,DP=482
  SPEC COLD TEMP=895
 REACTOR UID=R1,NAME=TUBREACT1
  FEED P30,P150
  PRODUCT V=P38
  OPERATION PHASE=V,PRES=3450,TEMP=970,ADIABATIC,TMIN=890,TMAX=1200
  CALCULATION CONVERSION,REFPHASE=V
  STOIC 1,-1/2,1/3,1/4,-1
  BASE COMPONENT 4
  CONVERSION 0.4,0,0
 REACTOR UID=R2,NAME=TUBREACT2
  FEED P38
  PRODUCT V=P40
  OPERATION PHASE=V,PRES=3450,TEMP=937,ADIABATIC,TMIN=890,TMAX=1200
```

```
 CALCULATION CONVERSION,REFPHASE=V
 STOIC 1,1/3,-2,/5,1
 BASE COMPONENT 3
 CONVERSION 0.0079,0,0
MIXER UID=M3,NAME=QUENCH
 FEED P40,P80
 PRODUCT M=P50
HX UID=HX10,NAME=COOLER
 HOT FEED=P50,M=P60,DP=200
 SPEC HOT TEMP=311
 CONFIGURATION U=426,TPASS=2
 UTILITY WATER,TIN=300,TOUT=322
FLASH UID=F1,NAME=FLASH
 FEED P60
 PROD V=P120,L=P70
 ADIA DP=150
SPLITTER UID=S1,NAME=PURGE
 FEED P120
 PRODUCT V=PURG,V=P130
 SPEC STRM=PURG,RATE=481.7
COMPRESSOR UID=E1,NAME=COMPRESSOR
 FEED P130
 PRODUCT V=GREC
 OPERATION POUT=3790,TOUT=328
MIXER UID=M1,NAME=GASMIX
 FEED GREC,HYD
 PRODUCT V=P140
 TPSPEC DP=10
HX UID=H1,NAME=GASHEATER
 COLD FEED=P140,V=P150,DP=50
 SPEC COLD TEMP=895
SPLITTER UID=S2,NAME=RCOOL
 FEED P70
 PROD L=P75,L=P88
 SPEC STRM=P75,RATE=120
PUMP UID=P2,NAME=QUENCHPUMP
 FEED P75
 PRODUCT L=P80
 OPERATION PRES=3450,EFF=70
VALVE UID=VAL1,NAME=EXPANDER
 FEED P88
 PROD L=P89
 OPER PRES=1120
HX UID=HX5,NAME=HEATSTAB
 COLD FEED=P89,M=P90
 SPEC COLD TEMP=410
COLUMN UID=C1,NAME=STABILIZER
 PARAMETER TRAY=15,SURE=25
 FEED P90,8
 PROD OVHD=FUEL,23.4,BTMS=P95,411.6
 COND TYPE=1,PRES=1102
 HEAT 1,1,-0.5/2,15,5.0
 PRINT KEYL=2,KEYH=3
```

```
  PSPEC TOP=1108,DPCOL=29
  ESTIMATE CTEMP=295,RTEMP=475,TTEMP=305,BTEMP=455,RRATIO=0.55
  SPEC STRM=FUEL,COMP=3,FRACTION=0.014
  SPEC STRM=P95,COMP=2,FRACTION=0.0000009
  VARI HEAT=1,2
  TOLERANCE BUBBLE=0.05,ENTHALPY=0.01,COMPONENT=0.01
$  PLOT PROFILE,XCOMP=2/3,YCOMP=2/3
 HX UID=CON1,NAME=STABCOND
  UTILITY WATER,TIN=288,TOUT=308
  ATTACHED COLUMN=C1,TYPE=1
  CONFIGURATION U=511,TPASS=1
 HX UID=REB1,NAME=STABREB
  UTILITY STEAM,TSAT=510
  ATTACHED COLUMN=C1,TYPE=2
$
 VALVE UID=VAL2,NAME=DROP
  FEED P95
  PROD L=P98
  OPER PRES=170
SHORTCUT UID=C2,NAME=BENZENECOL
  FEED=P98
  PROD STRM=P110,PHASE=L,RATE=265
  PROD STRM=P100,PHASE=L,PRESSURE=170
  CONDENSER TYPE=4,TEMPERATURE=347
  CALCULATION MODEL=1,TRIAL=25,KEYL=3,KEYH=4,RRMIN=1.3
  NOTRAYS=5
  SPEC STRM=P100,COMP=3,FRACTION=0.0050
  SPEC STRM=P110,COMP=4,FRACTION(V)=0.0003
 HX UID=HX2,NAME=BENZCOOLER
  HOT FEED=P110,L=BENZ,DP=30
  SPEC HOT TEMPERATURE=298
 SHORTCUT UID=C3,NAME=TOLCOL
  FEED=P100
  PROD STRM=LREC,PHASE=L,PRESSURE=130,RATE=33.7
  PROD STRM=DIPH,PHASE=L,PRESSURE=190,RATE=19.1
  CONDENSER TYPE=3
  CALCULATION MODEL=1,TRIAL=20,KEYL=4,KEYH=5,RRMIN=1.2
$  PRINT TRIAL
  NOTRAYS=4
  SPEC STRM=DIPH,COMP=4,FRACTION=0.01
  SPEC STRM=LREC,COMP=5,FRACTION=0.0001
$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$                                                              $
$    COMPUTATION OF EQUIPMENT COST, ENERGY COST, MATERIALS COST $
$    AND PROFIT BY MEANS OF CALCULATOR FUNCTIONS                $
$                                                              $
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
CALCULATOR UID=KAL1,NAME=HYDRSET
 $ THIS CALCULATOR DETERMINES THE RATE OF THE
 $ STREAM 'HYD' IN ORDER TO SATISFY THE CONDITION
 $ H2/OIL=5:1.
       RETRIEVE P(1),STRM=GREC,COMP=1,RATE
```

```
      RETRIEVE P(2),STRM=P30,COMP=3,5,RATE
 $ COMPUTATION TO SATISFY THE EQUATION
 $ H2(GREC)+0.95(HYD)=5(P30)
      PROCEDURE
      V(1)=5.0*P(2)
      V(1)=V(1)-P(1)
      V(1)=V(1)/0.95
 $ STORE RESULT
      R(1)=V(1)
      RETURN
     CALCULATOR UID=K01,NAME=PUMPS COST
$
$ THIS FUNCTION DETERMINES THE CAPITAL AND
$ OPERATING COST FOR COMPRESSOR AND PUMPS
      RETRIEVE P(1),UNIT=P1,WORK
      RETRIEVE P(2),UNIT=P2,WORK
      RETRIEVE P(3),UNIT=E1,WORK
$
      PROCEDURE
$ COMPUTATION FOR PUMP P1
      V(1)=P(1)/60.03
      V(2)=V(1)**0.5
      V(2)=V(2)*2189.0  $COST P1
      V(3)=V(1)*31508.0$POWER P1
$ COMPUTATION FOR PUMP P2
      V(4)=P(2)/1.56
      V(5)=V(4)**0.5
      V(5)=V(5)*421.0   $COST P2
      V(6)=V(4)*819.0   $POWER P2
$ COMPUTATION FOR COMPRESSOR E1
      V(7)=P(3)/532.0
      V(8)=V(7)**0.93
      V(8)=V(8)*50508.0 $COST E1
      V(9)=V(7)*279236.0$POWER E1
$ ADDING CAPITAL COSTS
      V(10)=V(2)+V(5)
      V(10)=V(10)+V(8)
$ ADDING POWER COSTS
      V(11)=V(3)+V(6)
      V(11)=V(11)+V(9)
$ STORING RESULTS
      R(1)=V(2)     $COST P1
      R(2)=V(5)     $COST P2
      R(3)=V(8)     $COST E1
      R(4)=V(3)     $POWER P1
      R(5)=V(6)     $POWER P2
      R(6)=V(9)     $POWER E1
      R(7)=V(10)    $TOTAL CAPTL COST
      R(8)=V(11)    $TOTAL POWER COST
      RETURN
     CALCULATOR UID=K02,NAME=FLASH COST
```

```
 $
 $ THIS CALCULATOR DETERMINES THE CAPITAL COST
 $ OF THE FLASH DRUM, BY MEANS OF THE EQUATION:
 $ COST=9071.*(VAPOR MOLAR RATE/3832.4)**0.52
 $
      RETRIEVE P(1),STRM=P120,RATE
 $
      PROCEDURE
      V(1)=P(1)/3832.4
      V(1)=V(1)**0.52
      V(1)=V(1)*9071.0
 $ STORE RESULT
      R(1)=V(1)
      RETURN
CALCULATOR UID=K03,NAME=REACTOR COST
 $ THIS FUNCTION CALCULATES THE COST OF THE REACTOR
 $ VESSEL BY MEANS OF THE EQUATION:
 $ COST=165778*(VOL/265.6)**0.63
 $ WHERE
 $ VOL=[ALOG((Z-2)/(Z+2))+2.887271]/Y
 $ AND Z=SQRT(5-X), BEEING X THE CONVERSION
 $ Y=-FA0/(3600*K*CA0**1.5)
 $ CA0: INLET TOLUENE MOLAR CONCENTRATION
 $ CA0=RATE TOL. P30/ HOTVOLUME(P150+P30)
 $ FA0: INLET TOLUENE RATE KGMOLE/HR
 $ K: RATE CONSTANT
 $ K=6.3E10*EXP(-26170/TAVG)
 $ WHERE TAVG=(TEMP.IN+TEMP.OUT)/2
 $ TEMP.IN=895 K
      RETRIEVE P(1),STRM=P40,TEMP          $ K
      RETRIEVE P(2),STRM=P30,COMP=4,RATE   $ KGMOLE/HR
      RETRIEVE P(3),STRM=P30,HOTVOL        $ M3/HR
      RETRIEVE P(4),STRM=P150,HOTVOL       $ M3/HR
      RETRIEVE P(5),UNIT=R1,CONVERSION,IDNO=1
 $ START COMPUTATIONS
      PROCEDURE
 $ COMPUTATION OF CONVERSION FUNCTION
      V(1)=5.0-P(5)
      V(1)=V(1)**0.5
      V(2)=V(1)-2.0
      V(3)=V(1)+2.0
      V(2)=V(2)/V(3)
      V(2)=ALOG(V(2))
      V(2)=V(2)+2.88727
      V(2)=V(2)/2.0
 $ COMPUTATION OF AVERAGE TEMPERATURE
      V(4)=P(1)+895.0
      V(4)=V(4)/2.0
 $ COMPUTATION OF RATE CONSTANT
      V(4)=-26170.0/V(4)
      V(4)=EXP(V(4))
      V(4)=6.3E10*V(4)
 $ CALCULATE INLET TOLUENE CONCENTRATION
```

```
      V(5)=P(3)+P(4)
      V(5)=P(2)/V(5)
      V(5)=V(5)**1.5
 $ COMPUTE REACTOR VOLUME
      V(6)=P(2)/V(5)
      V(6)=V(6)/V(4)
      V(6)=V(6)/3600.0
      V(6)=V(6)*V(2)
      V(6)=ABS(V(6))
 $ DETERMINE REACTOR COST
      V(7)=V(6)/265.58
      V(7)=V(7)**0.63
      V(7)=165778.0*V(7)
 $ RESULTS
      R(1)=V(6)       $ REACTOR VOLUME
      R(2)=V(7)       $ REACTOR COST
      RETURN
      CALCULATOR UID=K04,NAME=EXCHANGER COST
$ THIS CALCULATOR DETERMINES THE COST OF HX10,
$ HX5 AND HX2, AND THE CORRESPONDING UTILITIES
$ ORDER OF CONSTANTS:
$ I:BASE DUTY,I+1:UTILITY COST;I+2:EXCH. COST
      CONSTANT 159.0/682253./65002./*  $HX10
               5.67/33313./1885.2/*    $HX5
               1.65/15549./1444.       $HX2
$
      RETRIEVE P(1),UNIT=HX10,DUTY
      RETRIEVE P(2),UNIT=HX5,DUTY
      RETRIEVE P(3),UNIT=HX2,DUTY
$
      PROCEDURE
      IX4=0            $ COUNTER INDEX
      DO 10 IX1=1,7,3
      IX2=IX1+1
      IX3=IX2+1
      IX5=IX1-IX4
      V(IX1)=P(IX5)/C(IX1)
      V(IX2)=V(IX1)*C(IX2) $ UTILITY COST
      V(IX3)=V(IX1)**0.41
      V(IX3)=V(IX3)*C(IX3) $ EXCHANGER COST
      IX4=IX4+2
   10 CONTINUE
$ ADD CAPITAL COST
      V(10)=V(3)+V(6)
      V(10)=V(10)+V(9)
$ STORE RESULTS
$ ...UTILITY COST
      R(1)=V(2)    $ COOLWATER
      R(2)=V(5)    $ STEAM
      R(3)=V(8)    $ COOLWATER
$ ...EXCHANGER COST
      R(4)=V(3)    $ HX10
      R(5)=V(6)    $ HX5
```

```
      R(6)=V(9)    $ HX2
      R(7)=V(10)   $ TOTAL HX'S COST
      DUMP
      RETURN
CALCULATOR UID=K06,NAME=FURNACE COST
 $ THIS CALCULATOR DETERMINES THE COST OF UNITS
 $ H1 & H2 AND THE CORRESPONDING UTILITIES
 $
      RETRIEVE P(1),UNIT=H1,DUTY
      RETRIEVE P(2),UNIT=H2,DUTY
 $
      PROCEDURE
      V(1)=P(1)/93.63
      V(2)=V(1)*2.989E6    $FUEL COST H1
      V(3)=V(1)**0.75
      V(3)=V(3)*603278.0   $CAPTL COST H1
 $
      V(4)=P(2)/52.21
      V(5)=V(4)*1.667E6    $FUEL COST H2
      V(6)=V(4)**0.75
      V(6)=V(6)*323253.0   $CAPTL COST H2
 $ STORE RESULTS
      R(1)=V(2)     $ FUEL COST H1
      R(2)=V(5)     $ FUEL COST H2
      R(3)=V(3)     $ CAPTL COST H1
      R(4)=V(6)     $ CAPTL COST H2
 $
      RETURN
CALCULATOR UID=K07,NAME=STAB COST
$ THIS CALCULATOR DETERMINES THE CAPITAL AND OPERATING
$ COST OF THE STABILIZER COLUMN.
$ ASSUMPTION: A RIGOROUS MODEL IS USED WITH 14 TRAYS.
$
      RETRIEVE P(1),UNIT=C1,DUTY,IDNO=1
      RETRIEVE P(2),UNIT=C1,DUTY,IDNO=2
      RETRIEVE P(3),STRM=FUEL,TEMP
      PROCEDURE
$ CALCULATE COST OF COLUMN ASSUMING 14 TRAYS
      V(1)=P(2)/3.82
      V(2)=V(1)**0.533
      V(2)=27700.0*V(2)     $ COLUMN COST
      V(3)=V(1)**0.65
      V(3)=V(3)*1516.0      $ REBOILER COST
      V(4)=V(1)*204757.0    $ STEAM COST
      V(5)=ABS(P(1))
      V(5)=V(5)/0.422
      V(6)=V(5)**0.65
      V(6)=V(6)*1061.0      $ CONDENSER COST
$ USE COOLING WATER
      IF(P(3).GE.298.0)  V(5)=V(5)*3984.0
$ ELSE, USE REFRIGERANT
      IF(P(3).LT.298.0)  V(5)=V(5)*70704
$ ADD CAPITAL COSTS
```

```
      V(7)=V(3)+V(6)
      V(7)=V(7)+V(2)
$ STORE RESULTS
      R(1)=V(2)     $ COLUMNN COST
      R(2)=V(6)     $ CONDENSER COST
      R(3)=V(3)     $ REBOILER COST
      R(4)=V(5)     $ REFRIGERANT COST
      R(5)=V(4)     $ STEAM COST
      R(6)=V(7)     $ CAPITAL COST
      RETURN
$
      CALCULATOR UID=K10,NAME=MATERIAL COST
$
$ THIS CALCULATOR DETERMINES THE COST DIFFERENCE
$ BETWEEN PRODUCTS AND RAW MATERIALS
      CONSTANT -1.255464E6/-3.902276E3/2.03537E6/*
               4.7556E5
$ CONSTANTS HAVE UNITS OF $ HOUR/(M3 YEAR)
$ THE CONSTANT FOR HYDROGEN IS MULTIPLIED BY A DENSITY FACTOR
$ RHO=0.121217 KG/M3
      RETRIEVE P(1),STRM=TOL,RATE(V)
      RETRIEVE P(2),STRM=HYD,RATE(W)
      RETRIEVE P(3),STRM=BENZ,RATE(V)
      RETRIEVE P(4),STRM=DIPH,RATE(V)
      RETRIEVE P(5),STRM=FUEL,COMP=1,RATE(W)
      RETRIEVE P(6),STRM=FUEL,COMP=2,RATE(W)
      RETRIEVE P(7),STRM=PURG,COMP=1,RATE(W)
      RETRIEVE P(8),STRM=PURG,COMP=2,RATE(W)
$
      PROCEDURE
$ CALCULATE VALUE OF STREAMS TOL,HYD,BENZ & DIPH
      V(10)=0.0
      DO 10 IX1=1,4
      V(IX1)=C(IX1)*P(IX1)
$ ADDING VALUES
      V(10)=V(10)+V(IX1)
   10 CONTINUE
$ CALCULATE VALUE OF STREAMS PURG AND FUEL; PREVIOUSLY
$ THE NET HEATING VALUE OF THE STREAMS HAS TO BE DETERMINED
      DO 20 IX2=5,7,2
      IX3=IX2+1
      V(IX2)=P(IX2)*113807.0    $ HYDROGEN HEATING VALUE
      V(IX3)=P(IX3)*47443.      $ METHANE HEATING VALUE
      V(IX3)=V(IX3)+V(IX2)      $ STREAM HEATING VALUE
$ 7200 HR/YEAR*1.65 DOLLARS/1.E6 BTU = 0.01188
      V(IX3)=V(IX3)*0.01188     $ STREAM COST
   20 CONTINUE
$ ADD VALUES OF STREAMS
      V(10)=V(10)+V(6)
      V(10)=V(10)+V(8)
$ STORE RESULT
      R(1)=V(10)
      DUMP
```

```
      RETURN
$
      CALCULATOR UID=K11, NAME=ENERGY COST
$ THIS FUNCTION DETERMINES COST OF ENERGY IN THE PLANT
      RETRIEVE P(1),UNIT=K06,RESULT,IDNO=1     $ FUEL
      RETRIEVE P(2),UNIT=K06,RESULT,IDNO=2     $ FUEL
      RETRIEVE P(3),UNIT=K01,RESULT,IDNO=8     $ POWER
      RETRIEVE P(4),UNIT=K04,RESULT,IDNO=2     $ STEAM
      RETRIEVE P(5),UNIT=K04,RESULT,IDNO=1     $ WATER
      RETRIEVE P(6),UNIT=K04,RESULT,IDNO=3     $ WATER
      RETRIEVE P(7),UNIT=K07,RESULT,IDNO=4     $ REFRIG
      RETRIEVE P(8),UNIT=K07,RESULT,IDNO=5     $ STEAM
$
      PROCEDURE
      V(1)=P(1)+P(2)          $FUEL
      V(2)=P(4)+P(8)          $STEAM
      V(3)=P(5)+P(6)
      V(3)=V(3)+P(7)          $WATER
      V(4)=P(3)               $POWER
$ TOTAL ENERGY COST
      V(5)=0.0
      DO 10 IX1=1,4
      V(5)=V(5)+V(IX1)
   10 CONTINUE
$ STORE RESULTS
      R(1)=V(1)     $ FUEL
      R(2)=P(3)     $ POWER
      R(3)=V(2)     $ STEAM
      R(4)=V(3)     $ WATER
      R(5)=V(5)     $ TOTAL
      DUMP
      RETURN
$
      CALCULATOR UID=K12,NAME=CAPITAL COST
$ THIS FUNCTION CALCULATES THE TOTAL COST OF EQUIPMENT
      RETRIEVE P(1),UNIT=K01,RESULT,IDNO=8   $PUMP/COMPR
      RETRIEVE P(2),UNIT=K02,RESULT,IDNO=1   $FLASH
      RETRIEVE P(3),UNIT=K03,RESULT,IDNO=2   $REACTOR
      RETRIEVE P(4),UNIT=K04,RESULT,IDNO=7   $EXCHANGERS
      RETRIEVE P(5),UNIT=K06,RESULT,IDNO=3   $FURNACE
      RETRIEVE P(6),UNIT=K06,RESULT,IDNO=4   $FURNACE
      RETRIEVE P(7),UNIT=K07,RESULT,IDNO=6   $STAB COLUMN
$
      PROCEDURE
      V(1)=0.0
      DO 10 IX1=1,7
      V(1)=V(1)+P(IX1)
   10 CONTINUE
$ STORE RESULT
      R(1)=V(1)
      RETURN
$
      CALCULATOR UID=K13,NAME=LEVEL 3
```

```
$ THIS CALCULATOR COMPUTES THE ECONOMIC POTENTIAL
$ INCLUDING THE REACTOR AND COMPRESSOR COST.
      RETRIEVE P(1),UNIT=K10,RESULT,IDNO=1 $MATERIAL COST
      RETRIEVE P(2),UNIT=K03,RESULT,IDNO=2 $REACTOR COST
      RETRIEVE P(3),UNIT=K01,RESULT,IDNO=3 $COMPRESSOR COST
      RETRIEVE P(4),UNIT=K01,RESULT,IDNO=6 $POWER COST
$
      PROCEDURE
      V(1)=P(1)
      DO 10 IX1=2,4
      V(1)=V(1)-P(IX1)
   10 CONTINUE
$ STORE RESULT
      R(1)=V(1)  $ LEVEL 3 COST
      RETURN
$
      CALCULATOR UID=K14,NAME=LEVEL 4A
$ THIS FUNCTION CALCULATES THE ECONOMIC POTENTIAL INCLUDING
$ THE LOSSES OF VALUABLE MATERIAL IN THE STREAMS PURG AND FUEL
$
      CONSTANT -2.03537E6/-1.255464E6
      RETRIEVE P(1),STRM=FUEL,COMP=3,RATE(V)
      RETRIEVE P(2),STRM=FUEL,COMP=4,RATE(V)
      RETRIEVE P(3),STRM=PURG,COMP=3,RATE(V)
      RETRIEVE P(4),STRM=PURG,COMP=4,RATE(V)
      RETRIEVE P(5),UNIT=K13,RESULT,IDNO=1
$ CALCULATION  OF MATERIAL LOSSES COST
      PROCEDURE
      DO 10 IX1=1,3,2
      IX2=IX1+1
      V(IX1)=P(IX1)*C(1)     $ BENZENE LOSSES
      V(IX2)=P(IX2)*C(2)     $ TOLUENE LOSSES
      V(IX2)=V(IX2)+V(IX1)   $ STREAM LOSSES
   10 CONTINUE
      V(5)=V(2)+V(4)
      V(6)=P(5)+V(5)
$ STORE RESULTS
      R(1)=V(2)    $ STREAM FUEL
      R(2)=V(4)    $ STREAM PURG
      R(3)=V(5)    $ FUEL + PURG
      R(4)=V(6)    $ LEVEL 4A
      RETURN
      CALCULATOR UID=K15,NAME=PROFIT
$ THIS FUNCTION DETERMINES THE ANNUAL PROFIT
      RETRIEVE P(1),UNIT=K10,RESULT,IDNO=1
      RETRIEVE P(2),UNIT=K11,RESULT,IDNO=5
      RETRIEVE P(3),UNIT=K12,RESULT,IDNO=1
      RETRIEVE P(4),UNIT=K14,RESULT,IDNO=3
$
      PROCEDURE
      V(1)=P(1)-P(2)
      V(1)=V(1)-P(3)
      V(1)=V(1)+P(4)
```

```
        SM
PROCESS   INPUT LISTING - PAGE 11

$ STORE RESULT
      R(1)=V(1)
      RETURN
RECYCLE DATA
 ACCEL TYPE=DEM,STRM=P150


             SM
PROCESS   SIMULATION PROGRAM - VERSION 0484


       SM
PROCESS   OUTPUT DIRECTORY =  BENZENE3       CASE 4.1
                              L.MIRANDA      07-11-86

UNIT STREAM RELATIONS - P.   1
INPUT IN ORDER

UNIT   1, M2  ,      SOLVED
UNIT   2, P1  ,      SOLVED
UNIT   3, H2  ,      SOLVED
UNIT   4, R1  ,      SOLVED
UNIT   5, R2  ,      SOLVED
UNIT   6, M3  ,      SOLVED
UNIT   7, HX10,      SOLVED
UNIT   8, F1  ,      SOLVED
UNIT   9, S1  ,      SOLVED
UNIT  10, E1  ,      SOLVED
UNIT  11, M1  ,      SOLVED
UNIT  12, H1  ,      SOLVED
UNIT  13, S2  ,      SOLVED
UNIT  14, P2  ,      SOLVED
UNIT  15, VAL1,      SOLVED
UNIT  16, HX5 ,      SOLVED
UNIT  17, C1  ,      SOLVED
UNIT  20, VAL2,      SOLVED
UNIT  21, C2  ,      SOLVED
UNIT  23, C3  ,      SOLVED
LOOP  1 NOT SOLVED AFTER   1 TRIALS
STRM: LREC T= 392.7 P=  130.0 RATE= 308.8      DTEMP=  -0.34 DCOMP=  -0.0445
STRM: P150 T= 895.0 P= 3730.0 RATE= 7704.      DTEMP=   0.00 DCOMP=  -0.0216
STRM: P80  T= 311.0 P= 3450.0 RATE= 120.0      DTEMP=   0.00 DCOMP=   0.8904
UNIT   1, M2  ,      SOLVED
UNIT   2, P1  ,      SOLVED
UNIT   3, H2  ,      SOLVED
UNIT   4, R1  ,      SOLVED
UNIT   5, R2  ,      SOLVED
UNIT   6, M3  ,      SOLVED
UNIT   7, HX10,      SOLVED
UNIT   8, F1  ,      SOLVED
UNIT   9, S1  ,      SOLVED
UNIT  10, E1  ,      SOLVED
UNIT  11, M1  ,      SOLVED
UNIT  12, H1  ,      SOLVED
```

APPENDIX D

RESULTS FROM THE SIMULATION OF THE EXAMPLE PROBLEM

This appendix presents the results of the simulation of the example problem: the hydrodealkylation of toluene to produce benzene.

TABLE D.1: NET VALUE OF PRODUCTS

This table presents the variation of the net value of products (NVP) in terms of the reaction conversion (X) and of the hydrogen concentration of the gas recycled to the reactor (yH2). The units of NVP are 1,000 $/year. The value of NVP has been determined by means of the material balance equations (4.3) through (4.7).

X	yH2				
	0.4	0.5	0.6	0.7	0.8
0.10	10,415	9,606	8,334	6,044	712
0.20	10,395	9,586	8,314	6,024	681
0.30	10,367	9,558	8,286	5,996	654
0.40	10,368	9,517	8,245	5,956	614
0.50	10,265	9,455	8,183	5,894	552
0.60	10,159	9,350	8,078	5,789	445
0.70	9,955	9,146	7,874	5,586	245
0.75	9,767	8,958	7,686	5,398	59
0.80	9,444	8,635	7,364	5,077	- 261

TABLE D.2: RESULTS OF SIMULATION OF THE REFERENCE STRUCTURE

The values of NVP, Level 4, Energy, Capital and Profit are given in million dollars per year. The values were calculated for a ratio of actual reflux with respect to minimum reflux (R/Rmin) of 1.15 for column C2 and 1.10 for column C3.

X	yH2	H2/oil	NVP	Level 4	Energy	Capital	Profit
.75	.40	5.0	8.995	7.709	8.291	1.692	-0.989
.75	.59	4.9	6.596	5.208	6.739	1.295	-1.438
.75	.79	5.0	-2.371	-4.818	5.874	1.008	-9.253
.30	.50	5.9	7.378	5.784	26.101	3.329	-22.052
.40	.45	5.0	9.821	8.447	18.113	2.624	-10.916
.50	.43	4.8	9.715	8.449	13.644	2.178	- 6.108
.60	.43	5.1	9.469	8.213	10.963	1.947	- 3.441
.80	.41	4.9	8.571	7.300	7.519	1.614	- 0.562
.75	.40	5.0	8.995	7.709	8.481	1.691	- 1.177
.75	.59	4.9	6.596	5.208	6.928	1.274	- 1.605

The last two rows correspond to R/Rmin values of 1.45 for C2 and 1.30 for C3.

TABLE D.3: RESULTS OF THE SIMULATION OF THE MODIFIED STRUCTURE

The values of NVP, energy cost, capital cost and profit are given in millions of Dollars per year.

X	yH2	H2/oil	NVP	Energy	Capital	Profit
.50	.42	4.3	10.038	9.759	2.002	-1.723
.75	.40	4.2	10.259	7.076	1.612	1.570
.75	.43	4.9	9.718	7.261	1.672	0.785

TABLE D.4: EVALUATION OF THE REACTOR

X	yH2	H2/oil	Vol m3	Cost k$/year	T out K	H out MJ/h	Del H MJ/h
.30	.50	5.9	292.1	176.0	912	364	11.4
.40	.45	5.1	255.4	161.8	919	272	11.9
.50	.43	4.8	234.4	153.2	927	216	11.9
.60	.43	5.1	250.8	159.9	933	186	11.7
.75	.40	4.9	282.8	172.5	941	158	11.8
.75	.59	4.9	119.1	100.0	962	116	11.7
.75	.79	5.0	61.8	66.2	982	94	11.4

TABLE D.5: EVALUATION OF THE STABILIZER (C1)

X	yH2	Total flow Kgmol/hr	Cost of steam K$/year	Capital cost K$/year
.30	.40	898.8	698.0	58.1
,40	.40	687.4	482.2	47.7
.50	.40	552.6	359.8	40.8
.60	.40	461.5	279.6	35.7
.75	.40	373.1	204.2	30.2
.75	.60	367.2	203.6	30.0
.75	.80	354.8	199.4	29.4

TABLE D.6: EVALUATION OF THE DISTILLATION COLUMN (C2)

X	yH2	Total flow Kgmol/hr	Benzene Flow rate Kgmol/hr (F1)	Toluene Flow rate Kgmol/hr (F2)	F1/F2	Cost of steam K$/year	Capital cost K$/year
.30	.40	852.2	247.7	595.2	0.42	1569.8	225.8
.40	.40	649.3	263.2	384.8	0.68	1253.9	197.1
.50	.40	521.7	262.4	257.8	1.02	1046.0	177.0
.60	.40	436.3	261.5	172.5	1.52	903.7	162.3
.75	.40	352.3	260.2	87.5	2.97	769.3	150.0
.75	.60	351.6	258.6	88.6	2.91	767.2	149.8
.75	.80	344.9	251.7	89.0	2.83	750.8	148.1

TABLE D.7: EVALUATION OF THE DISTILLATION COLUMN (C3)

X	yH2	Total flow Kgmol/hr	Toluene Flow rate Kgmol/hr (F3)	Diphenyl Flow rate Kgmol/hr (F4)	F3/F4	Cost of steam K$/year	Capital cost K$/year
.30	.40	607.4	595.1	9.2	64.5	9845.6	131.1
.40	.40	387.9	384.8	1.2	319.6	6102.7	114.1
.50	.40	260.6	257.7	1.6	164.4	4154.4	87.3
.60	.40	175.5	172.4	2.2	77.3	2835.7	66.4
,75	.40	92.4	87.4	4.5	19.2	1511.0	44.2
.75	.60	93.4	88.6	4.3	20.4	1524.4	44.4
.75	.80	93.6	88.9	4.2	21.4	1525.9	44.5

APPENDIX E

PRICE OF CHEMICALS

The price of chemicals for the example process system (hydrodealkylation of toluene to produce benzene) has been determined based on two sources: the relative prices given in the 1967 AIChE Student Contest Problem (SCP, 1967) and the current prices.

The current prices in US Dollars reported by the Chemical Marketing Reporter (January 6, 1986; March 17, 1986; and, May 19, 1986), are the following:

CHEMICAL	UNIT	JAN.	MARCH	MAY
Benzene	gln	1.30	0.90	0.85
Toluene	gln	0.95	0.66	0.72
Diphenyl	lb	0.74	0.74	0.74

The prices in US Dollars given in the 1967 SCP are the following:

CHEMICAL	UNIT	PRICE
Benzene	gln	0.26
Toluene	gln	0.16
Diphenyl	gln	0.06
Hydrogen	1000 ft3	0.45
Fuel Gas	MM BTU	0.40

The price of hydrogen is referred to 1000 cubic feet at standard conditions. The price of the fuel gas is based on million BTU of net heating value.

Assuming an actual toluene price of $ 0.66 and computing an index that compares this current price with the one given in the 1967 SCP, we have:

INDEX = 0.66/0.16 = 4.125

The prices used in the simulation calculations have been determined by updating the 1967 SCP prices with the above index. These current prices in US Dollars are:

CHEMICAL	UNIT	PRICE
Toluene	m3	174.37
Benzene	m3	282.69
Diphenyl	m3	66.05
Hydrogen	std. m3	0.0657
Fuel	MM BTU NHV	1.65

A density of 1024 kg/m3 has been used to compute the price of diphenyl.

The net heating value of the streams PURG and FUEL is calculated with the following formula:

qStream = mH2 qH2 + mCH4 qCH4

where: mH2 and mCH4 represent the molar rates of hydrogen and

methane, respectively. qH2 and qCH4 represent the hydrogen and methane heating values, respectively. qH2 is 113,807 BTU/kg and qCH4 is 47,443 BTU/kg [Perry, 1974, p. 9-16].

APPENDIX F

PRICE OF SERVICES

To determine the price of services for the example problem the formulas provided by Ulrich [1984], have been used. As a basis, the price of residual fuel oil has been obtained from the Monthly Energy Review [December 1985, Energy Information Administration, Washington D.C.].

The price per gallon of residual fuel oil is $ 0.609 and the heat content is 6.287 million BTU per barrel (reported by the Monthly Energy Review). Therefore, the price of residual fuel oil can be expressed as $ 3.856 per GJ.

The "CE index" for January 1986 is 323.5 [Chem Eng,.....]

In summary, cost of fuel: FUEL = 3.856 $/GJ
CE index: CE = 323.5

Cost of Electricity.

For on-site power charge to process module the following formula is used:

Ce = 1.4E-4 CE + 0.011 FUEL
Ce = 0.0877 $/kWh

Cooling Water.

For Process Module
Cw = [0.0001 + 3.0E-5/Qw] CE + 0.0056 FUEL
Assume the total auxiliary water capacity (Qw) as 10 m3/s,
Cw = 0.0549 $/m3

Refrigerant.

For Process Module
Cr = 6.0E6 CE/(Qr**0.7 T**5) + 1.1E6 FUEL/T**5
Assuming a total auxiliary cooling capacity (Qr) of 300 kJ/s and a temperature (T) of 280 K:
Cr = 2.327E-5 $/kJ

Process Steam.

For process module
Cs = 2.7E-5 CE/m**0.9 + 0.0020 P**0.14 FUEL
Assuming a total auxiliary boiler steam capacity (m) of 10 kg/s and a pressure (P) of 30 barg:
Cs = 0.01329 $/kg.

NOTE.- The current cost of electricity, in December 1985, sold to commercial consumers is 0.0729 $/kWh [Monthly Energy Review], which is 16.9 % lower than the calculated value.

APPENDIX G

COST MODELS FOR THE MAJOR OPERATIONAL UNITS

This appendix presents the formulation of the cost models for the major operational units included in the simulation program for the example problem presented in Chapter Four. Table G.1 at the end of this appendix lists the cost models for the major operational units. The details of the formulation of the cost models are presented in what follows.

Reactor Cost Model.

The sizing and costing of the reactor is based on the following reaction:

$$2\ C_6H_5CH_3 + H_2 \longrightarrow 2\ C_6H_6 + 2\ CH_4 \qquad (G.1)$$

The reaction takes place in gaseous phase at a temperature of 895 K and a pressure of 3450 kPa. The rate equation for this reaction is:

$$r = -k\ Ca\ Cb^{**}0.5 \qquad (G.2)$$

and $k = 6.3E10\ (gmol/l)^{**}-0.5/s\ \exp[-52{,}000\ cal/gmole\ /RT]$ (G.3)

R = 1.987 cal/(gmole K)
Ca= Toluene concentration
Cb= Hydrogen concentration

Since the number of moles of reactants and products of equation (G.1) is constant, the reaction takes place at constant volume. Expressing equation (G.2) as a function of conversion, we have:

$$r = -k\ Cao^{**}1.5\ (1 - X)\ (M - X)^{**}0.5 \qquad (G.4)$$

where Cao represent the toluene initial concentration and M the ratio of the initial hydrogen concentration to the initial toluene concentration. For the example problem M = 5.

In the example problem an adiabatic plug flow reactor is used. The design equation for a plug flow reactor is:

$$V/Fao = 0\ INT\ X\ [dX/-r] \qquad (G.5)$$

where the symbol "0 INT X" represents the integral from 0 to X; V is the reactor volume and Fao is the molar feed rate to the reactor. Replacing equation (G.4) into equation (G.5), we get:

$$V/Fao = Cao^{**}-1.5 \int dX/[k(1-X)(5-X)^{**}0.5] \qquad (G.6)$$

To determine the value of the integral, because the reactor is not isothermal, select several values of conversion X. For each value of X, by means of energy balance compute the corresponding temperature. With the calculated temperature compute

the corresponding rate constant k. Then, for each X compute the value of the integrand function of equation (G.6) [k(1-X)(5-X)-**0.5]. Finally, integrate numerically.

Since usually the adiabatic line is straight, a simplified procedure is to calculate the temperature values corresponding to each X value from a straight line. In the example problem this straight line has the following end points: (X=0, T=895) and (X=0.75, T=940). The equation that correlates these points is:

$$T = 880 + (X + 0.25)/0.01667 \qquad (G.7)$$

Consequently, for each value of X, with Equation (G.7) the corresponding temperature is computed. Using Equation (G.3) the corresponding k value is calculated. With these values of X and k the integrand of Equation (G.6) is computed. Applying a modified Simpson's rule algorithm [Pachner, 1985], within the interval of conversion 0 to 0.75, the value of the integral was determined to be 23.3. So, equation (G.6) was reduced to:

$$V/Fao = 23.3/Cao^{**1.5}\ (mole/l)^{**0.5}\ s \qquad (G.8)$$

For base-case conditions (X=0.75, yH2=0.4), Fao=358 kgmoles Toluene/hr and Cao=4.238E-5 kgmole Toluene/lt. Then, V=265.6 m3. For a reactor length to diameter ratio of 6:1, the reactor diameter is equal to 3.8 m and the reactor length is equal to 23.0 m.

Since the PROCESS simulator was used, it was not possible to perform the numerical integration to find the reactor volume. The reactor model had to be simplified. It was assumed that the reactor operates under isothermal conditions at a temperature equal to the arithmetic mean of the inlet and outlet temperatures. This assumption has been proved to be correct with a small percent error. Under isothermal conditions the k value is constant and can be taken out of the integral function. Such an equation can be analytically integrated using formula 135, page A-122 of the CRC Handbook of Chemistry and Physics [56th edition]. The resultant expression is:

$$V/Fao = -1/(2\ k\ Cao^{**1.5})\ \ln\{[SQRT(5-X)-2]/[SQRT(5-X)+2]\}$$

between limits X=0 and X=X. (G.9)

To estimate the cost of the reactor for the base-case the following conditions have been assumed:

- reactor volume: 265.6 m3
- reactor diameter: 3.8 m
- reactor length: 23.0 m
- reactor material: Stainless steel 304
- reactor wall thickness 0.75 in [SCP, 1967]
- reactor weight: 12000 lb/ft
- reactor total weight: 90000 lb (Ws)

The cost of the reactor shell has been determined by the method proposed by Mulet, Corripio and Evans [1981]

$$C = \exp [6.823 + 0.14178(\ln Ws) + 0.02468 (\ln Ws)^{**}2 + 0.0158(L/D) \ln(Tb/Tp)] \quad (G.10)$$

where: Tb: shell thickness at bottom of tower
Tp: shell thickness at design pressure

Assuming L/D=6 and Tb/Tp=1, the cost of the reactor is:
Cr = $ 114,925.

The cost of the reactor at January 1986 is:
Cr(1986) = Cr CE(1986)/CE(1979) = 114,925 (323.5/250)
Cr(1986) = $ 148,713

The cost of the reactor installed is:
Cr (Ins) = Cr * F(Ins), where the factor of installation (F(Ins)) for reactors is 4.0 for a carbon steel shell [Hall et al., 1982]. For a stainless steel shell a material correction factor (Fm) has to be applied and it is equal to 1.7 [Mulet et al., 1981]. Therefore, the actual reactor cost is:

Cr = 148,713 * 4.0 * 1.7
Cr = $ 1'011,248

The annualized cost of the reactor (for a pay out period of 6.1 years) is equal to $ 165,778.
The cost model for the reactor [Guthrie, 1969] is:
Cr = 165,778 (V/265.6)**0.63

Estimation of Distillation Towers Cost.

The correlations used to calculate the cost of the shell of distillation columns, the cost of platforms and ladders, as well as the cost of trays has been taken from Mulet, Corripio and Evans [1981].

The shell cost of distillation towers is estimated using Equation (G.10). The cost of platforms and ladders is estimated with equation (G.11):

$$Cpl = 151.81\ Di^{**}0.63316\ Lt^{**}0.80161 \quad (G.11)$$

The cost per carbon steel tray is computed with:

$$Cbt = 278.38 \exp (0.1739\ D) \quad (G.12)$$

The number of trays factor is:

$$Fnt = 2.25/(1.0414)^{**}Nt \quad (G.13)$$

The material of construction cost factor for Stainless Steel 304 is:

$$Ftm = 1.189 + 0.0577\ D \qquad (G.14)$$

The total cost of a distillation tower (first quarter 1979) is:

$$Ct = CbFm + Nt\ Cbt\ Ftm\ Ftt\ Fnt + Cpl \qquad (G.15)$$

where:

Cb: cost of carbon steel shell, calculated by eq. (G.10)
Fm: material of construction factor, for carbon steel=1.0
Cbt: cost per carbon steel tray, eq. (G.12)
Nt: number of trays
Ftm: material of construction tray factor, eq. (G.14)
Ftt: Type of trays factor, for valve trays Ftt=1.0
Fnt: Number of trays factor, eq. (G.13)
Cpl: Cost of patforms and ladders, eq. (G.11)

The wall thickness for the distillation tower shell is determined from the table shown in page 11 of the AIChE SCP [1967]. The shell weight per linear foot is estimated from Figure 2 of the AIChE SCP [1967]. The installation factors (F(Ins)) are those recommended by Hall et al., page 82 [1982]. For distillation columns F(Ins)= 4.0.

The current cost of the distillation column (January 1986) is found by multiplying the cost obtained from the correlations, which is valid for the first quarter of 1979, by the January 1986 CE index (323.5) and dividing the result by the CE index corresponding to the first quarter of 1979 (250.0).

STABILIZER COLUMN (C1)

Operational conditions determined from the simulation:

. Pressure = 1120 kPa
. Condenser temperature = 290 K
. Reboiler temperature = 465 K
. Number of trays = 14
. Trays spacing = 24 in
. Type of trays = valve
. Column diameter = 42 in
. Free space at bottom of tower = 4 ft.
. Shell material = carbon steel
. Trays material = Stainless Steel 304

Cost of tower:

. Column height = 2 * 15 + 4 = 34 ft
. Wall thickness = 1/4 in
. Shell weight = 120 lb/ft
. Total shell weight = 4080 lb
. Shell cost, eq.(G.10), Cb= 17,838, assuming Tb/Tp=1.7
. Cost of platforms and ladders, eq.(G.11), Cpl=5,668

. Cost per carbon steel tray, eq.(G.12), Cbt=512
. Material of construction tray cost factor, Ftm=1.39
. Number of trays factor, eq.(G.13), Fnt=1.275
. Total cost of tower, eq.(G.15), Ct=$ 32,645
. Cost of tower at January 1986, Ct =$ 42,243
. Cost of tower including installation expenses, Ct=$ 168,972

BENZENE COLUMN (C2)

Operational Conditions determined from the simulation:

. Pressure = 170 kPa
. Condenser temperature = 347 K
. Reboiler temperature = 406 K
. Number of trays = 20
. Tray spacing = 24 in
. Type of trays = valve
. Column diameter = 6.5 ft
. Free space at bottom of tower = 6 ft
. Shell material = carbon steel
. Trays material = Stainless Steel 304

Cost of Tower

. Column height = 2*21 +6 =48 ft
. Wall thickness = 5/8 in
. Shell weight = 550 lb/ft
. Total shell weight = 26400 lb
. Shell cost = 54,447
. Cost of platforms and ladders = 11,059
. Cost per carbon steel tray = 862
. Material of construction tray cost factor, Ftm = 1.564
. Number of trays cost factor, Fnt = 1.0
. Total cost of tower, Ct = 92,501
. Total cost of tower at January 1986, Ct = 119,696
. Total cost of installed Tower, Ct = 478,784

TOLUENE COLUMN (C3)

Operating conditions

. Pressure = 170 kPa
. Condenser temperature = 390 K
. Reboiler Temperature = 553 K
. Number of trays = 25
. Tray spacing = 24 in
. Tray type = valve
. Column diameter = 3 ft
. Free space at bottom of tower = 4 ft
. Shell material = carbon steel
. Trays material = carbon steel

Cost of tower

. Column height = 56 ft
. Shell wall thickness = 1/4 in
. Shell weight = 100 lb/ft
. Total shell weight = 5600 lb
. Shell cost = 22,959
. Cost of platforms and ladders = 7669
. Cost of carbon steel tray = 469
. Number of trays factor Fnt = 0.816
. Total cost of tower Ct = 40,196
. Total cost of tower at January 1986, Ct= 52,013
. Cost of installed tower, Ct = 208,052

Condenser Cost Estimation.

The basic parameters for the cost estimation of the condensers are: the condenser temperature, the condenser duty and the overall heat transfer coefficient.

CONDENSER	TEMPERATURE K	DUTY GJ/H	U J/(m2 s K)
C1	298.0	0.4220	511
C2	360.0	21.64	738
C3	390.0	3.095	738

The values of U have been taken from the AIChE SCP [1967].

The cost of the condensers have been determined fron the charts of Hall et al. [1982]. To update the prices obtained from the charts, the CE index January 1986 and 1982 are correlated. An installation factor of 3.5 has been assumed [Hall et al, 1982].

The cost of the condensers are:

CONDENSER	COST, $
C1	6,470
C2	53,918
C3	11,144

Reboiler Cost estimation.

The main parameter to estimate the cost of a reboiler is the reboiler duty. For the reboilers of columns C1, C2 and C3 a constant heat flux of 31,546 J/(m2 s) is assumed [AIChE SCP, 1967]. The reboilers are kettle type. The material of construction of shell and tubes is carbon steel. The cost of the reboilers has been determined from the charts of Hall et al. [1982]. A kettle type reboiler is estimated to cost approximately 25 % more than an equivalent heat exchanger [Perry, 1974]. The installation factor is 3.5.

The price of the reboilers are presented below.

REBOILER	DUTY, GJ/h	COST, $
C1	3.820	25,160
C2	15.33	58,860
C3	3.124	20,220

Cost Models for the major operational units.

The cost model for the reactor has been already presented. The cost model for distillation columns has the following form [Douglas, 1985]:

C = Cref (N/Nref)**0.802 (V/Vref)**0.533

where N is the number of trays and V is the vapor flow rate. The subscript "ref" denotes a reference value.

For condensers and reboilers the cost model has the following form [Douglas, 1985]:

C = Cref (Q/Qref)**0.65

The utility consumption for condensers and reboilers is represented by:

C = Cref (Q/Qref)

For heat exchangers the cost model is [Ulrich, 1984, p.267]:

C = Cref (A/Aref)**0.41

For furnaces the cost model is similar to the one for heat exchangers, but instead of correlating the heat transfer area it correlates the duty, and the exponent is 0.78, instead of 0.41.

A summary of the actual cost models for the major operational units involved in the simulation of the reference structure is presented in Table G.1

TABLE G.1

COST MODELS FOR THE OPERATIONAL UNITS OF THE REFERENCE STRUCTURE

The costs have units of dollars per year.

PUMP P1

Pump cost:	2,189 [z kW/60.03]**0.5
Electricity cost:	31,508 [z kW/60.03]

```
     PUMP P2
Pump cost:                  421 [z kW/1.56]**0.5
Electricity cost:           819 [z kW/1.56]

     COMPRESSOR E1
Compressor Cost:            50,508 [z kW/532]**0.93
Electricity Cost:           279,236 [z kW/532]

     FLASH SEPARATOR
Flash drum cost:            9,071 [V kgmole/h vapor/3832.4]**0.52

     REACTOR
Reactor Cost:               165,778 [V/265.6 m3]**0.63
Reactor volume:
V = -Fo [ln ((a-2)/(a+2)) +2.8873]/[3600 k (Co)**1.5]
where: a = SQRT(5 - X)
       Fo = kgmoles/h toluene feed to reactor
       Co = kgmoles toluene feed/m3 total feed
       k = 6.3E10 exp [-26170/Tavg]
     Tavg= [Tin + Tout]/2

     FURNACE H1
Furnace cost:          603,278 [Q kJ/h / 93.63E6]**0.75
Fuel Cost:             2.989E6 [Q kJ/h / 93.63E6]

     FURNACE H2
Furnace cost:          323,253 [Q kJ/h / 52.21E6]**0.75
Fuel Cost:             1.667E6 [Q kJ/h / 52.21E6]

     HEAT EXCHANGER HX 10
Heat exchanger cost: 65,002 [A/734 m2]**0.41
     A = Q/(U delta T ln) = Q/[426J m-2 S-1 K-1* 141.2K]
     In this special case "delta T ln" is constant since all the
     temperatures are specified.  Therefore:
Heat exchanger cost: 65,002 [Q/159E06 KJ/h] ** 0.41
Cooling water cost : 682,253 [Q/159E06 KJ/h]

     HEAT EXCHANGER HX 2
     As in HX 10 "delta T ln" is constant.
Heat exchanger cost: 1,444 [Q/1.647E06 KJ/h] ** 0.41
Using ethilene glycol as refrigerant:
Refrigerant cost    : 275,904 [Q/1.647E06 KJ/h]
Using water at 288 K, as refrigerant:
Refrigerant cost    : 15,549 [Q/1.647E06 KJ/h]

     HEAT EXCHANGER HX 5
Assuming "delta T ln" constant as for HX 10.
Heat exchanger cost: 1885.2 [Q/5.67E06 KJ/h] ** 0.41
Steam cost:  33,313 [Q/5.67E06 KJ/h]

     DISTILLATION COLUMN  "C1": STABILIZER
Distillation column cost:
     27,700 [(N/14) ** 0.802] * [(qR/3.82E06) ** 0.533]
Condenser cost : 1,061 [-qC/0.422E06] ** 0.65
```

Using ethylene glycol as refrigerant for the condenser.
Refrigerant cost : 70,704 [-qC/0.422E06]
Reboiler cost : 1,516 [qR/3.82E06] ** 0.65
Steam cost : 204,757 [qR/3.82E06]

DISTILLATION COLUMN "C2" : BENZENE COLUMN
Distillation column cost:
123,093 [(N/34)**0.802]*[(R+1)D/670.5]**0.533 =
123,093 [(N/34)**0.802]*[(qC/22.39)]**0.533
Condenser cost : 9,055 [qC/22.39]**0.65
Cooling water cost : 96,388 [qC/22.39]
Reboiler cost : 9,885 [qR/16.12]**0.65
Steam cost : 852,915 [qR/16.12]

DISTILLATION COLUMN "C3" : TOLUENE COLUMN
Distillation column cost:
35,935 [(N/27)**0.802]*[(R+1)D/90.67]**0.533 =
34,107 [(N/27)**0.802]*[qC/3.043]**0.533
Condenser cost : 1,806 [qC/3.043]**0.65
Cooling water cost : 13,047 [qC/3.043]
Reboiler cost : 3,277 [qR/3.056]**0.65
Dowtherm fluid cost : 1'515,015 [qR/3.056]

APPENDIX H

HEAT INTEGRATION CALCULATIONS

This appendix presents the bases and the results of the heat integration procedure applied to the "reference structure" and to the "modified structure".

H.1 HEAT INTEGRATION OF THE REFERENCE STRUCTURE

The heat integration of the reference structure has been performed under the following basic conditions:
. minimum approach temperature: 10 K
. conversion X = 0.75.
. hydrogen concentration of the gas recycled yH2=0.4

Stream information:

STREAM No.	HEAT MJ/h	Cp MJ/h/K	TYPE	Tsource K	Ttarget K
P140-P150	93820	164.6	cold	325	895
P20-P30	52082	91.4	cold	325	895
P50-P60	158922	274.5	hot	890	311
Reboiler C1	3809	216.6	cold	450	468
Reboiler C2	14540	969.3	cold	390	405
Reboiler C3	3048	203.2	cold	538	553

Applying the technique proposed by Linhoff and Hindmarsh [1983] the following results have been obtained:
. minimum hot utility: 16,261.3 MJ/h
. minimum cold utility: 7,790.5 MJ/h
. pinch temperature: 405 K

In order to achieve the minimum utility requirements, at the hot end of the network, the specific heat of the hot stream should be less than or equal to the specific heat of the cold stream for each pinch match. This design rule is not satisfied by the reference structure, therefore the minimum utility target cannot be achieved.

H.2 HEAT INTEGRATION OF THE MODIFIED STRUCTURE

Basic conditions:
. minimum approach temperature: 10 K
. conversion: 0.75
. hydrogen concentration, yH2: 0.43

Stream Information:

STREAM No.	HEAT MJ/h	Cp MJ/h/K	TYPE	Tsource K	Ttarget K
P25-P30	160232	284.1	cold	331	895
P50-P60	174600	300.0	hot	893	311
Reboiler C1	4502	300.1	cold	460	475
Reboiler C2	12650	702.8	cold	402	420
P89-P90	7673	70.4	cold	311	420

Minimum utility requirements:

. minimum hot utility: 6,685.9 MJ/h
. minimum cold utility: 9,000.0 MJ/h
. pinch temperature: 402 K

There are several alternatives to construct the heat exchanger network for the modified structure. The selected alternative is shown in Figure 4.9.b. This alternative satisfies the design rules of the procedure proposed by Linhoff and Hindmarsh [1983], and has a minimum number of units.