Alternative Routes from Fossil Resources to Chemical Feedstocks

Dobrowolski, G., Kopytowski, J.A., Wojtania, J. and Zebrowski, M.

IIASA Research Report
September 1984

Dobrowolski, G., Kopytowski, J.A., Wojtania, J. and Zebrowski, M. (1984) Alternative Routes from Fossil Resources to Chemical Feedstocks. IIASA Research Report.

ALTERNATIVE ROUTES FROM FOSSIL RESOURCES TO CHEMICAL FEEDSTOCKS:

The Problem, a Methodological Approach, and the Case of Methanol

G. Dobrowolski, M. Żebrowski
Systems Research Department of the Institute for Control and Systems Engineering (Academy of Mining and Metallurgy) and of the Industrial Chemistry Research Institute, Cracow, Poland

J. Kopytowski
Industrial Chemistry Research Institute, Warsaw, Poland

J. Wojtania
Prosynchem Engineering Co., Gliwice, Poland

RR-84-19
September 1984

INTERNATIONAL INSTITUTE FOR APPLIED SYSTEMS ANALYSIS
Laxenburg, Austria

International Standard Book Number 3-7045-0073-9

Printed by Novographic, Vienna, Austria

FOREWORD

The research described in this report was initiated in 1981 within the framework of collaboration between IIASA and the Academy of Mining and Metallurgy in Cracow, Poland. At IIASA two research groups were particularly involved in the study: The Resources and Environment Area (Mineral and Energy Resources Task), which was concerned with the relationship between the natural resource base and structural change in different industries, and the System and Decision Sciences Area, in connection with its work on decision support systems.

This report is concerned with the general issue of industrial structural change and the related resource problems, focusing particularly on the chemical industry and its sources of hydrocarbon feedstocks. Most of the hydrocarbons currently used in the chemical industry are obtained by processing natural gas and crude oil, which are also of fundamental importance to the energy sector. However, these resources are not inexhaustible, and several countries are trying to overcome this problem by exploring the technical and economic feasibility of using gaseous and liquid hydrocarbons derived from coal as substitutes for natural gas and crude oil. This report considers the implications of such changes in the resource base for the chemical industry. Obviously there can be no easy answers to a question of this complexity. What the report attempts to do, however, is to develop a methodology capable of identifying the possible ways of restructuring industrial production processes in response to changes in the resource base. The use of the proposed methodology is illustrated by an analysis of the alternative routes to the production of methanol. The results of this case study show that the proposed methodology provides a powerful tool for examination of the alternatives available to industrial planners and may also be used to describe many of the impacts that changes in the resource base can have on individual industries.

A.P. WIERZBICKI
Chairman
System and Decision Sciences
Program

J.KINDLER
Leader
Institutions and
Environmental Policies
Program (formerly
Resources and Environment
Area)

SUMMARY

The chemical industry depends very heavily on hydrocarbon feedstocks, which are presently derived almost exclusively from crude oil. Although only about seven percent of the hydrocarbons suitable for chemical processing are actually used in this way, it is already clear that there is a potential conflict between the needs of the energy sector and those of the chemical industry: they are competing for increasingly scarce liquid hydrocarbon resources.

The authors suggest that the supply of hydrocarbon feedstocks to the chemical industry could be protected against the effects of changing patterns of energy use by modifying the underlying industrial structure. They have developed an approach which takes a variety of production processes (either in use or under development), compares their efficiency, their consumption of different resources, etc., and finds the combination of technologies that best satisfies a particular demand while staying within the limits imposed by resource availability. This approach uses the techniques of interactive decision analysis to incorporate the unquantifiable social and political factors that must influence any development decision. By way of illustration, the method is applied to one very small part of the problem area: the different routes to the production of methanol.

This report does not attempt to provide any final answer to the problem of feedstock supply, but rather to explain one possible approach to the problem and discuss some intermediate results. It is addressed not only to researchers, but also, and in particular, to all decision makers and industrial consultants facing problems of this type.

CONTENTS

1 INTRODUCTION 1

2 PROBLEM IDENTIFICATION 4
  2.1 Substitution of Hydrocarbon Feedstocks 4
  2.2 Working Scenarios and Decomposition of the Problem Area 10
  2.3 Measures and Data 12

3 AN APPROACH TO PROBLEM SOLUTION 14
  3.1 Toward a Formal Representation of the Problem Area 14
  3.2 General Model of a PDA 16

4 THE CASE OF METHANOL 19
  4.1 The Methanol Industry and its Future 19
  4.2 Production of Methanol from Fossil Resources 24
  4.3 Results of Simulation Experiments 31

5 METHODOLOGY 36
  5.1 Scope 36
  5.2 Concordance as a Multiobjective Problem 37
  5.3 Methodological Implications of the General Model 39
  5.4 The Attainable Performance Area and Critical Resource Area of a PDA 42
  5.5 Steps in Problem Solution 42
  5.6 Methodological Interpretation of the Methanol Experiments 44

6 CONCLUSIONS 49

ACKNOWLEDGEMENTS 50

APPENDIX 50

REFERENCES 52

1 INTRODUCTION

The world is currently passing through a period of great economic, social, and technological change. Recognition of this fact, and of the need to control the forces of change, has stimulated international interest in the problems of change and methods for coping with them. Nowhere is the need for management of change more crucial than in the industrial sector, where many factors can affect the growth or decline of individual industries and the resulting industrial structure. This paper will concentrate on the chemical industry and the problems it faces as a result of global change, particularly as a result of changing patterns of energy use.

The importance of the chemical industry is often greatly underestimated. Not only does it provide soaps, detergents, and medicines, but also pesticides, fertilizers, synthetic rubbers, plastics, synthetic fibers,... – in fact, our modern technological society could be said to be founded on the chemical industry. One of the most surprising facts about this industry is that a large proportion of its many products are derived from only a very small number of starting materials, of which hydrocarbons are probably the most important. Hydrocarbons are chemical compounds containing only carbon and hydrogen; they can exist in complicated ring structures as well as long chain formations; some of them react easily with other elements and compounds while others are extremely inert. Hydrocarbons occur naturally as components of gas and crude oil – most of those used in the chemical industry are obtained by processing crude oil. Thus it is immediately apparent that there is a potential conflict between the needs of the energy sector and those of the chemical industry: they are competing for an increasingly scarce resource – crude oil.

In view of the importance of the chemical industry, it is clear that the supply of hydrocarbon feedstocks should not be allowed to run dry. The main aim of our research is to develop a methodology capable of proposing possible restructuring in various sectors of industry which would ensure that this type of situation could not arise. The approach chosen takes a variety of interrelated and alternative production processes (either in use or under development), compares their efficiency, their consumption of different resources, etc., and finds the combination of technologies that best meets a particular need while staying within the limits imposed by the availability of resources. If this methodology is successful in solving the problems of feedstock supply, then it could also be helpful in the analysis of synfuel production since it leads to a better understanding of the dynamics of industrial structural change.

In recent years there has been much discussion of future levels of liquid fuel consumption, the availability of resources, and the economic and political factors affecting their production and consumption. The realization that the supply of natural hydrocarbons is not infinite, taken in conjunction with the production and pricing policies of OPEC and other producers, has led to a more careful investigation of the balance of future supply and demand. The main result of these considerations has been greatly increased research into methods of producing synthetic hydrocarbons, with especial emphasis on synfuels. Many large-scale research programs have been set up to investigate whether the energy currently obtained from liquid fuels could be replaced by nuclear or solar energy, biomass-derived energy, coal or lignite. One of the main aims in energy-oriented research is the production from coal or lignite of gaseous and liquid hydrocarbons that could be used as substitutes for natural gas and crude oil; these "synthetic" hydrocarbons may be loosely termed synfuels.

It is difficult to predict where the major investments in new energy technologies will be made because:

1. Most of the technologies are at an early stage of development, and investors prefer to wait for some technological breakthrough before committing their resources.
2. The various technologies (e.g., solar, nuclear, biomass, coal-based) are comparable in terms of the energy produced for a given capital expenditure; therefore, it is not clear which technology or combination of technologies a given country or region will choose to adopt.

Complete substitution of crude oil (at current levels of use) by products derived from coal would require 10,000–12,000 million metric tons of coal per year, assuming the present coal liquefaction technology. This means that it would be necessary to at least quadruple the current annual world production of coal. The investment required to process the coal is also very high. To process 10 million metric tons of crude oil in a full-treatment refinery costs about $1,500 million. By way of comparison, studies show that to obtain the equivalent products from coal it would be necessary to build conversion facilities capable of handling 40–50 million tons of coal per year, requiring capital investment in the range $10,000–12,000 million. To completely substitute crude oil by coal-based products on a global scale would require capital investment of the order of $\$(2.0–3.6) \times 10^{12}$, and this is clearly out of the question.

These considerations alone lead us to the conclusion that the synthetic fuels industry is not likely to develop very rapidly. However, such a situation would pose a threat to all developed economies because the chemical industry would be forced into dangerous competition for hydrocarbons with the gasoline producing sector, where profit margins are always very high. This has been recognized by IUPAC and was singled out in the recommendations made by the IUPAC Conference held in Toronto in 1978 (St. Pierre 1978):

> "In monetary terms it has been estimated that the output of the organic chemical industry (with the crude oil origin feedstock) of the world amounts to three hundred billion US dollars annually. In addition, it is essential to perhaps a third of the world's gross product. Any major change in this industry will utterly change living patterns as we know them today. Nevertheless, people generally, political leaders, and influential citizens seem unaware of these facts and their significance for the future quality of life on earth."

This is the first report from a research project focusing on the problems identified above. The research was sponsored by the Polish Government Program on Coal Processing and carried out under a collaborative agreement between IIASA and the Academy of Mining and Metallurgy (AMM) in Cracow, Poland;* most of the collaboration on the IIASA side has involved the Resources and Environment group, with partial support from the System and Decision Sciences Area. This report does not attempt to provide answers to the problems of feedstock supply, but rather to explain one possible approach to the problem and discuss some intermediate results. Emphasis is placed on the general philosophy behind the approach rather than on the technical or mathematical details, which are described in full elsewhere (Dobrowolski et al. 1980a,b, 1982, Kopytowski et al. 1981, Gorecki et al. 1982).

The report is addressed not only to researchers but also, and in particular, to decision makers and industrial experts facing the problems outlined above. It is also directed to funding institutions, in the hope that their attention will be drawn to the need to allocate resources for research in this very important area.

The report falls into five main parts.

The first part (Section 2) deals with identification of the problem: it begins with a summary of our work on alternative industrial structures, which will perhaps give the reader a better understanding of the complexity and nature of the system being studied. Various aspects of the production of hydrocarbon feedstocks are discussed and the connections between this activity and those in other sectors are revealed, with especial emphasis on energy resources. We also propose a natural decomposition of this whole area of chemical production into subareas (Production/Distribution Areas, or PDAs, see later); this disaggregation can be continued right down to areas based on individual chemical products such as methanol. The importance of data collection is emphasized and the type of data used in the analysis is discussed.

The second part of this paper (Section 3) describes the approach developed to analyze the problem. We first give a generalized description of the chemical industry, which provides an introduction to our simple formal representation of the industrial structure. The idea of a Production/Distribution Area (PDA) is then explained and developed mathematically; this is the basis of our methodological approach.

Having identified the problem area and presented a way of finding feasible feedstock production strategies, Section 4 considers how our approach may be applied to one very small part of the problem area – the production of methanol. The reasons behind the choice of methanol are elaborated and some general information on production technologies, conversion processes, and possible developments is given. We then use the PDA model to carry out a comparative analysis of seven different methanol production processes, and the results obtained under various scenarios are discussed.

---

*The actual group involved is the Systems Research Department of the Institute for Control and Systems Engineering in the AMM and of the Industrial Chemistry Research Institute. Prosynchem Engineering Co. also participated in the study.

Section 5 is concerned with the methodology developed to treat the fundamental problem of matching available resources with technologies (the concept of "concordance"). This methodology is based on the principles of interactive multiobjective analysis. Some of the results obtained in the previous section are then interpreted in the light of this methodological discussion.

Finally, we summarize our findings and draw a number of conclusions in Section 6.

2 PROBLEM IDENTIFICATION

2.1 Substitution of Hydrocarbon Feedstocks

It is not easy to obtain precise information on the world-wide consumption of hydrocarbons by the chemical industry, but some rough figures are available. It has been estimated that only about three percent of all the natural gas and crude oil produced annually is used as feedstocks in the chemical industry. However, since more than fifty percent of the refined material is unsuitable for this purpose, we may say that the chemical industry consumes approximately seven percent of the hydrocarbons available to it, most of this coming from light crude oil fractions. This figure seems marginal when compared to the total production volume, but represents an input of critical importance to the chemical industry and to the industrial structure as a whole.

Hydrocarbons derived from crude oil and used as feedstocks in the chemical industry are transformed by highly sophisticated technological processes into:

1. Compounds of low molecular weight, such as hydrocarbon monomers containing double and triple carbon–carbon bonds, aromatics, and alcohols of different chain lengths.
2. Compounds of high molecular weight:
    - plastics such as polyethylene, polypropylene, polyvinyl chloride, polystyrene, their copolymers, and a wide range of special plastics. The total global production of plastics is of the order of 60 million tons/year.
    - rubbers such as styrene–butadiene rubber (SBR), polybutadiene, polyisoprene, etc. The total world-wide production of rubbers is approximately 11.5 million tons/year.
    - fibers such as polyamides, polyesters, polyacrylonitryl, etc. The total production of fibers in the world is in the region of 10.5 million tons/year.
3. A great variety of other compounds which when processed are used in the production of many different types of goods and commodities.

In our preliminary report on this subject (Kopytowski et al. 1981) we warned that the production of these materials could be severely affected by changes in the level of production of hydrocarbon feedstocks caused by the lack of raw materials at acceptable prices. We stated:

> "The crisis in the synthetic fibers market has not been caused by lack of demand but by the losses incurred in the production process ... The prospective crisis in the synthetic plastics and rubber industries is another illustration of the effects caused by an unstable hydrocarbon market. Far-sighted industrialists are now selling the facilities used to make these products."

The scale of the problems facing the chemical industry has even reached the pages of the popular press. *Le Monde* (June 20, 1982) reports:

> "The situation in the high-tonnage plastics industry is much worse than we could have anticipated, with the total losses incurred by French manufacturers in 1981 exceeding 3 billion francs. This loss is essentially associated with the more widely used plastics (which represent 67 percent of total consumption volume), in particular the five thermoplastics (PVC, high and low density polyethylene, polypropylene, and polystyrene). This loss corresponds to 20 percent of the global sales of the industry (15 billion francs) and represents 75 percent of the total losses incurred by the chemical industry as a whole (4 billion francs)."

And a few lines later *Le Monde* gives the view of M. Schun, Chairman of the Syndicate of Plastics Manufacturers, that

> "the main cause lies in the prices, which are 25 percent lower than their equilibrium level. A long period of fierce competition between European manufacturers has created a situation of deadlock and has not allowed them to respond to a fantastic increase in the demand for raw materials derived from crude oil."

Further on we read that:

> "The difficulties have caused a general crisis, with even the great German trio (Hoechst, BASF, and Bayer) registering a total deficit of 1.5 billion francs. The combined losses of all European plastics manufacturers are estimated at 8–13 billion francs."

A few months later, *The Economist* (October 9, 1982) tells us:

> "Europe's synthetic fibers industry is braced for a fresh round of cuts in capacity. Manufacturers plan to sign an agreement in late October to shut down 17 percent of the industry's capacity by the end of the year."

The article concludes:

> "But most basic industries are finding that the gains from moving into cleverer, high-profit and low-volume products are still offset by losses on their much bigger bulk-commodities businesses."

Just two weeks later *The Economist* (October 23, 1982) reports some more bad news for the chemical industry:

> "The bosses of Europe's petrochemical industry commiserated with each other at their annual beanfeast in Brussels this week: their companies are losing between them 200 million dollars a month."

We could give many more quotes from other newspapers and periodicals, but these would only serve to emphasize what has already been said. When this sort of information starts to appear in the popular press it means that the time left for finding a solution is running out; the temporary drop in oil prices should not be understood to mean that the danger has disappeared. The heart of the matter is much more complex and only a new structural development strategy can help us to overcome the problem.

To move toward a solution of these problems we have to consider various ways of designing an industrial structure which would robustly fulfill the requirements of the chemical industry. The aim is to develop such an industrial structure at a low investment cost and, with the cooperation of the fuel industry, to ensure stable feedstock prices and supplies.

It is clearly impossible to carry out such an analysis on a global scale. Rather, we should examine the balance between hydrocarbon demand and supply in individual countries or regions, taking into account the raw materials available and the processes by which they can be transformed.

We can summarize the various steps in problem solution as follows:

1. Development of some means of determining the demand vector in the consumption sector – this is a typical scenario type of problem.
2. Development of some means of identifying an appropriate industrial structure (i.e., an appropriate combination of production and conversion processes).
3. Investigation of the environmental constraints, the availability of resources, the final distribution of products, etc.

Hydrocarbons can theoretically be obtained from any substance containing carbon. The higher the hydrogen content, the lower the cost of its transformation to a specific hydrocarbon compound. The aim of our research is to develop a method which would identify the best way of substituting natural hydrocarbons derived from crude oil by hydrocarbons from other materials containing carbon (i.e., coal, lignite, oil shales, etc.). Unfortunately the hydrogen content of these materials is no more than 4–5 percent, compared with 10–12 percent in the natural hydrocarbons currently used as feedstocks in the chemical industry. The technological processes used to convert coal to liquid and gaseous hydrocarbons (and coke) are summarized in Table 1. Combinations of these and conventional production possibilities must be analyzed, taking into account both construction and operating costs. To make the method more universal and less susceptible to changes in relative prices, we estimate "costs" in terms of basic natural resources, i.e., water, energy, land, materials, and manpower (the WELMM approach) as suggested by Grenon and Lapillone (1976) and Häfele et al. (1982). When a final decision has been made, the costs can also be evaluated in monetary terms under the

TABLE 1 Technological processes for coal conversion and the resulting products.

Process	Product
Extraction of coal and lignite by gases under supercritical conditions Extraction of coal by liquid solvents	Mixture of light and heavy oils (syncrude)
Hydrogenation of coal extracts Hydrotreatment of coal suspensions	Mixture of light and heavy oils (syncrude)
Flash pyrolysis of coal and heavy oil mixtures Flash pyrolysis of coal	Syncrude and coke
Coking	Tars and coke
Carbide production	Acetylene
Gasification of coal (oxidation)	Synthesis gas

particular conditions prevailing at the time. Two cases are shown in Figure 1 – the present situation (a) and the most robust solution possible in the future (b).

We begin our search for a suitable method by investigating some of the options. Figure 2 illustrates one possibility based on the assumption that hydrocarbons are divided between the energy sector and the chemical sector according to priority of demand. In this situation, therefore, a temporary lack of feedstocks may occur and lead to disruption in the production of plastics, rubbers, and fibers.

The option most popularly believed to represent a possible solution is illustrated in Figure 3. It is based on the supposition that a lack of liquid fuels would provide an incentive for large-scale investment in the extraction of hydrocarbons from solid fossil resources, and that this would lead to a natural division of available resources between chemical and energy sectors. This implies that the production of feedstocks for the chemical industry would become totally dependent on the equilibrium in the fuel sector, and could also lead to a situation in which the hydrocarbons supplied to the chemical industry would not be in the most thermodynamically efficient form for chemical processing.

Figure 4 shows another approach to the problem. In this case it is assumed that there is a set of specific technological processes which could provide the basis for an industry whose only function is to produce feedstocks for the chemical industry. This industry would cooperate with the fuel sector, buying products obtained by the processing of fossil resources and selling certain byproducts which could be used in the fuel sector. The supply of feedstocks to the chemical industry would thus be assured by optimal investment strategies for specific processes, which would be time and market dependent. Feedstocks would be produced efficiently and, although there would be certain links with the fuel sector, feedstock production would certainly not be controlled by it.

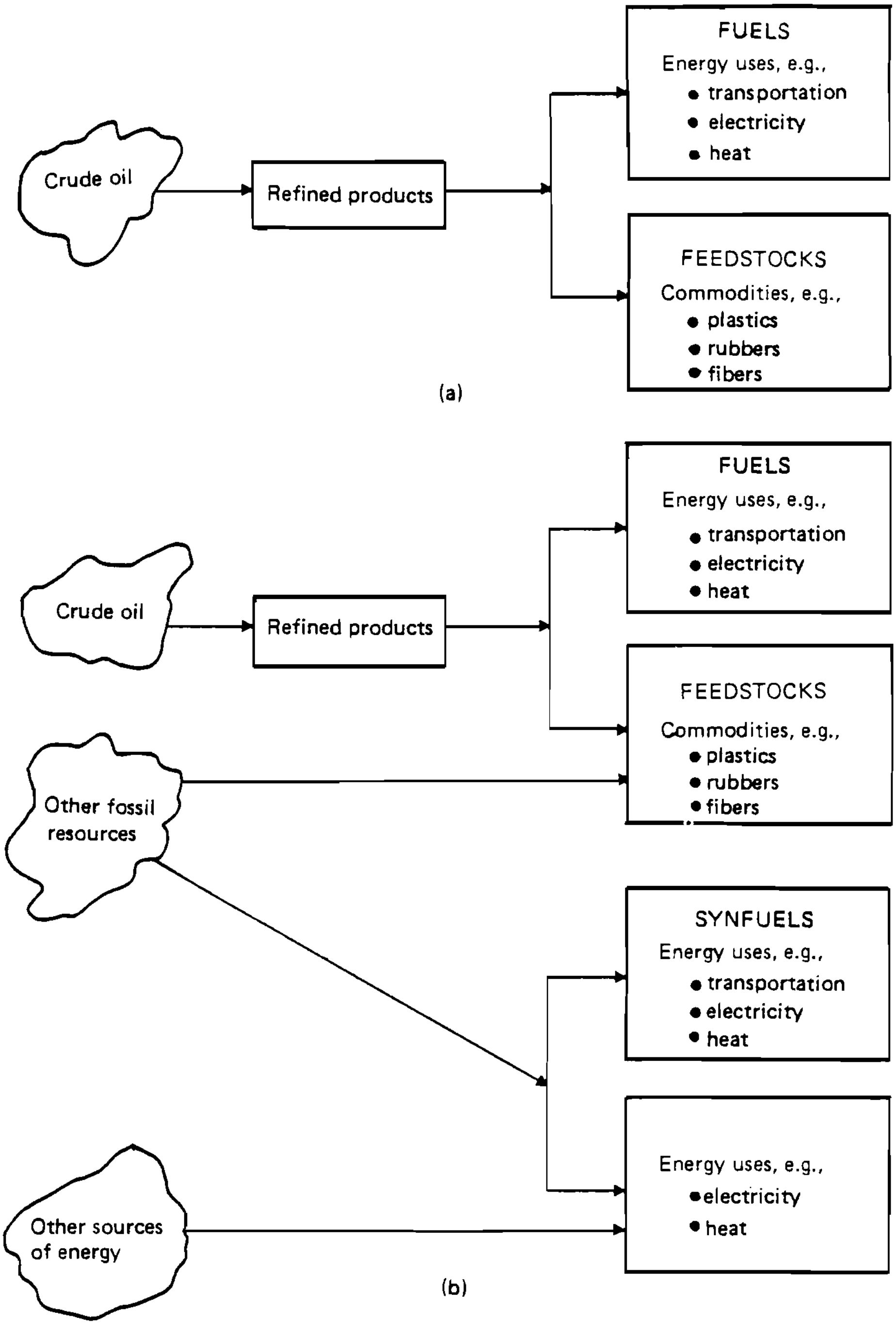

FIGURE 1 Two possible routes from resources to fuels and feedstocks: (a) the present situation; (b) the most robust solution possible in the future.

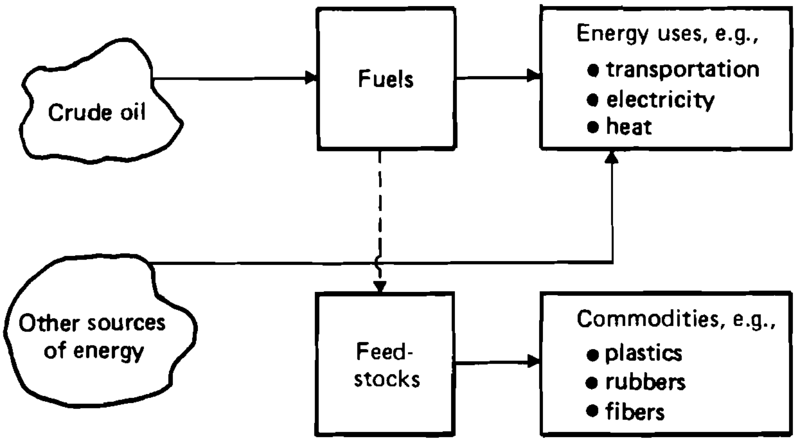

FIGURE 2 Route from resources to fuels and feedstocks based on the assumption that hydrocarbons are divided between the energy sector and the chemical sector according to priority of demand.

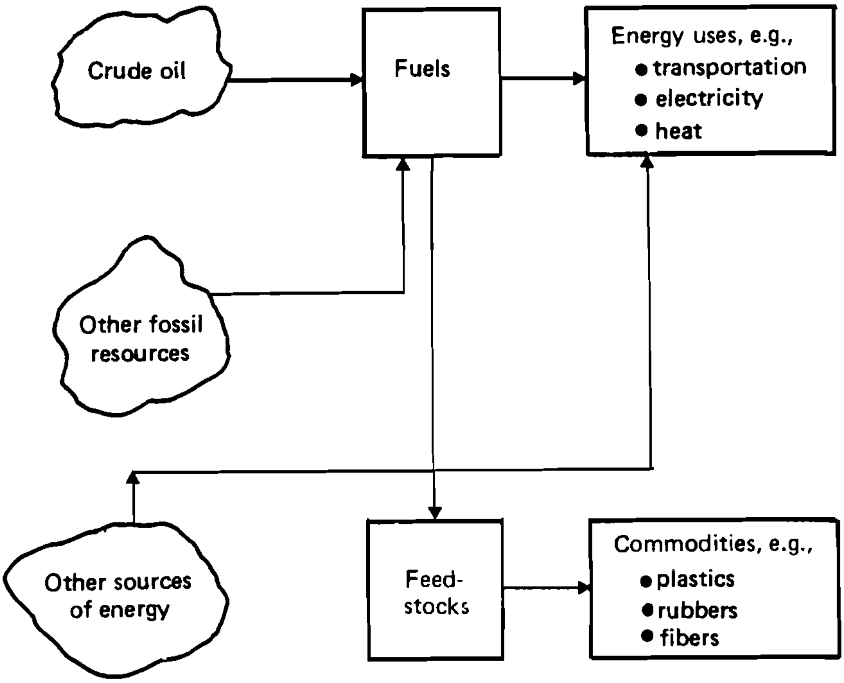

FIGURE 3 Route most popularly believed to represent a solution to the problem of fuel/feedstock allocation of hydrocarbons.

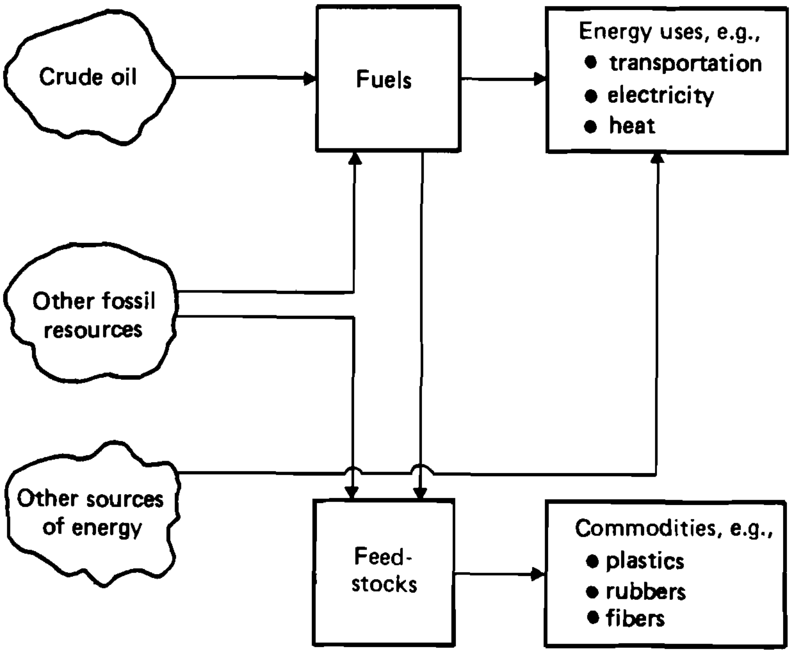

FIGURE 4 Route from resources to fuels and feedstocks suggested by the authors.

2.2 Working Scenarios and Decomposition of the Problem Area

Our approach to the problem outlined above is based upon an analysis of the different ways of producing chemical feedstocks and synfuels. We consider various technological possibilities, and scenarios such as:

- present and future demand will be met by hydrocarbons derived from crude oil only (an extreme case);
- hydrocarbons derived from crude oil will be used to meet the present level of demand; any increase in demand must be covered by hydrocarbons derived from hard coals and lignite.

Different assumptions concerning the level of future demand and the availability of resources are examined to see how these factors influence the structure of production. It is also necessary to consider the various methods of energy production in this and other sectors, not only to compare the efficiency of energy use, but also to establish possible tradeoffs between the different industrial sectors.

Since the area covered by the problem is so large and complex and requires such a vast amount of data, it is virtually impossible (and could be misleading) to treat it as a single system. We therefore break it down into a number of smaller areas (called Production/Distribution Areas or PDAs), each concerned with a particular closely related group of products. One such PDA could be defined as follows:

PDA 1: gasoline, jet fuels, diesel oil, fuel oil, simple monomers, simple aromatics, fuel gas (natural gas or SNG), methanol and the higher alcohols, naphtha, and ammonia.

This could be broken down still further to form a smaller PDA:

PDA 2: simple monomers, simple aromatics, methane (SNG), methanol, naphtha, and ammonia.

The way in which these PDAs can be constructed is treated in some detail later in the report.

One very important advantage of this decomposition is that various methodological approaches may be developed and tested using the smaller areas before applying them to the problem as a whole. Another is that the smaller the area considered, the easier it is to examine the influence of changes in technology or resource use – cause and effect relationships can be identified more clearly in simple systems. Finally, decomposition also allows us to obtain the solution to a particular complex problem in several simpler stages; we can treat the case of methanol (see Section 4) as one of these steps.

Returning to the overall problem once again, it is clear that there cannot be a single solution which holds for all countries and economic regions. Different countries have different demand vectors and access to different fossil resources. The transformation of coal, lignite, etc. into hydrocarbons would therefore require a different industrial structure in different countries and/or regions.

In parallel with the generation of different industrial structures, we carry out an analysis of the various alternatives to determine which of them minimizes the consumption of basic natural resources. Since the analysis involves several criteria, we use a multiobjective optimization technique (see Section 5).

There are two main approaches to our problem:

1. Simulation of a number (usually in the range 20–30) of different production processes composed of different technological units; these simulations should consider the transformation of all possible grades of fossil resources. The simulations are compared and the best feasible solution is identified in an interactive fashion.
2. Simulation of all possible combinations of technologies; the optimization procedure selects several close-to-optimal solutions (in terms of resource use), which are then analyzed by a multiobjective optimization model.

The first approach requires more work preceding computerized analysis, but can be applied to the problem under all sorts of different conditions. This method will be discussed in more detail later in the report.

An automated system such as that required by the second approach would involve prior development of a large number of different technological models, some of which may turn out to be useless or irrelevant in the final analysis. This type of approach should therefore be limited to rather narrow areas, such as the methanol study mentioned earlier.

In practice, the method adopted will be a compromise between (1) and (2) which will depend on the particular case under consideration: the more complex the industrial structure, the closer the approach will be to (1).

2.3 Measures and Data

In order to construct a model it is necessary to establish some means of identifying not only the variables and parameters of the model, but also its constraints and objective function.

Three distinct types of values have been chosen to characterize a specific technological process or group of processes: natural resource requirements, technological parameters, and secondary parameters.

The first group reflects the requirements of a process for natural resources such as water, energy, land, materials, and manpower, the availability of which determines whether a given process is feasible in a particular environment. These factors have an important effect on the economic efficiency of the process.

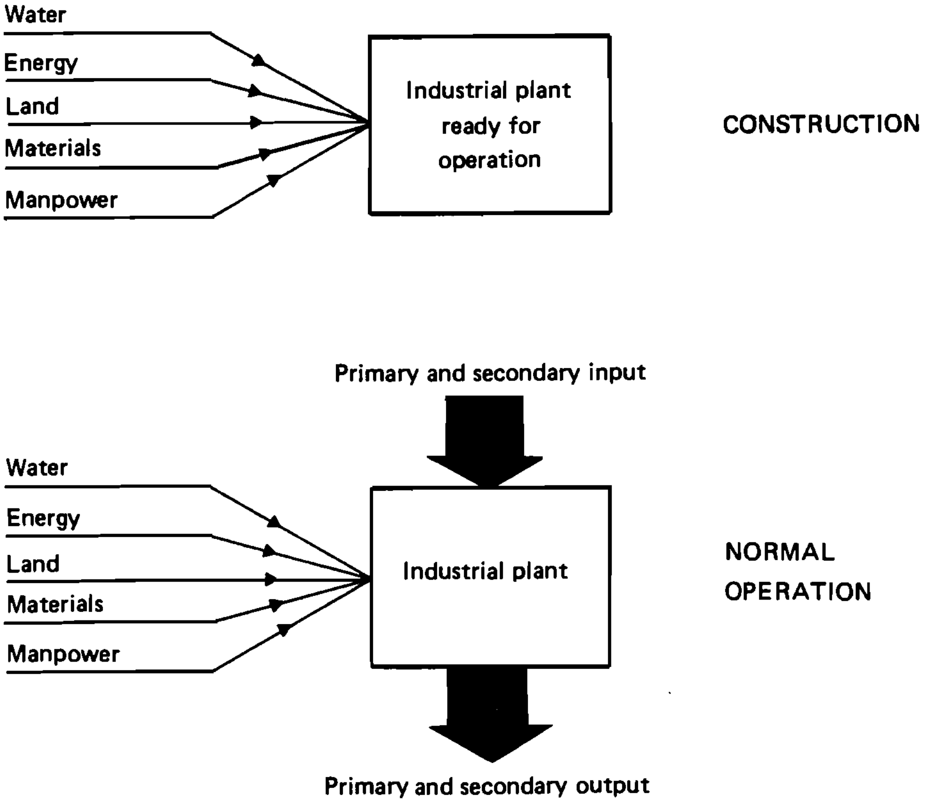

FIGURE 5 Resources required in the construction and normal operation of an industrial plant.

Figure 5 shows that resource requirements can be estimated for two distinct phases of plant activity: the construction (or implementation) phase and normal operation. The various factors considered in each phase are explained in more detail below.

Construction phase

Materials: Equipment, pipes, valves, steel structures, concrete, steel reinforcements, and other material necessary on site.

Manpower: Numbers of manhours required for construction (can also be expressed as a number of men working for a specified length of time).

Land: Amount of land necessary for siting plant and facilities.

Energy: Electrical, mechanical (fuels), and thermal energy necessary to carry out the construction work.

Water: Water required for sanitary and construction purposes.

Normal operation

Materials: This includes the primary and secondary materials consumed in the process and the materials used in normal operation (replacement valves, lubricating oils, etc.). The former are mostly either primary energy carriers (crude oil, coal, natural gas) or secondary energy carriers (synthesis gas, naphtha), and could also be considered as specific forms of energy (see below).

Manpower: Labor directly employed at the plant.

Land: Amount of land occupied by plant, buildings, and facilities.

Energy: Electrical energy for driving machinery, heating, and lighting; thermal energy (steam) for heating and driving machinery, and fuels used in industrial furnaces.

Water: This includes the water used in the process, the water used for cooling, and the water used for sanitation. It is sometimes also important to specify the quantity of water lost, i.e., consumed in the process or lost to the atmosphere through evaporation.

This is basically the approach developed by the WELMM group to analyze energy strategies and options (Grenon and Lapillone 1976) and also has similarities to the Bechtel model (Gallagher and Zimmerman 1978). We worked closely with the Resources and Environment group at IIASA on our application of the WELMM approach, although we structured our data in a slightly different way so that it would be more flexible for practical purposes and compatible with our model (see Sections 3 and 4). However, this restructuring did not in any way restrict the range of application of the data base.

The second group of values used to characterize the process are the technological parameters. These include the total consumption of raw materials, the level of output of final products, capacities, and the kinetic or thermodynamic parameters of the production process.

The last group of values are what we call the secondary parameters of the process, and can be determined only by combining and manipulating the information in the data base. These are coefficients such as the consumption of materials and energy per unit output, the productivity of labor (manhours per unit output), operational demands, investment per unit output, and efficiency. The experiments considered here are mostly described in terms of this third group of parameters, which makes it possible to consider elements from classical economics, such as the return on investment or the net present value of the chosen project alternative.

Data collection and evaluation are obviously very important parts of the study. In the particular case of methanol, the information came largely from operating data and the literature, but special technical studies also had to be carried out to make the data consistent and to fill in gaps in the parameter estimates. The same data base was used to derive all three groups of parameters; the first two groups can be extracted directly but the third requires some initial manipulation of the data.

3 AN APPROACH TO PROBLEM SOLUTION

3.1 Toward a Formal Representation of the Problem Area

Our aim is to construct a model describing the production structure of the chemical industry which could then be used to generate various development alternatives. In order to do this we have to look at the industry as a whole and identify the crucial features that must be included in the model. There has been much research on this topic. Our own research goes back several years (see Borek et al. 1978, 1979) and is still in progress (Dobrowolski et al. 1982). Another approach that leads to very interesting results is described by Stadtherr and Rudd (1976) and Sophos et al. (1980). The book by Kendrick and Stoutjestijk (1978) also proposes an interesting alternative process-type model.

Chemical production can be viewed basically as a sequence of processes that change certain starting materials into end products that are quantitatively and qualitatively (physico-chemically) very different from the input material. The flow of material through the production process can be considered continuous, even in the case of periodic reactions. There are usually a number of ways of producing a given compound, most of which involve not one reaction but a whole chain of them. The same compound may be used in a number of reactions in any given production chain and may also be used in other chains; these chains therefore form a network. Compounds going into or produced by reactions in the middle of chains are called semiproducts or intermediates, and there is a very large market for these materials within the chemical industry itself. However, it must be said that this market depends greatly on the strength of the demand for final products.

Thus the industry, by its very nature, is composed of a great number of elements that are very strongly interdependent, both technologically and economically.

Consider Figure 6, which shows how the resource vector X may be mapped onto the demand vector Y in a given economic environment. The demand vector may either be based on observed data or modeled according to some scenario. Using this demand vector and assuming that it excludes

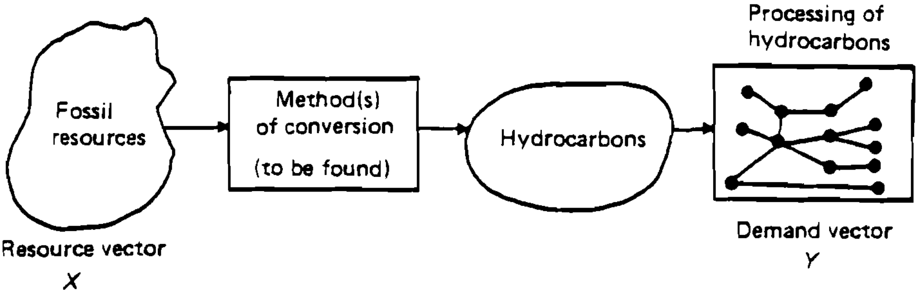

FIGURE 6 The problem: to map resource vector X onto demand vector Y in a given economic environment.

wasteful consumption, it is possible to determine the production structure for commodities that meets this demand. Then, working backwards, and using information on the chemical precursors of each commodity, it is possible to determine the chemical production structure that underlies the production of this combination of commodities.

It is important to realize at this point that we should not expect substantial changes in large, investment-intensive areas of the industrial structure in the next 10–15 years – industry simply cannot afford it, financially or technically. Too many resources and too much technical know-how are tied up in existing plants and processes to allow massive reorganization. On the other hand, we have the fossil resources and must decide how best to utilize them.

We may therefore formulate the problem as follows (see Figure 6): given the demand vector Y and some vector X of available resources, we have to find the combination of fossil resource → hydrocarbon conversion processes that represents the optimal transformation, bearing in mind the existing industrial structure, the associated environmental impacts, and so on. This is done using the previously described data on the various production processes and technologies in conjunction with the procedures described in Section 5.

However, we have already pointed out that the area of chemical production is much too large and complex to be treated as a whole; it must be divided into more manageable areas based on a small number of closely related products and processes. We call these smaller areas Production/Distribution Areas (PDAs) because they are largely concerned with the production and distribution of a particular chemical or group of chemicals. There must be a certain amount of freedom in selecting or marking the PDA boundaries, although the relative density of technological connection is perhaps one of the most important factors to be considered here. Others include organizational factors and market, labor, maintenance, transport, and supply conditions.

In fact, PDAs often correspond roughly to the areas of production covered by the individual large chemical companies; it makes sense for each company to deal with a particular closely related group of chemicals because they can then coordinate the flow of intermediates, feedstocks, etc. through a set of linked processes with the minimum of dependence on external suppliers. These companies wish to maximize their profits by developing the most efficient production structure for a given economic/social/political environment; but, since this environment is constantly changing, the production structure must evolve to keep pace with it. The companies try to adapt to the new conditions by selling old plant, investing in new plant, and reallocating resources, but generally the change in production structure lags behind the changes in operating conditions, leading to a loss of efficiency and hence of profits. The scale of the problem is illustrated very clearly by the quotes from the press given in Section 2. One very important application of our PDA model could therefore be to help in determining the best production structure for an individual company under various operating conditions. In addition, by adjusting the boundaries of the PDA it is possible to determine how individual companies could broaden their range of activities most effectively. Of course, the same sort of results can also be obtained for PDAs that cross these company boundaries and involve activities intersecting with those of several established production groups.

It should be emphasized that the simplified model of the PDA described in the next section includes only the easily quantifiable physical elements of the system; it does not attempt to take into account the sometimes very important but unquantifiable social and political factors that will affect any development decision. The relative importance of these factors can only be assessed by the decision maker; this is why it is important to use an *interactive* decision support system (see Section 5) in conjunction with this model.

3.2 General Model of a PDA

We regard the chemical industry as being divided into a number of subsectors, each dealing with a group of closely related chemicals. These subsectors are called Production/Distribution Areas (PDAs) because they basically comprise a network of production processes and distribution flows for a very specific group of chemicals. The PDAs are linked to each other and to other industrial sectors through the buying and selling of chemicals. Our general model of a PDA must therefore take into account:

- the processing and flow of chemicals within the PDA;
- the flow of chemicals into and out of other areas or industries, representing the marketing or business activity of the PDA;
- the flow of investment, revenue, and other resources such as energy, manpower, etc.

The model is given below in its basic form so that its structure may be more easily understood; however, the complexity of the full computer implementation should not be underestimated. We first define the links of the PDA with its environment (see Figure 7).

From Figure 7, we can write the following equation describing the outflow of any chemical j:

$$y_j = y_j^{\mathrm{ms}} - y_j^{\mathrm{mp}} + y_j^{\mathrm{cs}} - y_j^{\mathrm{cp}} \quad , j \in J \tag{1}$$

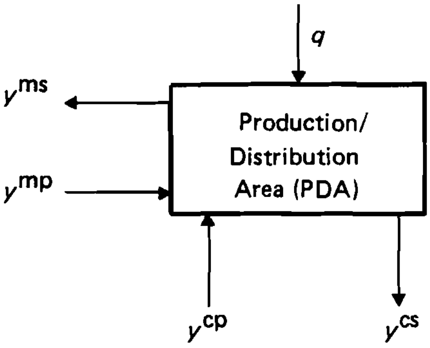

FIGURE 7 The links between a Production/Distribution Area (PDA) and its environment.

where

y_j^{ms} – market sale of chemical j
y_j^{mp} – market purchase of chemical j
y_j^{cs} – coordinated sale of chemical j
y_j^{cp} – coordinated purchase of chemical j
J – set of indices representing the chemicals under consideration.

Here we introduce the concept of a coordinated flow, i.e., agreed buying and selling of chemicals among PDAs. This makes it possible to achieve some form of inter-PDA coordination.

Note that we cannot usually describe this coordination by the formal decomposition of a larger problem containing a number of areas. This can be illustrated by the situation that arises when the source of an intermediate is a different PDA: the second PDA may not be willing to reveal to the first all of the data that would be necessary for optimization over all the PDAs involved.

Resources other than chemicals required for network activities are denoted in Figure 7 by q, and include inputs such as energy, labor, and water.

The particular formulation of the performance functions depends on the strategy and policy adopted by the industry and does not influence our considerations until we are ready to solve the optimization problem.

Now let us briefly look at the form of the production/distribution network within the PDA. The network is formed by two types of elements:

- process elements, which represent chemical processing;
- balance nodes, which represent the total flow of any chemical j .

We shall denote by J^* the set of indices describing chemical processes taking place in the PDA under consideration.

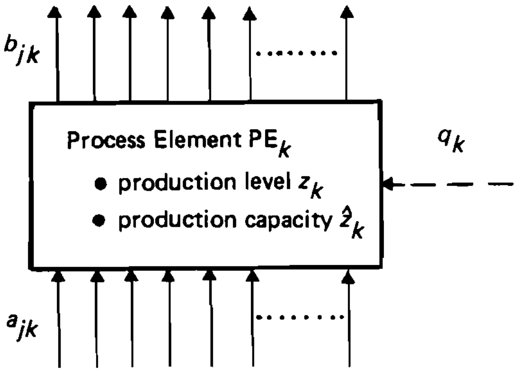

FIGURE 8 Process element PE_k and the associated variables and parameters.

The way in which the network is constructed ensures that all of the conditions concerning links to and from the environment are taken into account, regardless of the number of process elements and balance nodes.

Let us consider a process element $PE_k, k \in J^*$ (see Figure 8). The variables used in Figure 8 may be defined as follows:

z_k – production level of PE_k
$\hat{z}_k$ – production capacity of PE_k
$a_{jk} z_k$ – quantity of chemical j consumed by PE_k
$b_{jk} z_k$ – quantity of chemical j produced by PE_k
$q_k(z_k)$ – necessary resources.

For the balance nodes we may write an equation of the following type:

$$y_j = x_j^+ - x_j^- \tag{2}$$

for each chemical j, where

y_j – total outflow of j
x_j^+ – total production of j
x_j^- – total consumption of j.

The network is constructed from process elements and balance nodes in a way that reflects all of the technological connections present in the system. Of course, a process element may be connected to other process elements only through balance nodes.

Having defined the network, we may formulate the following equations: Total production of chemical j :

$$x_j^+ = \sum_{k \in J^*} b_{jk} z_k \quad , \quad j \in J \tag{3}$$

Total consumption of chemical j :

$$x_j^- = \sum_{k \in J^*} a_{jk} z_k \quad , \quad j \in J \tag{4}$$

Substitution of (3) and (4) into (2), and combination of the result with (1) leads to

$$y^{ms} - y^{mp} + y^{cs} - y^{cp} = (B-A)z \tag{5}$$

To complete this somewhat simplified description of the internal PDA network, we have to add the constraints imposed by production capacity. The form of these constraints will depend on the type of chemical process concerned, and may, for example, include a number of alternative technologies. The idea of new technologies is fundamental to this approach since it opens the way to technological change in the structure of the area. (Data on all relevant new technologies are included in the parameter set discussed in Section 2.)

Note that the version of the model implemented describes all possible modes of production, including alternative ranges of products made at a given installation, recycling of semiproducts, and coupled production of a number of chemicals at one plant.

This model provides us with a basis for formulating decision problems concerned with the generation of efficient development alternatives for a PDA. It is obviously necessary to add a set of criteria and some additional constraints reflecting the preferences or goals of the decision maker as well as physical limits on resource availability, and this generally leads to the formulation of a multiobjective optimization problem.

4 THE CASE OF METHANOL

4.1 The Methanol Industry and its Future

In this section we focus on a particular PDA – that dealing with the production and distribution of methanol. We chose methanol not only because of its industrial importance – it is manufactured in great quantities and used extensively in the chemical and energy sectors – but also because data on the various production technologies are relatively easy to obtain. There are also good methodological reasons for choosing the methanol PDA: it is a relatively simple system whose behavior can easily be analyzed by conventional techniques, thereby providing a means of testing and improving new methodology. In fact, our methodology was developed precisely by studying simple systems such as this and the pesticides PDA (Dobrowolski et al. 1982). We begin with a brief overview of the historical development of methanol production and consumption, and then consider the prospects for the future.

World production of methanol has grown very rapidly over the last 30 years or so (see Table 2). A crucial increase in investment over the period 1967–1970 may be attributed to the introduction of a new low-pressure process, which is cheaper, more efficient, and consequently more economically desirable than the high-pressure process previously in use. Further improvements in methanol production technology are still being sought.

At present, the world produces about 10.5 million metric tons of methanol per year, 3 million metric tons of it in western Europe (Nowak 1982). Experts predict that world production of methanol will rise to about

TABLE 2 Levels of methanol production in various countries.

Country	Methanol production (10^3 t/year)						
	1950	1955	1960	1965	1970	1975	1980
USA	409	609	893	1306	2240	2975	2992
Japan		63	205	470	934	762	
FRG	74	163	334	604	863	887	
Italy	8	28	63	162	209	232	
France		24	70	123	212	375	
Soviet Union			231	482	810	1680	1809[a]
GDR	38	60	73	114	120	246	249[a]
Czechoslovakia	14	29	44	77	98	99	110[a]
Poland	1	9	20	71	72	201	197

[a] Data from 1978.
Source: Nowak (1982).

17.6 million metric tons in 1985, with only about 4 million metric tons of this coming from western Europe. This growth in global production is expected to result from new plants in the Soviet Union, Canada, and Mexico, i.e., nations which are rich in the traditional raw material base – natural gas and crude oil. Western Europe, Japan, and even the USA will probably be net importers of methanol in the 1990s, with the result that methanol trade will assume much greater importance.

TABLE 3 Levels of methanol consumption in various countries and economic regions, and in the world as a whole.

Country or economic region	Methanol consumption[a] (10^3 t/year)							
	1950	1955	1960	1965	1970	1979	1985	1990
USA	236	510	804	1217	2108	3362		
Japan				404	864			
FRG	74	151	348	605	827			
Italy	8	21	60	119	330			
France	17	31	74	114	231			
Western Europe						3259	4345[b]	5625[b]
World	609	1022	2064	3566	5700	13000	17000[b]	23000[b]

[a] Only traditional uses of methanol are considered.
[b] Forecasted values.
Source: Nowak (1982).

The development of methanol consumption in a number of different countries and in the world as a whole is summarized in Table 3. The differences between the amounts of methanol produced and consumed (see Tables 2 and 3) also give an indication of the volume of trade. The present structure of methanol consumption in western Europe is outlined in Table 4, together with some forecasts of how this may change in the future.

TABLE 4 Structure of methanol demand in western Europe.

End uses of methanol	1979		1985		1990	
	10^9 t/year	%	10^9 t/year	%	10^9 t/year	%
Traditional uses						
Production of:						
Formaldehyde	1590	48.8	1840	42.4	2080	37.0
Dimethyl terephthalate (DMT)	160	4.9	185	4.3	200	3.6
Methyl methacrylate (MMA)	110	3.4	130	3.0	150	2.7
Methyl halides	110	3.4	145	3.3	175	3.1
Methyl amines	155	4.8	180	4.1	210	3.7
Miscellaneous	807	24.7	990	22.8	1170	20.8
Subtotal	2932	90.0	3470	79.9	3985	70.9
New uses						
Production of:						
Methyl tertiary butyl ether (MTBE)	70	2.2	180	4.1	240	4.2
MTBE blending component	30	0.9	75	1.7	100	1.8
Gasoline blending	200	6.1	200	4.6	200	3.6
Acetic acid	25	0.8	260	6.0	550	9.7
Single-cell protein (SCP)	2	0.1	160	3.7	550	9.8
Subtotal	327	10.0	875	20.1	1640	29.1
Total	3259	100.0	4345	100.0	5625	100.0

Source: Sherwin (1981).

Most of the traditional end uses of methanol are of a chemical nature. Quite a number of important chemical products are based on methanol, as illustrated by the following examples:

1. Thermosetting and thermoplastic resins and synthetic glues are produced from formaldehyde which, in turn, is obtained by oxidation of methanol (approximately 40–50 percent of all methanol produced is converted to formaldehyde). Phenolic and melamine resins are also obtained in this way.
2. Alkyl resins are produced from pentaerythriol, which is also derived from methanol via formaldehyde.
3. Polyester fibers and films are produced from dimethyl terephthalate, which is synthesized from *p*-xylene and methanol.
4. Chlorine derivatives of methane, which are intermediates in the production of silicones and methyl cellulose, can be obtained by treatment of methanol.
5. Methylamines, which may be derived from methanol, are intermediates in the production of pesticides and insecticides, surfactants, pharmaceuticals, and solvents.

The oil price increases in the early 1970s opened the way to a number of new energy-related applications:

1. In motor fuels
   - by using methanol/gasoline mixtures containing up to 15 percent methanol, although there are some problems concerning phase separation;
   - by designing vehicles to run on 100 percent methanol. This would require only slight modification of a conventional internal combustion engine;
   - by conversion of methanol to gasoline with an octane number of between 90 and 100 using a zeolite-type catalytic process;
   - by the synthesis of methyl tertiary butyl ether (MTBE), the blending and antiknock agent for gasoline, from methanol.
2. Power production can be increased at peak periods by the use of gas turbines, and methanol is potentially an excellent turbine fuel.
3. It has been suggested that methanol could be used as a source of "reducing gas" and hence of hydrogen. Methanol could easily be transported from distant production areas, catalytically converted to a mixture of carbon monoxide and hydrogen ("reducing gas") and used, for example, to reduce iron ore.
4. Methanol can be used in sewage treatment as a food for bacteria which are able to convert nitrogenous wastes into gaseous nitrogen and carbon dioxide.
5. Single-cell protein (SCP) can be obtained from methanol and used to produce animal feed.
6. Methanol can be used in the production of fuel cells.

TABLE 5 New and potential uses of methanol in the chemical industry.

Product	Process	Prospects	Methanol requirement (tons of methanol per ton of product)
Ethylene	Catalytic cracking of methanol	Commercial operation before 1990	3.47–3.89
Ethylene glycol	Carbonylation of formaldehyde	A syngas route to commercial operation by 1990	0.61
Acetic anhydride	Carbonylation of methyl acetate	Already in commercial operation	0.35
Vinylacetate	Reaction of syngas and methyl acetate	Rather poor	0.97
Ethanol	Homologation of methanol	Rather poor	0.77
Styrene	Methylation of toluene	Fair	0.35
Methyl methacrylate	Condensation of formaldehyde and methylpropionate	Fair	0.73
MTBE	n-Butene isomerization to isobutylene	Commercial operation before 1985	0.36

Source: Sherwin (1981).

These new and potential uses of methanol could, if widely adopted, have a strong influence on future methanol requirements, possibly even leading to an increase in demand by several orders of magnitude.

Finally, it should be pointed out that methanol is a "pure" fuel. It contains essentially no sulfur and in combustion produces 70 percent less nitrogen oxides than conventional fuels. New and potential uses of methanol in the chemical industry are listed in Table 5.

Methanol is likely to play a more important role in the future, as crude oil becomes increasingly scarce; the remaining resources (coal, lignites, peat, and wood) are all potential sources of syngas, and hence of methanol.

4.2 Production of Methanol from Fossil Resources

Methanol is usually produced industrially from syngas, a 1:2.2 mixture of carbon monoxide (CO) and hydrogen (H_2), in the presence of a catalyst and under specific temperature and pressure conditions. In practice, this means either a zinc–chromium catalyst at high temperature and pressure (600–700°C and 30 MPa) or a copper–zinc–chromium (or copper–zinc–aluminium) catalyst under milder conditions (<600°C and 5–15 MPa).

Syngas may be obtained from any raw material containing carbon, and therefore all fossil resources are potential starting materials. The following are the most commonly used:

- natural gas;
- natural gas combined with a source of carbon monoxide, such as the residual gas from carbide ovens;
- light fractions of crude oil (naphtha);
- heavy fractions and the heavy residues from distillation of crude oil;
- hard coals and lignite.

The choice of raw material depends largely on the resources and conversion technologies available. We believe that this is a very important decision, and have made the quest for a concordance between resources and technologies a main theme of our research. To analyze this question in more depth we have formulated it as a multiobjective decision problem (see Section 5.2) in which the alternatives to be evaluated are the various routes from natural resource to methanol. We considered seven possibilities:

1. From natural gas to methanol through steam reforming of methane (see Figure 9).
2. As above, but with the addition of (carbon-monoxide containing) residual gases from carbide ovens (Figure 10).
3. From light fractions of crude oil (naphtha) to methanol through steam reforming of the naphtha (Figure 11).
4. From coal to methanol through low-pressure gasification of the coal (Koppers–Totzek-type process – Figure 12).

5. From coal to methanol through medium-pressure gasification of the coal (Lurgi-type process I – Figure 13).
6. From coal to methanol through medium-pressure gasification of the coal, followed by SNG (synthetic natural gas) production and subsequent steam reforming of methane (Figure 14).
7. From heavy residues to methanol through partial oxidation of the heavy residues (Figure 15).

A production unit of 500,000 tons/year capacity has been designed for each of the above processes, and used as a basis for technological comparison. The processes are characterized by three groups of parameters, which have already been described in some detail in Section 2.3. Using this information, and some additional parameters introduced to describe the amount of a critical resource required to obtain one unit of product, it is possible to determine the process (or combination of processes) that best fulfills a given objective (or objectives) under specified conditions. In essence, therefore, we are carrying out a comparative study of methanol production processes under a number of different scenarios.

The experiments described below are based on consideration of the following parameters:

- amount of investment, measured in monetary units (m.u.);
- consumption of natural gas, measured in millions of normal cubic meters (Nm^3);
- energy consumption, measured in tons of coal equivalent (t.c.e.);
- financial efficiency, measured in monetary units (m.u.).

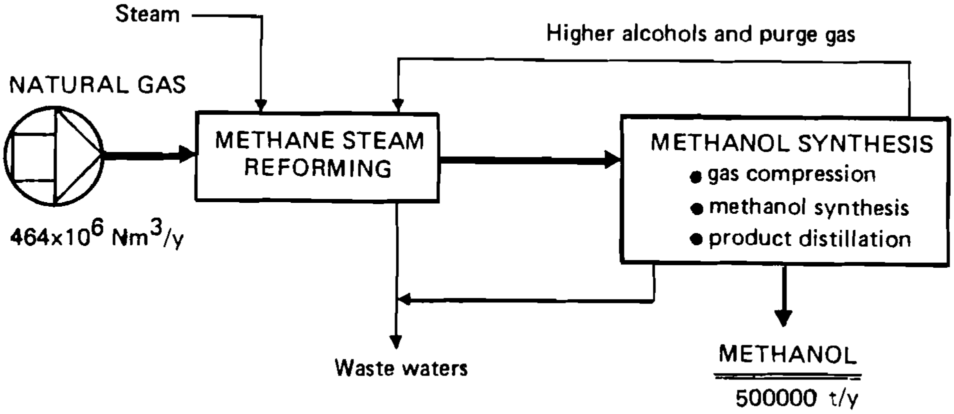

FIGURE 9 Production of methanol from natural gas (steam reforming).

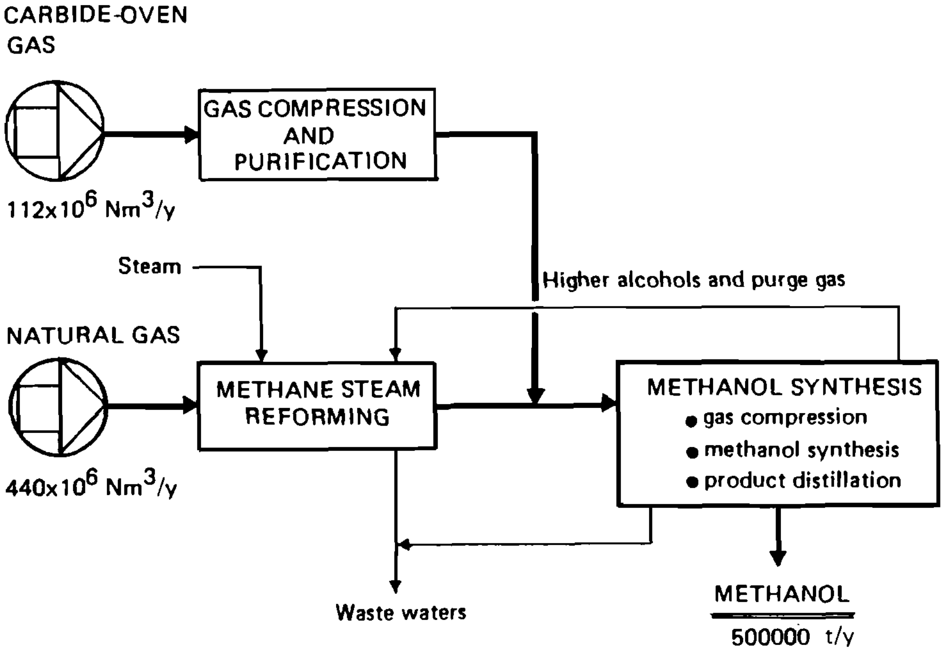

FIGURE 10 Production of methanol from natural gas and (CO-containing) gases from carbide ovens (steam reforming).

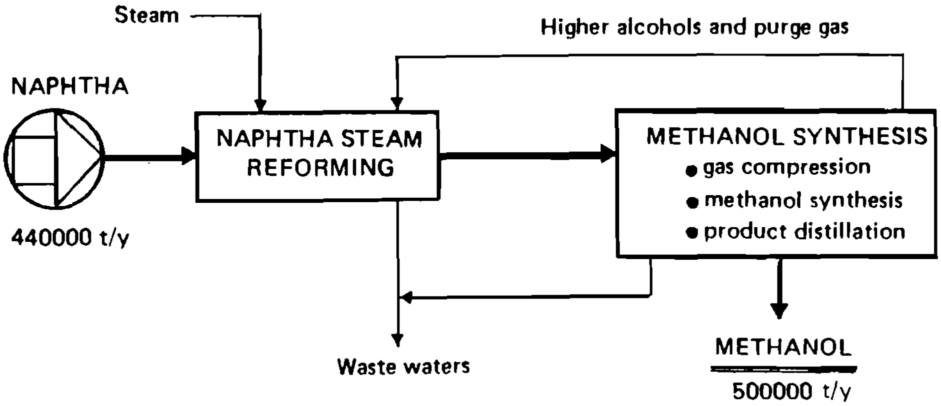

FIGURE 11 Production of methanol from naphtha (steam reforming).

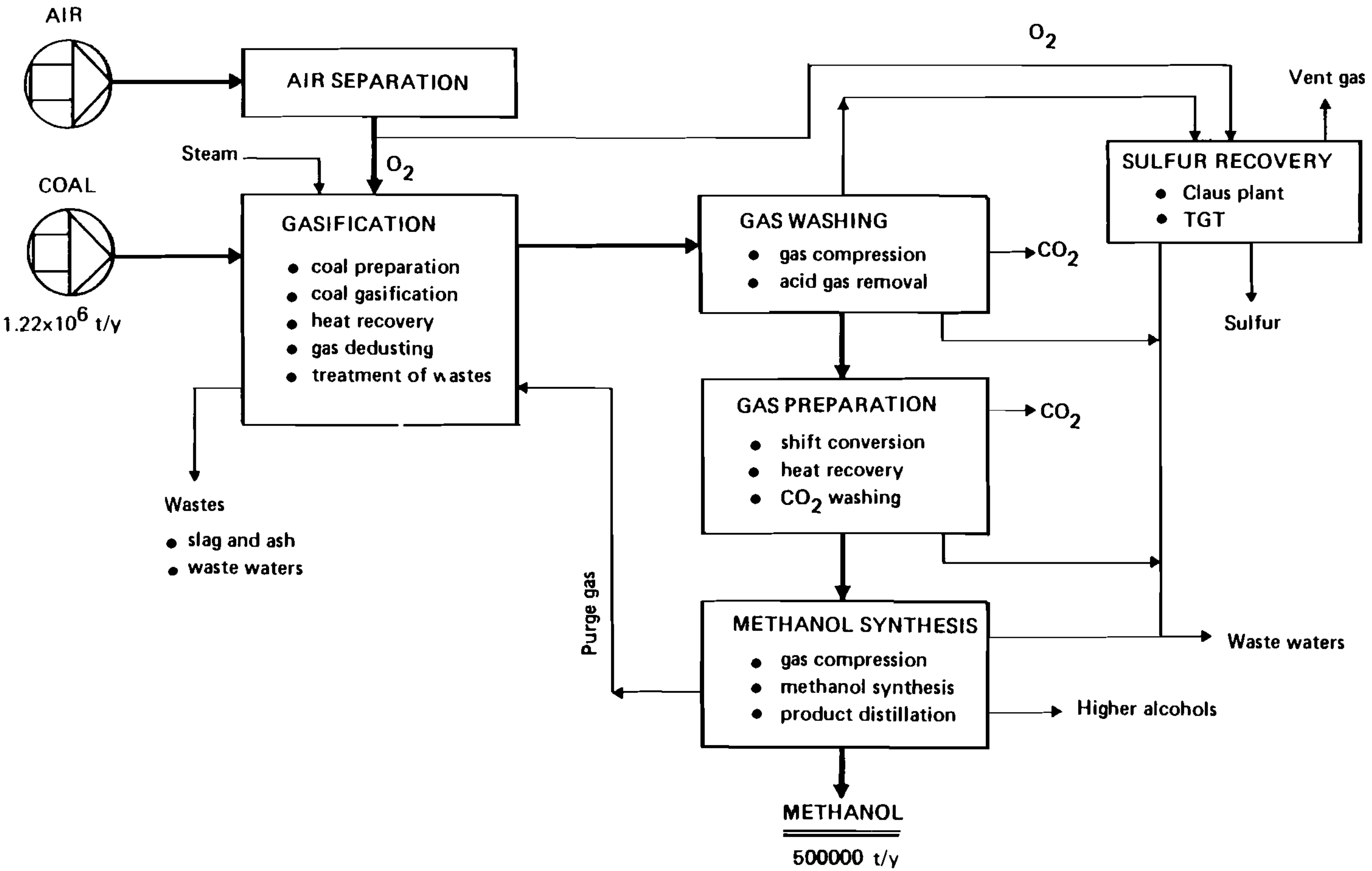

FIGURE 12 Production of methanol from coal (Koppers–Totzek process).

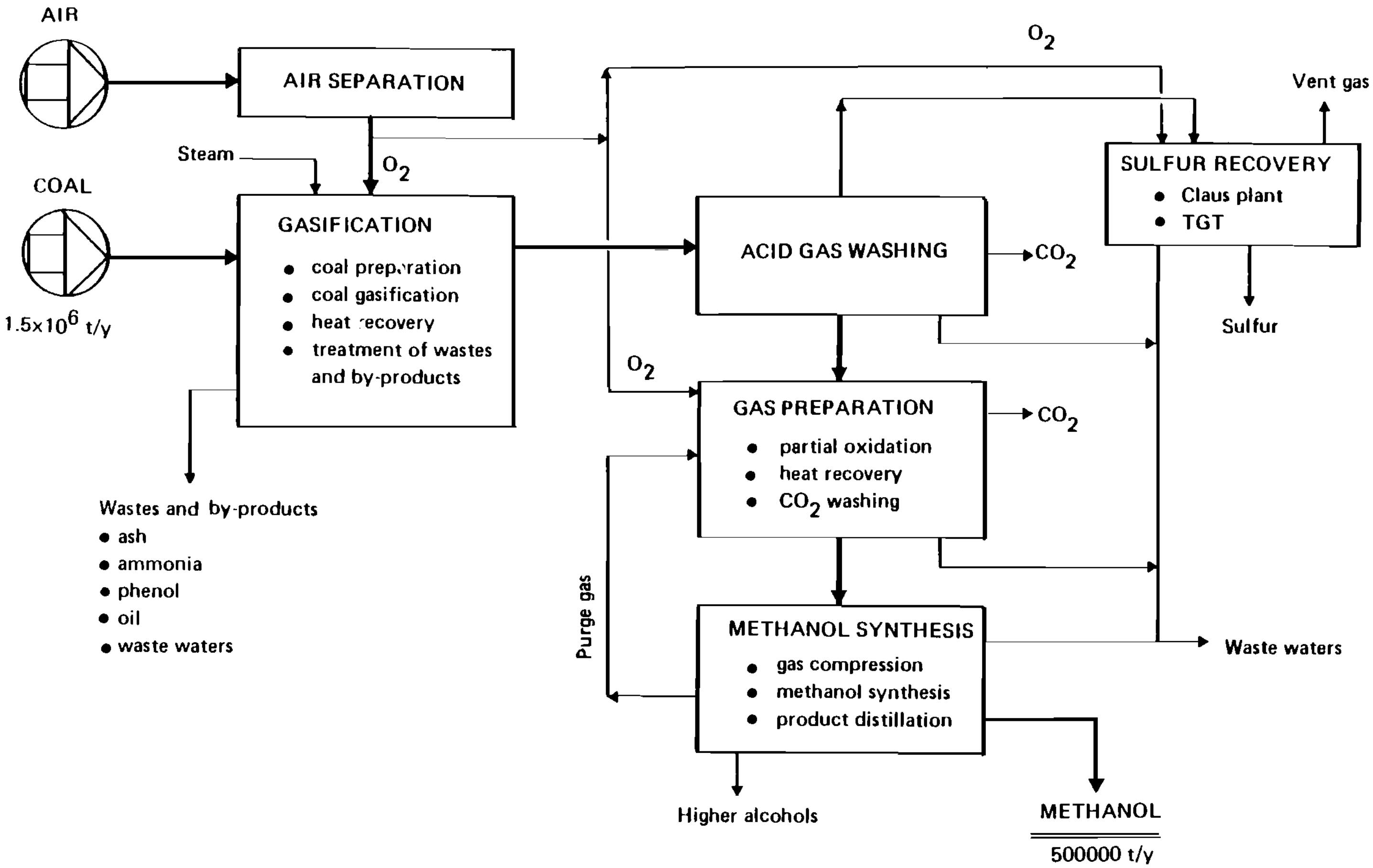

FIGURE 13 Production of methanol from coal (Lurgi process).

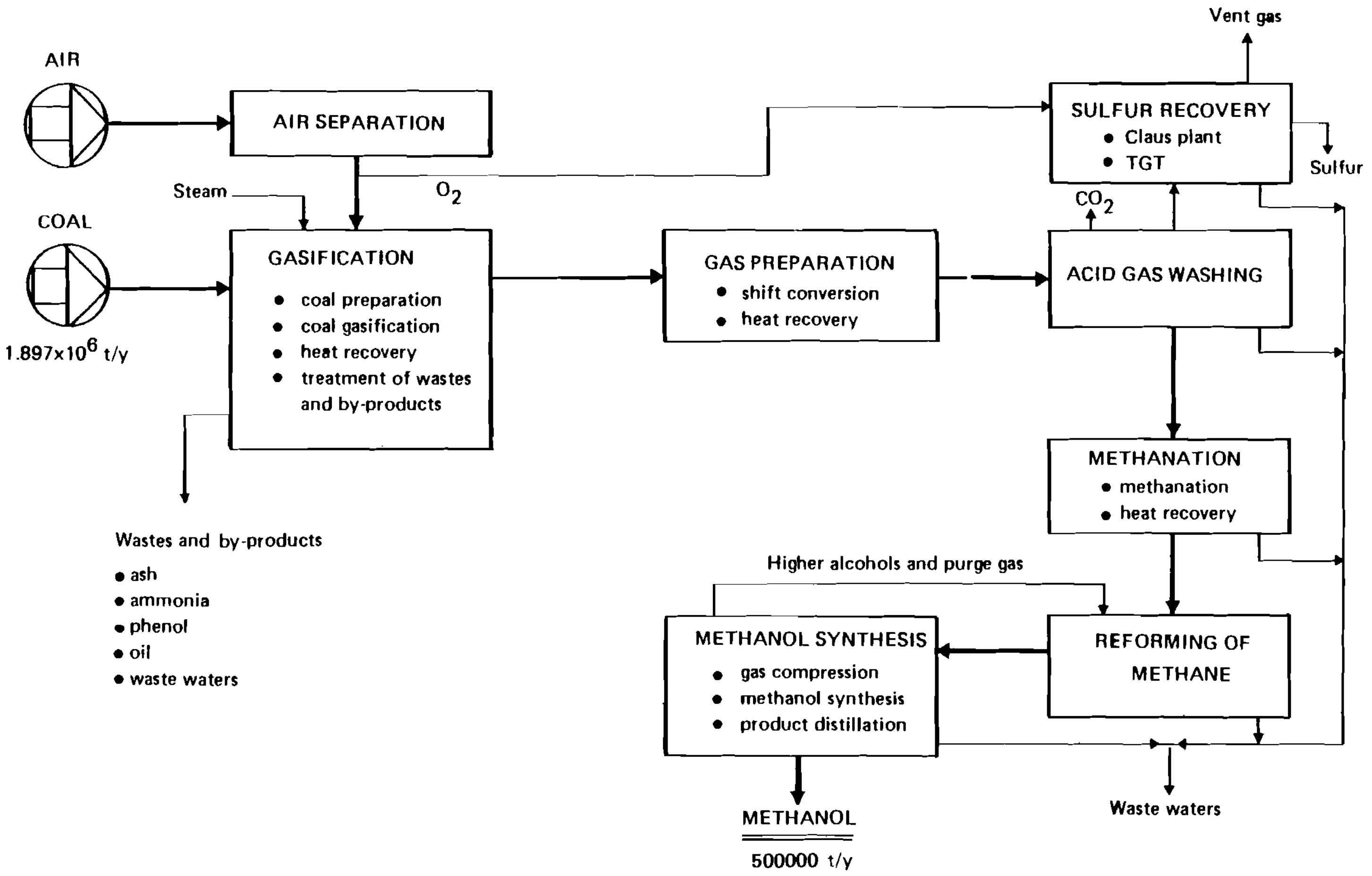

FIGURE 14 Production of methanol from coal (Lurgi process, SNG production, and steam reforming).

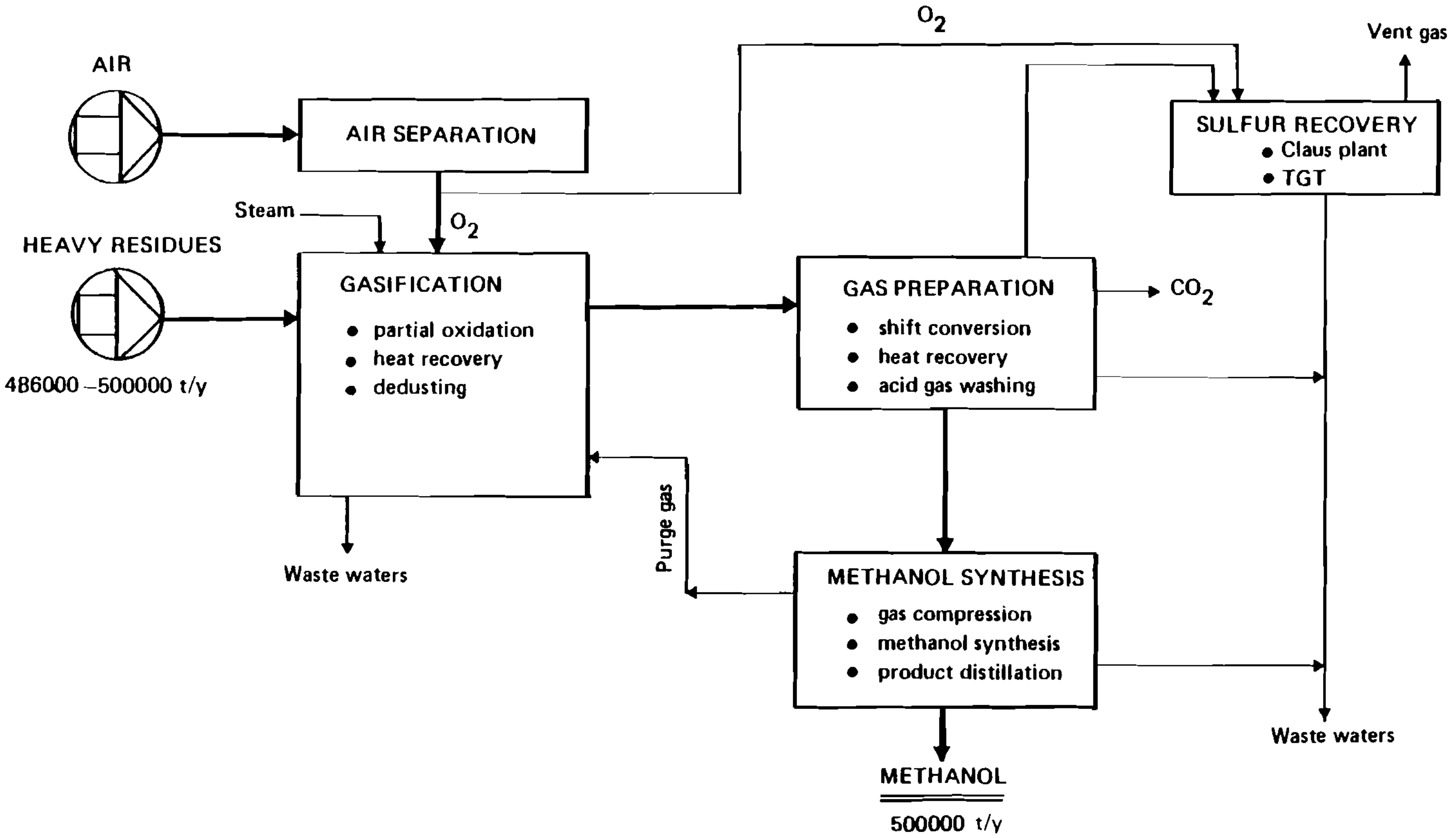

FIGURE 15 Production of methanol from heavy residues (partial oxidation).

4.3 Results of Simulation Experiments

What we have actually done in the case of methanol is to carry out a comparative study of various production technologies. Two factors are emphasised: financial efficiency and investment. In order to make the analysis independent of the value of the discount rate and the corresponding time horizon, financial efficiency and investment should be treated in a way that reveals the properties of the PDA with these two factors taken as objectives. Here we define financial efficiency as the net yearly financial flow for the whole PDA, i.e., the difference between the value of the resources obtained from the PDA and the value of the resources consumed in production. This gives some indication of the value added, and opens the way to further economic analysis.

This approach is illustrated by three examples. Although we come back to the results obtained in these experiments in more detail in the section dealing with methodology, it is worth noting here that this methodology is designed to help the decision maker find out what is "the best" that can be attained from a given PDA.

Further evaluation of the individual investment projects can be performed using the standard tools of microeconomic analysis (discount rates, rates of return, net present values, etc.).

Case 1. Maximization of efficiency under constraints on investment

In this case we are looking for the combination of methanol production technologies that maximizes efficiency at different fixed levels of investment. It is assumed that there are no constraints on the availability of raw materials. Table 6 gives a summary of the results obtained at five different fixed investment levels, together with the corresponding efficiency/investment ratios (Experiments 1–5). The solution is given in terms of the total amount of each raw material consumed, together with the corresponding energy consumption and methanol production levels. Table 7 shows how this consumption of raw materials relates to the levels of use of the individual production processes; the values are given in terms of the percentage utilization of installed capacity. These figures give some idea of the order in which the various processes should be introduced as investment is increased, and may also be used to draw conclusions about economies of scale.

Thus, for a given set of constraints and objective function, this type of analysis can yield information on

- the order in which different raw materials should be used for methanol production;
- the order in which the individual production processes should be introduced;
- the levels of methanol production and resource consumption;
- the performance of the industry as compared with others (as reflected in the efficiency/investment ratio).

TABLE 6 Maximization of efficiency under constraints on investment.

	Experiment				
	1	2	3	4	5
Limited resources					
Investment (10^9 m.u.)	20	30	40	50	62.4
Optimal value of objective function					
Maximum efficiency (10^9 m.u.)	9.4	12.7	15.3	17.2	19.2
Resources corresponding to optimal solution					
Consumption of coal (10^3 tons)	1183	2380	3412	3805	4634
Consumption of heavy residues (10^3 tons)	0	0	108	496	496
Consumption of natural gas (10^3 Nm^3)	901	901	901	901	901
Energy consumption (10^3 t.c.e.)	139	345	737	1163	1560
Methanol production (10^3 tons)	1310	1660	2110	2660	3000
Efficiency/investment ratio	0.470	0.423	0.38	0.344	0.308

TABLE 7 Utilization of methanol production processes (as a percentage of installed capacity) corresponding to the solution given in Table 6.

Methanol production process	Experiment				
	1	2	3	4	5
Coal					
Lurgi process, SNG synthesis, and steam reforming of methane	62	100	100	100	100
Lurgi process	0	32	100	100	100
Koppers–Totzek process	0	0	0	32	100
Heavy residues					
Partial oxidation	0	0	22	100	100
Natural gas					
Steam reforming of methane	100	100	100	100	100
Steam reforming of methane and CO-carrying gas	100	100	100	100	100

Case 2. Maximization of efficiency under constraints on investment, energy consumption, and natural gas availability

We are again seeking to maximize efficiency, but in this case we have constraints not only on investment but also on energy consumption and the availability of natural gas. The various situations considered are summarized in Table 8. In experiments 1 and 7 we examine the effect of reducing the availability of natural gas to zero, with investment limited to 20×10^9 m.u. in both cases. We find that the lack of natural gas in experiment 7 leads to a dramatic drop in methanol production compared with the control experiment (1), and that energy consumption rises markedly (by a factor of 2.5). The substitution of raw materials and processes caused by the nonavailability of natural gas is shown clearly in Table 9. In experiments 8 and 9 we again examine the effect of reducing the availability of natural gas to zero, but this time with the constraints on investment replaced by constraints on energy consumption. We again find a spectacular decline in methanol production in the zero natural gas situation (experiment 9); Table 9 shows that production from natural gas in experiment 8 (the control experiment) is replaced entirely by production from coal in experiment 9.

TABLE 8 Maximization of efficiency under constraints on investment, energy consumption and natural gas availability.

	Experiment			
	1	7	8	9
Limited resources				
Availability of natural gas (10^3 Nm^3)	901	0	901	0
Investment (10^9 m.u.)	20	20	–[a]	–[a]
Energy consumption (10^3 t.c.e.)	–[a]	–[a]	500	500
Optimal value of objective function				
Maximum efficiency (10^9 m.u.)	9.4	6.8	13.8	8.3
Resources corresponding to optimal solution				
Consumption of coal (10^3 tons)	1183	2273	2878	3030
Consumption of heavy residues (10^3 tons)	0	114	0	0
Investment (10^9 m.u.)	–[b]	–[b]	34.3	25.3
Energy consumption (10^3 t.c.e.)	139	341	–[b]	–[b]
Methanol production (10^3 tons)	1340	740	1820	873
Efficiency/investment ratio	0.47	0.34	0.40	0.33

[a] Not limited – see below.

[b] Limited – see above.

TABLE 9 Utilization of methanol production processes (as a percentage of installed capacity) corresponding to the solution given in Table 8.

Methanol production process	Experiment			
	1	7	8	9
Coal				
Lurgi process, SNG synthesis, and steam reforming of methane	62	100	100	100
Lurgi process	0	25	65	74
Heavy residues				
Partial oxidation	0	23	0	0
Natural gas				
Steam reforming of methane	100	0	100	0
Steam reforming of methane and CO-carrying gas	100	0	100	0

Case 3. Optimization with respect to two criteria

In both of the previous cases we have been concerned simply with aximizing one criterion – efficiency. We shall now consider the problem of finding the production structure for which the values of two criteria, such as efficiency and investment, lie simultaneously within certain admissible ranges. This is one way of treating the problem of "concordance". Table 10 shows the results of four such experiments in which it was required to find a production structure for which the efficiency and the investment lie within specified ranges, and are respectively as large and as small as possible. It is also required that the supply of methanol should be maintained at or above some minimum level. [Note that in Table 10 there is an apparent contradiction between the constraint imposed on the methanol supply (740×10^3 tons) and actual methanol production. This will be explained in Section 5.6.] The results show that under these conditions only natural gas is used as a source of methanol; the breakdown into individual production processes in given in Table 11. A similar problem in which it is assumed that the availability of natural gas is limited is considered in Table 12. Here we are required to find the production structure for which the consumption of natural gas and the efficiency simultaneously lie within specified ranges and are respectively as small and as large as possible. There are again boundary constraints, this time for both the minimum level of methanol supply and the maximum level of investment. The breakdown into individual processes is given in Table 13. We will come back to these results again in Section 5.6.

TABLE 10 The results obtained in four experiments with different admissible ranges for efficiency (which should be as large as possible) and investment (which should be as small as possible).

	Experiment			
	11	12	13	14
Admissible ranges for criteria				
Efficiency (10^9 m.u.)	2–4	2–6	6–10	1–2
Investment (10^9 m.u.)	5–10	5–10	5–10	5–10
Conditions				
Minimum methanol supply level (10^3 tons)	740	740	740	740
Optimal value of criteria				
Efficiency (10^9 m.u.)	3.13	4.0	5.84[a]	2.28[b]
Investment (10^9 m.u.)	5.87	7.08	10.16[a]	4.71[b]
Resources corresponding to optimal solution				
Consumption of natural gas (10^3 Nm^3)	526	628	889	426
Energy consumption (10^3 t.c.e.)	156	241	457	943
Methanol production (10^3 tons)	575	690	985	460
Efficiency/investment ratio	0.533	0.565	0.575	0.484

[a] The admissible range is not attainable.

[b] The levels obtained are better than those proposed in the admissible ranges.

TABLE 11 Utilization of methanol production processes (as a percentage of installed capacity) corresponding to the solution given in Table 10.

Methanol production process	Experiment			
	11	12	13	14
Steam reforming of natural gas	100	100	100	92
Steam reforming of natural gas and CO-carrying gas	16	38	97	0

TABLE 12 The results obtained in four experiments with different admissible ranges for efficiency (which should be as large as possible) and consumption of natural gas (which should be as small as possible).

	Experiment			
	15	16	17	18
Admissible ranges for criteria				
Efficiency (10^9 m.u.)	8–10	10–12	2–6	2–6
Consumption of natural gas (10^3 Nm^3)	300–500	300–500	300–500	300–500
Constraints				
Minimum methanol supply level (10^3 tons)	–[a]	–[a]	–[a]	740
Maximum investment level (10^9 m.u.)	20	20	20	20
Optimal value of criteria				
Efficiency (10^9 m.u.)	8.35	9.5[b,d]	6.92[b,c]	6.88[b,c]
Consumption of natural gas (10^3 Nm^3)	400	901[b,d]	0[b,c]	0[b,c]
Resources corresponding to optimal solution				
Consumption of heavy residues (10^3 tons)	0	0	0	114
Consumption of coal (10^3 tons)	1862	1182	2415	2273
Energy consumption (10^3 t.c.e.)	1791	1394	3094	3415
Actual investment (10^9 m.u.)	20	20	20	20
Actual methanol production (10^3 tons)	945	1320	671	740
Efficiency/investment ratio	0.418	0.475	0.346	0.344

[a] There are no constraints on methanol supply in these cases.
[b] These solutions lie at a vertex of the Pareto set.
[c] The levels obtained are better than those proposed in the admissible ranges.
[d] The admissible ranges are not attainable.

The multiobjective method used to solve these problems has also been used to generate efficient alternatives for the development of the chemical industry as a whole (Dobrowolski et al. 1982), and is described in some detail in Section 5.2.

The results presented above may seem trivial to chemical technologists, especially those specializing in syngas production. However, to see if our approach really works in practice it is necessary to begin by applying it to small, familiar systems such as methanol production so that our results can be verified by other methods. When the approach has been shown to work well for these simple systems, it can be applied to the analysis of more complex PDAs involving more fossil resources and more final products. Our ultimate aim is to use this method to find a robust production structure for an industry that would provide raw materials for the organic chemicals sector.

TABLE 13 Utilization of methanol production technologies (as a percentage of installed capacity) corresponding to the solution given in Table 12.

Methanol production process	Experiment			
	15	16	17	18
Natural gas				
Steam reforming of methane	0	100	0	0
Steam reforming of methane and CO-carrying gas	91	100	0	0
Heavy residues				
Partial oxidation	0	0	0	23
Coal				
Lurgi process	0	0	34	25
Lurgi process followed by synthesis of SNG and steam reforming of methane	98	62	100	100

5 METHODOLOGY

5.1 Scope

The development of methodology is an important part of the research described in this report, and our main methodological findings are summarized in this section. Although the approach described here has demonstrated its usefulness in many theoretical and practical ways, it should be regarded as fairly elastic and subject to further development and modification. We shall therefore consider only the basic elements of the methodology, concentrating on the philosophy behind the approach rather than the mathematical tools deployed within it.

The underlying problem is one of interactive decision making, and therefore we must make use of interactive decision support methods. There are many possible approaches, one of the most interesting of which is based on the reference point approach developed by Wierzbicki (1980), and Kallio, Lewandowski, and Orchard-Hays (1980). This is the IIASA decision support package DIDASS (Dynamic Interactive Decision Analysis and Support System), which we have already used in planning the development of the chemical industry (see Dobrowolski et al. 1982). This methodology may also be used to analyze the production structure of a PDA, although comparison of the approach proposed there and the one discussed here goes beyond the scope of this report. Note, however, that these are only two of the possible methodological options consistent with the proposed philosophy.

What can the decision maker expect from our methodology? We have already stated that the approach to the decision problem should be interactive, which means that the decision maker is able to experiment directly with the model, learn from the results, and refine his expectations (and the solution) accordingly. In terms of overall development strategy, the decision maker may expect to obtain results relating to system design rather than to system implementation or maintenance. It should also be pointed out that the whole interactive process must be embedded in the management system, or at least in that part of the management system which is responsible for development (see Dobrowolski et al. 1982, Borek et al. 1978).

In essence, the methodology described here is designed for use in solving the problems identified earlier in this report. These problems are stated in terms of a single multiobjective decision problem, which is solved interactively. We also point out the methodological implications and restrictions of the general model of a PDA described in Section 3.2. The concepts of a Critical Resource Area (CRA) and an Attainable Performance Area (APA) in resource space are introduced; the latter is defined by the performance ratios of the set of available technologies. These considerations lead us to formulate methodological steps in problem solution, which are then presented and discussed.

5.2 Concordance as a Multiobjective Problem

We now recall some of the points made in Section 1, and expand on these ideas using the concepts developed in subsequent sections. It was shown that changes in patterns of energy use have led to a crisis in the supply of hydrocarbon feedstocks for the chemical industry. We suggest that this problem could be overcome if the PDAs dependent on hydrocarbon feedstocks could adjust their industrial structure to follow changes in the availability of resources more closely. Thus, we describe the fundamental problem as one of finding concordance between available resources and technologies (see also Gorecki and Kopytowski 1980, Gorecki et al. 1982).

It has already been emphasized that the problem of choosing the most appropriate industrial structure, given the available technologies, resources, and demand for products, cannot be formulated as a single-criterion problem. The single criterion most frequently used in this type of problem, maximization of profits, depends on financial estimates of the resources to be invested in a given development program, and this is clearly undesirable in view of the unstable economic situation and the rapidly changing prices of fossil resources. In addition, the increasing scarcity of these resources is encouraging decision makers to be less single-minded in their pursuit of profits; they may wish to (simultaneously) minimize factors such as resource consumption and environmental pollution while maximizing (say) output and profits. Since these goals are at least partially conflicting, some sort of multiobjective procedure is required to find an acceptable compromise solution. In the approach described here, each criterion is given in terms of resources so that the whole analysis takes place in resource space.*

Thus, we shall describe the search for concordance as a multiobjective decision problem. The elements involved in this process are:

---

*The book by Kendrick and Stoutjestijk (1978) on the planning of industrial investment programs provides an extensive study of the methodological aspects of process-type models. Unfortunately it is one of very few publications on the subject.

- a decision maker, who has to make a final choice from the alternatives under consideration;
- a set of available technologies, described in terms of a model;
- a demand vector;
- a vector of available resources.

We have already pointed out that the multiobjective analysis should be interactive so that the decision maker can play an active role in the process. In an interactive procedure the system accumulates information about the wishes of the decision maker while the decision maker simultaneously "learns" from the system how changes in his preferences affect the results of the analysis.

In the particular case considered here the idea is to help the decision maker learn how the estimated resources and the relevant states of the model are related in criteria space. Each state of the model represents a particular subset of available technologies together with a particular level of technology utilization. We are interested in those states which belong to the so-called Pareto-optimal set in criteria space. The concept of Pareto-optimality is illustrated in Figure 16. This figure shows the set of states (combinations of technologies) that can be attained under the conditions and constraints specified in the model. Note that these states are specified here in terms of criteria Q_1, Q_2, which could be earnings ($Q_1 \rightarrow$ max) and investment ($Q_2 \rightarrow$ min), respectively, in a classical industrial minimax problem. The Pareto-optimal set comprises those attainable states for which an improvement in the value of one of the criteria automatically leads to a deterioration in the value of the other. This set therefore represents in some sense the best feasible compromise solutions, and the quest for a satisfactory concordance between technologies and resources becomes an analysis of geometrical relations.

Returning to our four elements of a multiobjective decision-making system, we have to transform three of them into criteria, constraints, and objectives in some way that would enable the decision maker (the fourth element of the system) to match available technologies with available resources by simple manipulation of parameters. This is usually achieved by allowing the decision maker to adjust both the set of technologies and the available (or assumed) quantities of resources, and is dealt with in more detail in Section 5.3.

The decision maker sometimes has to deal with considerable uncertainty in the data: examples include "apparent" availabilities of resources and estimated operating requirements for hypothetical plants based on new technologies. However, the reliability of these two types of information is not the same. A forecast of the future availability and price of oil is usually less reliable than technological information on a methanol plant based on a newly developed process. It may therefore be more realistic to assume that the technology is described relatively precisely, while the availability of resources may be expressed as a range. This procedure also enables the decision maker to set levels of acceptability for the estimated values; this is particularly important since it reflects a subjective factor in the decision-making process. The idea of an admissible range of resource availabilities

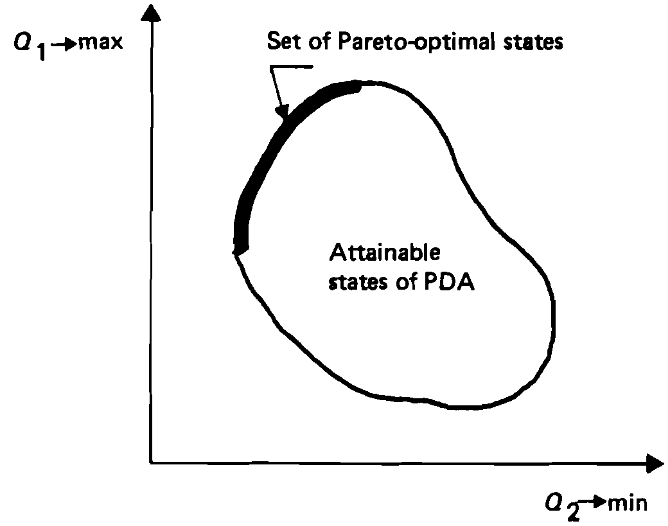

FIGURE 16 Attainable states and Pareto-optimal states of the PDA in criteria space.

was introduced and developed theoretically by Gorecki and his co-workers (Gorecki 1981, Gorecki et al. 1982). Without going into detail, the method is based on scalarization with respect to the "skeleton" of an Admissible Demand Set (ADS). The ADS is delimited by estimated ranges of the availability of critical resources, and the skeleton represents solutions which are equidistant from these limits. One of the more useful features of the procedure is that it enables the decision maker to evaluate the attainability of various estimates. This is discussed further (with reference to Case 3 from Section 4.3) in Section 5.6.

5.3 Methodological Implications of the General Model

A general model of a Production/Distribution Area was presented in Section 3.2. We now analyze the methodological implications of this model, taking as a starting point the philosophy behind the multicriteria decision problem considered.

A decision maker has to have information on the properties of the PDA network. The main characteristic of the network is that it contains a finite repertoire of possibilities described in terms of existing and possible (known) technologies, and this means that the information available for each model is restricted by the supply of technological data. It is clear that the accuracy of this information depends on the reliability of the information source. Given the availability of resources and his goals or preferences, the decision maker can experiment with various combinations of technologies within this finite repertoire of possibilities. The decision maker's range of options is limited further by consideration of critical resources, technological constraints, and complementary or auxiliary constraints.

These three categories are not specified formally in the model but are defined by the decision maker during the formulation of the decision problem. Critical resources are those which are seen by the decision maker as being particularly scarce or difficult to obtain; examples may be crude oil, manpower, energy, or capital. In practice the set of critical resources is also the set of criteria, since we try to find an optimal solution with respect to all critical resources. Technological constraints are quite easily identified and are related to factors such as production capacities and operating conditions. All the other constraints in the model, such as the demand for a particular product, the availability of (noncritical) raw materials, or prices, fall into the category of complementary or auxiliary constraints.

It is clear that whether a resource is treated as critical or not depends on the formulation of the decision problem. In fact, a resource can be moved from one category to the other by the decision maker and this makes the analysis much more flexible.

All of this assumes that the decision maker (and his staff) have access to the relevant information on the PDA. This requires some preparatory analysis, which falls into two main areas. The first deals with critical resources such as capital investment, energy, labor, and so on. This area of the analysis should enable the decision maker to evaluate "initial conditions" in terms of critical resources. The other area of the analysis should yield all kinds of market information, supply forecasts and the like, a specific example being the coordination variables describing the coordinated sale and purchase of chemicals between various PDAs. This kind of information is included in the form of auxiliary constraints in the general model described in the previous sections. The technological analysis furnishes forecasts concerning the nature of the processes expected to be developed, the date when they are expected to be available, and what their capacities, efficiencies, and other characteristics will be.

The preceding discussion has been concerned with the PDA model and the classification of constraints considered as limitations from the decision maker's point of view. We shall now consider a feature of the model which is strictly connected with its formal properties. It has strong implications for the solution of the problem and hence influences the methodology.

All the limitations (including constraints on critical resources) are taken to be constraints in the linear programming problem. Thus, monotonic results can be obtained for each constraint separately (within its range of activity), assuming all other constraints to be inoperative. To show how this feature may be incorporated in our methodology, we first consider two particular states of the general model. Both of these result from a situation in which there are no active constraints on critical resources, and represent the optimal industrial structure possible under these conditions. However, these states differ in that the first (unconstrained best present state or UBP) has its repertoire of technologies restricted to existing plants (this means that no investment is available); the second (unconstrained best future state or UBF) considers both existing plants and other known or potentially available technologies. The consequence of such an "ideal" unrestricted availability of critical resources is that we may in fact optimize the PDA model with respect to a single criterion such as economic efficiency or earnings. (It does not make sense to optimize with respect to something which is completely unconstrained.) These two solutions therefore represent the best possible outcomes for the smallest and largest repertoires of technologies that we shall consider.

Now we ask whether this "ideal" situation should really be regarded as ideal by the decision maker. An abundance of resources does not mean that they will be utilized efficiently, and these special cases tell us very little about the performance of different PDAs from the point of view of resource allocation. However, these cases provide very useful information about the properties of the structure described by the general model under the assumed market conditions (prices, demand for products, capacities, availability of noncritical resources, etc.). We can, for example, find out which technologies (existing or potentially available) are eliminated from the structure of the PDA even with no constraints on critical resources (see the results of the methanol study). This observation may lead to a number of conclusions: the critical resources were not identified correctly, a given technology does not fit the assumed structure, etc.

The problem is now to compare the set of solutions contained within the range between these two unconstrained best cases from the point of view of performance. This should be done in terms of critical resources, and in the way most convenient to the decision maker.

A decision maker who wants some way of assessing the PDA's performance will automatically turn to its input–output relations. The decision maker wants to know how much output he can expect from the (limited) resources which he may allocate (input) to the PDA under consideration. The most common performance measure is the ratio* of revenue to investment. Inverse ratios representing the amount of a critical resource necessary to obtain a unit of output are also used quite frequently, but fortunately these two types of ratios are equivalent from a mathematical point of view. A number of such performance ratios can be formulated using different critical resources, providing the decision maker with a range of information about the intensive properties of the modeled structure. Examples are the ratios of revenue to energy consumption or of output level to energy consumption. Performance measures may also be used as a basis for comparison of various structures within the repertoire of a given PDA or between different PDAs.

Having introduced the concept of performance ratios we may now describe another very important methodological implication of the model. It will be recalled from our description of the model that the solution of the single- or multiobjective problem corresponds to a particular PDA structure and to a particular state of flow within that structure. There is no reason why the performance ratio should not become one of the parameters of the model; this would in fact be very useful to the decision maker in his analysis of possible options. The important point here is that within the repertoire of a given PDA model there is only one solution which maximizes (or minimizes) any chosen performance ratio. Furthermore, this solution is not equivalent to either of the unconstrained best solutions discussed earlier. It is clear that this feature is a consequence of the previously described monotonic dependence of the solution upon the only active constraint.

---

*This procedure, based on optimization of the ratio of effects to consumed resources, is well established theoretically (see Bellman 1961).

This leads to the possibility of formulating the decision problem as a minimax problem based on performance ratios. For the sake of simplicity we usually concentrate on a set of ratios with a common denominator or numerator.

We should emphasize at this point that the preceding discussion does not limit the generality of the multiobjective problem formulation in any way. We have merely drawn methodological observations from the properties of the model and the problem of concordance described above, and pointed out the various ways in which they *could* be used. The use of performance ratios in the multiobjective problem is only one of these options.

5.4 The Attainable Performance Area and Critical Resource Area of a PDA

Since we have formulated the problem in terms of matching available resources and available technologies, we have to find some way of helping the decision maker to achieve this by mapping various combinations of technologies (industrial structures) onto the available resources.

The limits imposed by the (assumed) availability of critical resources define an area in resource space which we call the Critical Resource Area (CRA). These limits may be specified either in terms of a single numerical value, or as a range of admissible values for each critical resource. The latter approach is more practical in many cases, and a solution procedure based on this formulation of the multiobjective problem was developed by Gorecki and his co-workers (Gorecki 1981, Gorecki et al. 1982). One of the simulation experiments (Case 3) described in Section 4.3 is actually based on this concept of admissible ranges.

Having introduced the idea of a critical resource area, we now consider another area in resource space which is defined by the properties of the industrial structure (technologies). This area is called the Attainable Performance Area (APA) and is bounded by the values of chosen performance ratios attainable by various industrial structures. What can the decision maker gain from a study of the attainable performance area? He can learn what is the best potentially attainable performance of a PDA (measured in terms of specific performance ratios) when no resources are regarded as critical. This performance cannot be improved any further no matter how many resources the decision maker may wish to allocate to the PDA in question. The problem is therefore somewhat simplified and becomes a question of matching two areas, one defined by the availability of resources and the other by the attainable performance of the available technologies (which is also expressed in terms of critical resources).

5.5 Steps in Problem Solution

We shall now organize our observations into one possible series of methodological steps in problem solution. Figure 17 illustrates these steps in the form of a flow diagram – note, however, that the actual series of steps taken will vary from problem to problem and not all of the stages shown in Figure 17 will necessarily be required.

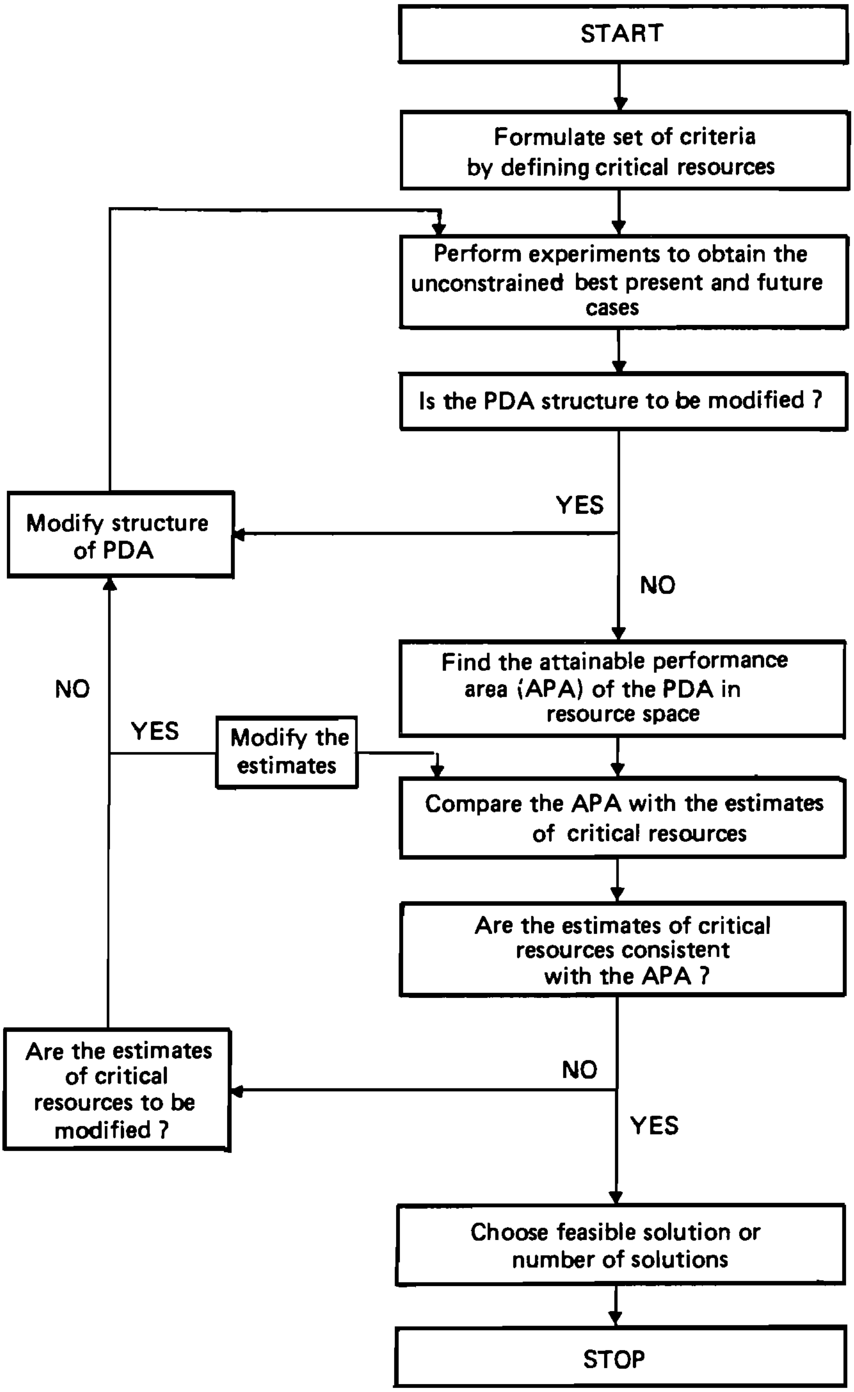

FIGURE 17 Steps in problem solution.

The very nature of the problem, concordance between available technologies and resources, implies that the analysis can be approached from two directions: from a given structure to the best use of resources or from a given set of resources to the best industrial structure. In general, the decision maker should experiment with both approaches in order to learn as much as possible about the relations between the industrial structure and the critical resources. However, the emphasis given to each direction of analysis will depend on the particular conditions of the problem being solved.

There are three main possibilities. First, the problem formulation phase may reveal that most of the restrictions are concentrated in technology, which means that the industrial structure is more critical than the resources. This also happens when it is very difficult to obtain reasonable estimates of available resources: one way of obtaining the estimates is to calculate the necessary ranges from the demand created by the industrial structure. In this type of situation we obviously concentrate on the technology-to-resources approach.

The second case arises when the availability of resources is given with some degree of certainty: for example, if the critical raw materials are to be obtained from specified sources in definite quantities. In this situation we concentrate on the resources-to-technology approach.

The third possibility is that both the industrial structure and the availability of resources impose constraints on the system. In this case, and in the situation where none of the available information is very reliable, we should use a combination of the two approaches. This enables the decision maker to learn as much as possible about the problem so that the compromise is established on the basis of the best available knowledge of the situation.

5.6 Methodological Interpretation of the Methanol Experiments

Armed with new insight from the above sections on methodology, we may now go back and re-examine the results of the simulation experiments described in Section 4.3.

Each of the three cases considered in that section illustrates a particular aspect of the methodology:

Case 1: Investment-oriented comparative study of methanol technologies
Case 2: Flexibility of the PDA with respect to the critical resources, i.e., tradeoff analysis
Case 3: Quest for concordance between available technologies and available resources, with a range of estimates of resource availability.

In the methanol study we have a specific PDA based on a set of technologies which offer alternative routes from various raw materials to methanol. This naturally brings the analysis down to the level of a comparative study of technologies. If the decision maker is "investment sensitive" we have a returns-to-investment problem; this is illustrated by Case 1. In the same way it would be possible to base the comparative analysis on the efficiency of energy use, raw material consumption, or manpower utilization of the various technologies.

Let us now take another look at the three cases described in Section 4.3.

Case 1. Investment-oriented comparative study

Table 6 shows the maximum efficiency that can be obtained at various levels of investment and the corresponding utilization of resources. This gives the decision maker some idea of the relation between investment and efficiency and, by inference, the combination of technologies best suited to a given level of investment. These technologies and their capacity utilization are given explicitly in Table 7. This information opens the way for further analysis, in particular of economies of scale, since quite often the proposed capacities do not meet the specified demand.

Experiment 5 corresponds to the state referred to in Section 5.3 as the unconstrained best future (UBF) state of the PDA.* It is interesting that no methanol is produced from gasoline even under these unconstrained conditions.

It should also be observed that for an industrial structure such as that described above, the performance of a particular combination of technologies can be measured by a single value. Thus the Attainable Performance Area (APA) in the space of resources for each possible strategy reduces to a single point. The performance measure simply indicates the production strategy that performs best from the point of view of the critical resources considered in the performance ratio.

Case 2. Flexibility analysis of the PDA

The effects of substituting one critical resource for another can be explored if the decision maker needs information about the efficiency of critical resource use. He will generally want to know what he can get from the PDA under investigation if one critical resource is replaced by another, or whether an acceptable combination of the two resources can be found. This sort of analysis provides information about the flexibility of the structure of the PDA with respect to critical resources, and may therefore be seen as an analysis of tradeoffs between the critical resources.

In this particular example we considered the substitution of natural gas by energy consumption** and of natural gas by investment (see Tables 8 and 9). Experiments 1 and 7 yield the most efficient production structures given maximum and zero availability of natural gas, respectively. Consumption of natural gas is replaced in experiment 7 by increased consumption of energy, coal, and heavy residues, with a corresponding decrease in both economic efficiency and methanol production. Naturally, both experiments were performed under the same constraint on investment; this may be derived from the analysis carried out in Case 1.

Experiments 8 and 9 illustrate a similar situation in which we observe how natural gas can be substituted by investment and other resources under a constraint on energy supply.

---

*Note that since only new technologies are considered the unconstrained best present (UBP) state does not exist.

**Note that the energy considered here is that actually used in the technological processes (steam, electricity, etc.).

Case 3. Quest for concordance

We have emphasized that learning is an important factor in the decision process that we define as a quest for concordance between available resources and technologies. Cases 1 and 2 represent learning steps in this process: they help the decision maker to acquire some understanding of the properties of the PDA in terms of critical resources. Some of the data used to facilitate learning and to provide a basis for the final decision should be treated with caution: there are obvious uncertainties associated with "apparent" availabilities of resources and estimated operating requirements of hypothetical plants.

The critical resources estimated may include: amount of raw materials (gas, coal, etc.) available for use, the amount of capital available for investment, and the desired levels of various processes or effects. All of these estimates are subject to analysis and may be obtained from various sources – they generally result from studies carried out by experts.

The most natural way of formulating the estimates is to express them in terms of ranges, as discussed earlier. Algorithms using this idea of admissible ranges for critical resources were used in Case 3, which also illustrates other important aspects of our methodology.

The essence of the quest for concordance is to find a compromise between the estimated availability of resources, the aspirations of the decision maker, and the capabilities of the technologies. The PDA is basically a structure that transforms inputs into outputs. The desired effects of this transformation are expressed by the criteria, while the environment in which it must take place is specified by the constraints. The purpose of the exercise is to obtain answers to the following questions:

1. What is the best structure of the PDA from the point of view of the various criteria?
2. Can the expectations of the decision maker be met?

The following situations may arise in connection with the second of these questions:

- The decision maker overestimates the potential of the system: his aspirations are too high and cannot be achieved;
- The decision maker underestimates the potential of the system: his aspirations can be fulfilled and even exceeded.

In the first case the computer informs the decision maker of the feasible solution closest to his expectations. The decision maker then either accepts this solution, revises his aspirations, or gives up.

In the second case the computer informs the decision maker of the best possible result, which actually exceeds his expectations. This does not mean that analysis of the estimates should now stop: the reason for the difference between estimates and results should be found. If the solution is better than expected, this provides some information about the estimation method used. The method is not necessarily wrong, it may simply be incompatible with the system.

There is actually a third possibility (and one to which the interactive process should ultimately lead): that the best solution lies within the estimated ranges. The safest course of action is to accept a solution which is equidistant from the limits imposed by the ranges (i.e., on the skeleton of the ADS – see Section 5.2). Even in this case the decision maker should carry out further analysis of the results, since these only confirm that the PDA is consistent with the estimates of resources.

The situations described above are illustrated by the results given in Table 10. In experiment 13 the possibilities have been overestimated, while in experiment 14 they have been underestimated. By contrast, experiments 11 and 12 are good examples of concordance. Comparison of these four experiments is very instructive since it illustrates the effects of subjective preferences or external factors (expressed by the admissible ranges). Recall that the results given in the table are "safe" in terms of equidistance from the limits of the ranges: comparison of experiments 11 and 12 shows that the higher expectation of efficiency in experiment 12 is fulfilled only at the cost of additional investment.

The above considerations are summarized and illustrated in Figure 18. This shows how the preferences of the decision maker (in terms of the ADS and the "safety" represented by its skeleton – see Figure 19) are transformed to yield the Pareto-optimal structure of the PDA.

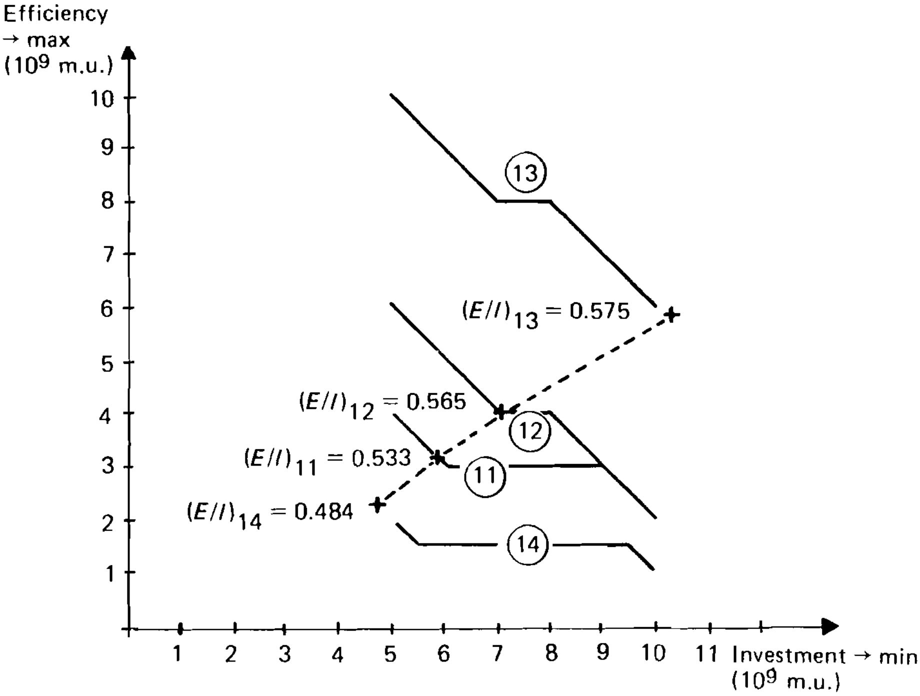

FIGURE 18 Graphical interpretation of sample experiments from Table 10. Here – ⓝ – is the skeleton of the ADS for experiment number n, + – – – + represents the approximation of the Pareto set, + represents the solution obtained in experiment number n and $(E/I)_n$ is the corresponding efficiency/investment ratio.

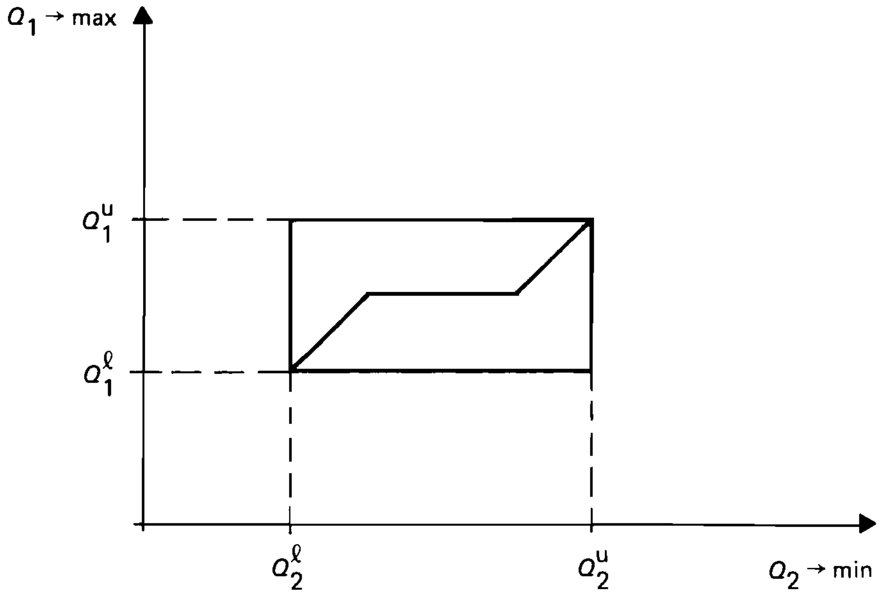

FIGURE 19 Graphical interpretation of the admissible demand set and its skeleton. Here Q_i^u and Q_i^l represent the upper and lower bounds of the admissible ranges (i = 1, 2).

The sequence of experiments shown in Figure 18 (see also Table 10) illustrates how the decision maker learns and adapts his preferences to attain the concordant solution. These experiments not only yield the values of objective functions but also identify the best structure of the PDA in terms of the criteria, specifying particular technologies and their parameters, production levels, amounts of resources, etc. (see the Appendix).

It is also worth looking at what happens when the preferences (aspirations) of the decision maker are incompatible with the properties of the PDA. Recall in particular that on p. 34 we pointed out the contradiction between the required minimum methanol supply level and actual methanol production in experiments 11, 12, and 14 (Table 10). In these cases there is no structure that simultaneously (i) belongs to the PDA, (ii) is the "best" in terms of the criteria, and (iii) meets the demand for methanol.

Table 12 provides another illustration of the problem of concordance, but in this case emphasis is placed on the availability of raw materials rather than on investment, which is simply given a fixed value. The critical raw material here is natural gas.

The type of data obtained from a typical experiment is illustrated in the Appendix.

6 CONCLUSIONS

This paper represents the first and possibly the most important step in our research on the problem of developing new sources of chemical feedstocks through industrial structural change.

The PDA concept provides a very useful way of structuring the problem, confirming expectations based on its use in earlier work (generating a development program for the chemical industry). This has given us a considerable degree of confidence in the PDA model. The methodology developed so far makes use of and develops our earlier concept of a quest for concordance between available resources and available technologies. Although further methodological work remains to be done, the theoretical basis of the approach appears to be sound, and the results obtained so far seem very encouraging.

The computer software developed in parallel with the methodology has also proved itself in practice, but will be modified in the future to accommodate changes in methodology or improvements suggested by further experiments. The data collected for the methanol study have proved very illuminating and are now also being used for other purposes.

Our results are in general agreement with papers dealing with the use of fossil resources for energy supply (see Häfele et al. 1982, Sassin 1982, Rogner 1982). We note with satisfaction that energy researchers are moving perceptibly closer to our area – the emerging common ground may be called energochemical processing of fossil resources. Since there is an explicit complementarity between these approaches, we expect to cooperate closely with the relevant IIASA projects (Patterns of Economic Structural Change and Industrial Adjustment, and particularly Energy Development and Investments) in the future.

For the dual reasons of clarity and limited space, this report does not include many of our findings. These are concerned with various problems based on prices and their evaluation using sensitivity analysis and postoptimal analysis, and will be published separately. Much important mathematical background has also been omitted.

We shall continue with this general line of research in the future, emphasizing not only tools and their methodological implications but also case studies of specific PDAs. We intend to pay special attention to the energochemical processing of lignite.

We are convinced by the results of our study that a temporary drop in oil prices should not deter decision makers and researchers from the pursuit of new sources of raw materials and energy, and new ways of deploying them. The world cannot afford to waste any time in this field. Should the present inefficient patterns of resource utilization continue, this waste of time will only be translated into a waste of resources.

ACKNOWLEDGEMENTS

We are grateful to all of the people who have helped us at various stages of the research reported here. However, we would like to express our especial gratitude to Professor H. Gorecki for his patient guidance through the theoretical problems that we encountered; to Professor A. Wierzbicki, who was always very supportive, both as leader of the System and Decision Sciences Program at IIASA and as our consultant in the area of multiobjective optimization and interactive methodology; and to Janusz Kindler, Leader of the Resources and Environment Area at IIASA, whose common-sense approach and help could always be relied upon.

H. Rogner pointed out several contentious points in an earlier draft, and we are also very grateful to the anonymous referees for their constructive comments, which were very helpful when revising the paper.

We should not forget our Editor, Helen Gasking, who patiently fought her way through our terrible manuscript and clarified it greatly.

Any remaining errors are, of course, ours.

APPENDIX

In Table A.1 we present the complete set of data obtained from one of the experiments described in Section 4.3. We have selected experiment 15 (see Tables 12 and 13) as our example, but the same type of information is available from all experiments 1–18.

It is clear that some of the information is concerned with the design of installations belonging to the PDA under investigation. These data become very important once a particular case (an experiment) has been chosen for further analysis, and could be obtained from an initial study carried out by a design office. These data may help the decision maker to reach the next stage in his investment decision or may lead him to reconsider the matter completely.

TABLE A.1 Set of data obtained from a typical experiment (based on experiment 15 from Tables 12 and 13).

Parameter	Value	Parameter	Value
General		*By-products*	
Efficiency	8.35×10^9 m.u.	Higher alcohols	17×10^3 tons
Energy consumption	1791×10^3 t.c.e.	Phenol	13×10^3 tons
Investment	20×10^9 m.u.	Fuel oil	88×10^3 tons
Labor	409 men	Sulfur	21×10^3 tons
Methanol production	945×10^3 tons		
		Waste products	
Raw materials		CO_2	629×10^3 Nm^3
Natural gas	400×10^3 Nm^3	Waste water	2724×10^3 m^3
Coal	1862×10^3 tons	Ash	216×10^3 tons
Carbide gas	102×10^3 Nm^3		
ZnO catalyst	62 tons	*Construction data*	
Reforming catalyst	31 tons	Weight of concrete	95,064 tons
Shift-conversion catalyst	44 tons	Weight of steel structure	12,363 tons
Methanation catalyst	59 tons	Weight of equipment	17,086 tons
CoMo catalyst	2 kg	Weight of pumps and compressors	2,565 tons
Air	1378×10^3 Nm^3		
Water	1384×10^3 m^3	Weight of pipes	9,671 tons

REFERENCES

Bellman, R. (1961) *Adaptive Control Processes – a Guided Tour.* Princeton University Press, Princeton, New Jersey.

Borek, A., Dobrowolski, G., and Żebrowski, M. (1978) GSOS – a growth strategy optimization system for the chemical industry. In *Advances in Measurement and Control – MECO-78*, Vol. 3, pp. 1128–1131. Acta Press.

Borek, A., Dobrowolski, G., and Żebrowski, M. (1979) *Applications of Systems Analysis in the Management of Growth and Development of the Chemical Industry.* Report CHEM/SEM.8/R.16, Chemical Industry Committee of the United Nations.

Dobrowolski, G., Kopytowski, J., and Żebrowski, M. (1980a) *Systems Analysis in Management of Optimal Strategy of Growth.* Paper presented at the 3rd IFAC/IFORS Conference, 16–19 June, Warsaw. In preprints of the 3rd IFAC/IFORS Conference on Dynamic Modelling and Control of National Economies, published by the Polish Academy of Sciences. Copies available from the Institute of Systems Research (Polish Academy of Sciences), Warsaw.

Dobrowolski, G., Kopytowski, J., and Żebrowski, M. (1980b) Development forecast of production structure. In the *Proceedings of the XIV Union of Polish Architects Congress*, 9–14 June, Zakopane, Poland, pp. 19–26.

Dobrowolski, G., Kopytowski, J., Lewandowski, A., and Żebrowski, M. (1982) *Generating Efficient Alternatives for Development of the Chemical Industry.* Collaborative Paper CP-82-54, International Institute for Applied Systems Analysis, Laxenburg, Austria.

Gallagher, J.M., and Zimmerman, R.G.J. (1978) *Coal in Transition: An Analysis of Development Programs Using the Bechtel Energy Supply Planning Model.* Published by Research and Engineering Bechtel National Inc., San Francisco, California. Prepared for the Energy Modeling Forum (ENP), 1 February 1978.

Gorecki, H. (1981) Problem of choice of an optimal solution in a multicriterion space. In the *Proceedings of the VIIIth Triennial World IFAC Congress*, 24–28 August, Kyoto, Japan, pp. 106–110.

Gorecki, H., and Kopytowski, J. (1980) *Polyoptimal Approach to the Problems of Design of the Production Structure in the Chemical Industry.* Paper presented at the 5th Italo–Polish Seminar on the Application of Systems Theory to Economics, Management and Technology, Torun. Copies available from the authors.

Gorecki, H., Dobrowolski, G., Kopytowski, J., and Żebrowski, M. (1982) The quest for a concordance between technologies and resources as a multiobjective decision process. In M. Grauer, A. Lewandowski, and A.P. Wierzbicki (Eds.), *Multiobjective and Stochastic Optimization.* Collaborative Proceedings CP-82-S12, International Institute for Applied Systems Analysis, Laxenburg, Austria.

Grenon, M., and Lapillone, B. (1976) *The WELMM Approach to Energy Strategies and Options.* Research Report RR-76-19, International Institute for Applied Systems Analysis, Laxenburg, Austria.

Häfele, W., Barnett, H., and Sassin, W. (1982) Künftige fossile Brennstoffe – Ihre Nutzung und Einbettung in moderne Energiesysteme (Future Fossil Fuels – Their Utilization and Embedding in Modern Energy Systems). *DFVLR-Nachrichten*, Mitteilungsblatt der Deutschen Forschungs- und Versuchsanstalt für Luft- und Raumfahrt E.V., 35: 8–19.

Kallio, M., Lewandowski, A., and Orchard-Hays, W. (1980) *An Implementation of the Reference Point Approach for Multiobjective Optimization.* Working Paper WP-80-35, International Institute for Applied Systems Analysis, Laxenburg, Austria.

Kendrick, D.A., and Stoutjestijk, A.J. (1978) *The Planning of Industrial Investment Programs. Vol. 1. A Methodology.* Published by Johns Hopkins University Press, Baltimore, M.D., for World Bank Research Publications.

Kopytowski, J., Wojtania, J., and Żebrowski, M. (1981) *Fossils as Key Resources of Hydrocarbons for the Chemical Industry – the Burning Problem of Industrial Development.* Collaborative Paper CP-81-20, International Institute for Applied Systems Analysis, Laxenburg, Austria.

Nowak, H. (1982) *Prospects for Methanol Production.* Unpublished report (in Polish). Institute for Industrial Chemistry, Cracow, Poland. Based on *Chemical Market Report,* Vol. 215, No. 266, p.5 (1979); *Chemical Age,* Vol. 118, No. 3122, p. 10 (1979); Sherwin (1981) – see below; *Inform. Chemie,* No. 166, p. 181 (1977).

Rogner, H.H. (1982) *Substitution of Coal and Gas for Oil – Some Global Considerations.* Paper presented at the first US–China Conference on Energy, Environment and Resources, 7–12 November, Beijing. Copies available from the Energy Group at the International Institute for Applied Systems Analysis, Laxenburg, Austria.

Sassin, W. (1982) *Fossil Energy and its Alternatives – a Problem Beyond Costs and Prices.* Paper presented at the International Economic Association, Conference on Economics and Alternative Sources of Energy, 27 September–1 October, Tokyo, Japan. Copies available from the Energy Group at the International Institute for Applied Systems Analysis, Laxenburg, Austria.

Sherwin, Martin B. (1981) Chemicals from methanol. *Hydrocarbon Processing* 60(3): 79–84.

Sophos, A., Rotstein, E., and Stephanopolous, G. (1980) Multiobjective analysis in modeling the petrochemical industry. *Chemical Engineering Science* 35(12): 2415–2426.

Stadtherr, M.A., and Rudd, D.F. (1976) Systems study of the petrochemical industry. *Chemical Engineering Science* 31(11): 1019–1028.

St. Pierre, L.E. (Editor) (1978) *Resources of Organic Matter for the Future. Perspectives and Recommendations.* Multiscience Publications Limited, Montreal, Canada.

Wierzbicki, A.P. (1980) *The Use of Reference Objectives in Multiobjective Optimization – Theoretical Implications and Practical Experience.* Working Paper WP-79-66, International Institute for Applied Systems Analysis, Laxenburg, Austria.