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FOSSILS AS KEY RESOURCES OF HYDROCARBONS  
FOR THE CHEMICAL INDUSTRY - The Burning  
Problem of Industrial Development

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## PREFACE

The future role of fossils in the world economy is a controversial problem which is being discussed among economists and engineers. Unfortunately, a variety of the reports already published describe solutions without detailed identification, and the data quoted are hardly comparable. Systems analysis may contribute substantially in such a case, and the research undertaken within the framework of the cooperative agreement between IIASA and the Academy of Mining and Metallurgy, Krakow, is an example of this. The preliminary results presented in this collaborative paper were discussed in January 1981 at a seminar held at IIASA.

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## ABSTRACT

Intensive research is being pursued world-wide to establish a methodology for industrial development. Many types of changes play an important role in the dynamics of the industrial structure in both large and small economies. The global energy supply and future substitution of crude oil are among the most important and widely investigated constraints. With the existing patterns of production and development strongly determined by the specific conditions in a given region, the development of various raw materials for the chemical industry is of great importance. The impact of changing production methods in feedstock hydrocarbons on industrial development requires further intensive research. A non-uniform demand vector and a variety of possible production processes, with a constrained supply of resources in different economic regions and countries, open a number of possibilities for new and non-conventional solutions. Further, hydrocarbon synthesis for the chemical industry should be a high priority research goal, not only because of the scale of demand, but because of the properties of the substances themselves. Provided the problem of production of hydrocarbon feedstock for the chemical industry can be solved successfully, the same methodology could also be used for the analysis of synfuel production: It would contribute to a better understanding of the dynamics of the industrial structure.



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INTRODUCTION

Hydrocarbons are extremely specific compounds. They exist as such or can be synthesized into long chain formations as well as into complicated rings, react easily with other elements of the earth's core, and not only is the human being based on this structure, but his civilization depends on it. It is easy to prove that the major and most important part of industry utilizes hydrocarbons or their derivatives. The problem then, of how to balance their supply and demand becomes the main hindrance to the process of development of an industrial structure. Hydrocarbons are obtained mainly from crude oil processing, therefore hydrocarbons for the chemical industry and for other sectors have the same origin. This creates competing demand between the chemical industry and the energy sector which has to supply energy for home heating, industrial boilers, automobiles, etc.

During the past few years, a large number of reports have appeared, discussing future levels of consumption of liquid fuels, the availability of resources, the economic as well as the political factors affecting their production and consumption. OPEC's policies instigated a more careful investigation of the future balance which led to the development of many research programs on synthetic hydrocarbons production, with more emphasis on synfuels. Large scale programs have been initiated for the substitution of energy from liquid fuels by nuclear, solar, and biomass-derived energy, coal and lignite. The main issue in energy-oriented technological and systems investigations is the production of gaseous and liquid hydrocarbons--in a narrow sense called synfuels--the compositions of which permit their use as substitutes for natural gas and crude oil.

It is difficult to predict the investments which will be made in this field because:

- (1) The technologies are far from being perfect, and every investor expecting a technological breakthrough waits for further research results so as to avoid severe risk.
- (2) Capital expenditures are high and comparable to other sources of energy (i.e., solar, nuclear, biomass); therefore, any economic region or country cannot be expected to employ only one universal transformation process for fossil fuels.

To substitute the present total production of crude oil by coal-derived products would require 10,000-12,000 million tons per year of different types of coal, at the current level of technology. This means that it would be necessary at least to quadruple the capacity of coal mines. Processing investments are also very high. For the processing of 10 million tons/year of crude oil in a full treatment refinery, it is necessary to spend about US\$1,500 million. Engineering studies show that for a corresponding result with coal, conversion facilities capable of handling 40-50 million tons/year are necessary, with investments in the range of US\$10,000-12,000 million. The worldwide figure of capital expenditures for the total substitution of crude oil by coal is in the range of US\$2.0 × 10<sup>12</sup> to 3.6 × 10<sup>12</sup> so there is no question about such substitution.

One cannot therefore expect a rapid development of the synthetic fuels industry. On the other hand, further delays would pose a threat to all developed economies because the production of chemicals based on hydrocarbons will enter into dangerous competition with gasoline production where profit margins are always very high. As stated in the recommendations of the IUPAC Conference held in Toronto in 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 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 expresses perfectly the global scale of the problem, therefore no comment is necessary.

## SUBSTITUTION OF THE HYDROCARBON FEEDSTOCK

Some effort is required to evaluate the world-wide consumption of hydrocarbons by the chemical industry, but rough figures are available. It has been shown that only about 3% of the total production of natural gas and crude oil serves as feedstock for the chemical industry. However, more than 50% of the refined products cannot be used directly as raw material for this industry. Therefore, for rough estimates, it is more reasonable to use the figure of 7% consumed by the chemical industry, mostly obtained from light crude oil fractions. When calculating this consumption, the figure seems to be marginal in comparison to total production. However, it is of critical importance to the chemical industry and to the overall industrial structure.

Hydrocarbons originating from crude oil and used as feedstock for the chemical industry are subject to transformations by highly sophisticated technological processes into:

- (1) Substances of low molecular weight, such as monomers (mostly double and triple bound hydrocarbons), aromatics, alcohols of different chain lengths, etc.
- (2) Substances of high molecular weight:
  - plastics such as polyethylene, polypropylene, polyvinyl chloride, polystyrene, their copolymers, and a wide range of special plastics. The total production of plastics in the world is in the range of 60 million tons/year.
  - rubbers such as SBR, polybutadene, polyisoprene, etc. The total world-wide production of rubbers is in the range of 11.5 million tons/year.
  - fibers, such as polyamides, polyesters, polyacrylonitril, etc. The total production of fibers in the world is in the range of 10.5 million tons/year.
- (3) Producer goods and commodities.

It could happen one day, that all this production could be stopped by lack of raw materials, at acceptable prices. The crisis in the synthetic fibers market has not been caused by the lack of demand but by the losses incurred in the production process. Substitution of polyester fibers by cotton needs twice as much energy, and also causes soil degeneration. The forthcoming crisis in the synthetic plastics and rubbers branches is another case in point of the impact of unstable hydrocarbon prices. Far-sighted industrialists are selling the appropriate production facilities.

In solving these problems an industrial structure specifically applicable to the chemical industry will be defined. The aim is to develop this industrial structure at a low investment cost and, in cooperation with the fuel industry, to assure stable feedstock prices.

It is impossible to find a solution applicable on a global scale. It is necessary to define the balance between the demand and supply of hydrocarbons country by country or region by region, as well as the raw materials and processes available for their transformations.

The internal logic and content of the problem indicates its systems character:

- (1) The methodology for determining the demand vector in the complex sector of consumption is to be developed--this is a typical scenario type of problem.
- (2) The methodology for identification of an appropriate industrial structure in the complex technological sector is to be developed.
- (3) The environmental constraints, the availability of resources, final distribution of the products, etc., have to be investigated.

The main task is to develop a method which would allow for implementation of the best approach to substitution of natural hydrocarbons from crude oil by other materials with a carbon content (i.e., coal, lignite, oil shales, etc.). Many possibilities must be analyzed, taking into account both construction and operation costs. To make the method more universal and less susceptible to monetary fluctuations, it would be interesting to estimate "costs" in terms of basic natural resources, i.e., Water, Energy, Land, Materials, and Manpower (the WELMM approach), as put forward by Grenon (1976) and Haefele (1981). After the choice of the proper solution has been made, the costs, if necessary, might be evaluated also in monetary units, but under particular time and site conditions. Two cases are shown in Figure 1--the present situation and the most morphogenic solution possible in the future.

To attain such a goal, it is necessary to investigate some potential options. Figure 2 shows Case A, in which the answer to the "7% question" discussed above has been approached in a traditional way. This case is based on the assumption that the priority of demands creates a special system of supply of hydrocarbons further used as feedstock for the chemical industry. Sometimes, the structure of such a system is seen as an actual pricing system, e.g., for agricultural products in the Common Market. Without going into a detailed discussion of the potential applicability of this system, it should be stressed that for a number of developed countries crude oil, in contrast to agricultural products, is an imported commodity. Therefore, it could be stated that in Case A, a temporary lack of resources and unstable profits in the production of plastics, rubbers, and fibers may appear.

Case B in Figure 3 presents the most popular concept of a possible solution to the problem. The case is based on the supposition that a deficit in fuels will provide an incentive for large investments in processing fossils to extract hydrocarbons, and thus the division of the market share will be natural. As a result, the production of feedstock for the chemical industry will be totally dependent on equilibrium in the fuel sector and will also lead to the situation where the structure of hydrocarbons (from the point of view of the molecular properties), would call for unnecessary transformations and additional loss of energy.

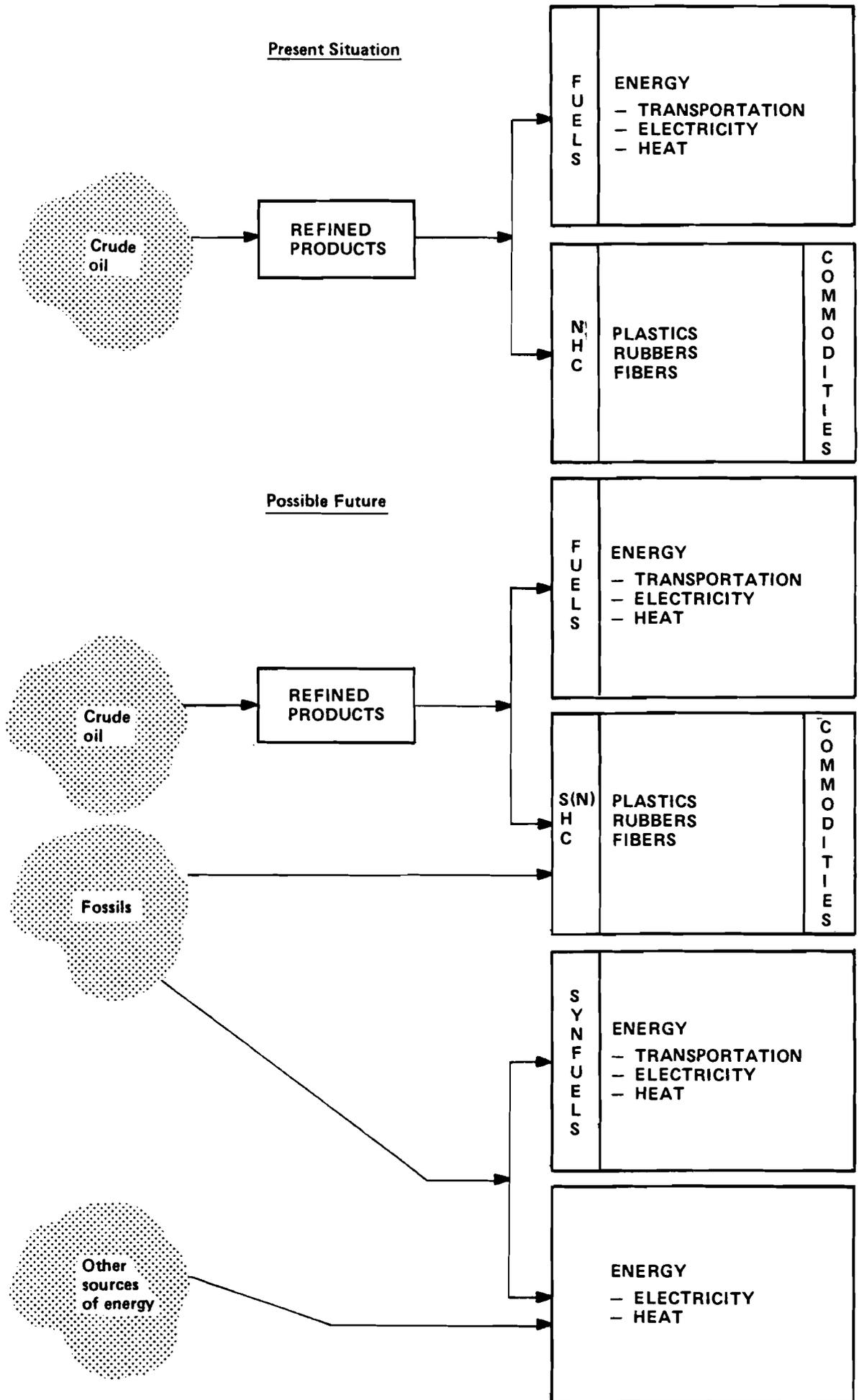


Figure 1. The way to substitution.

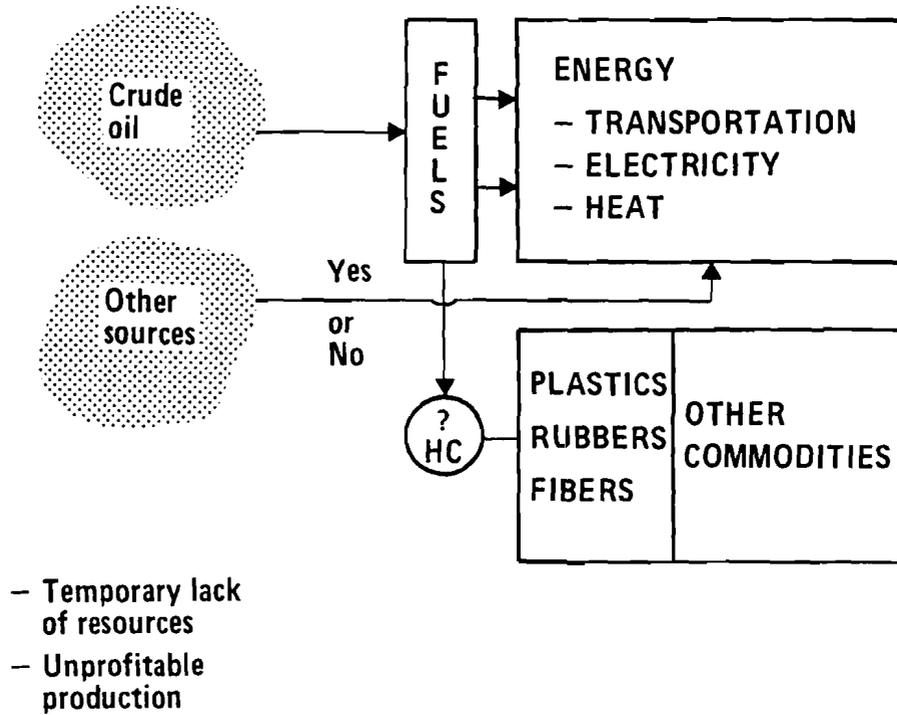


Figure 2. Case A: From where 7% can be obtained.

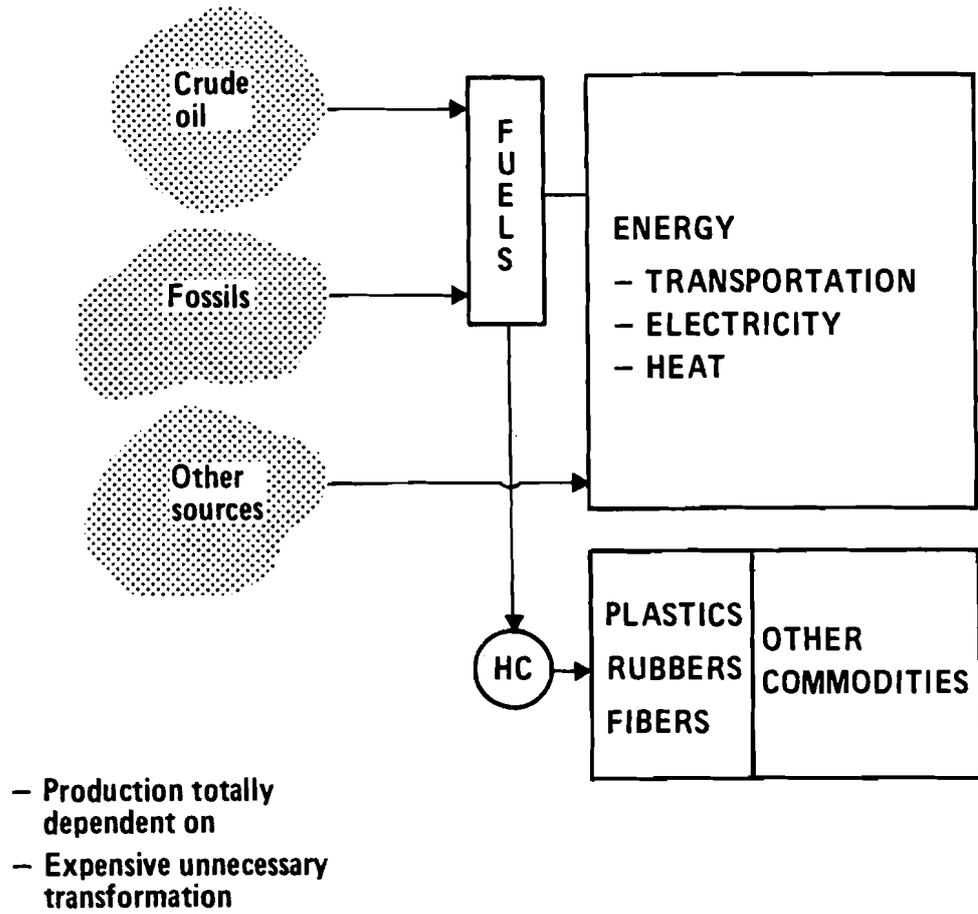


Figure 3. Case B: Most popular idea regarding HC supply.

Case C in Figure 4 analyzes another approach to the solution of the problem. The case is based on the assumption that a set of specific technological processes exists, leading directly to the robust structure of an industry producing feedstock for the chemical industry. This industry will cooperate with the fuel sector by buying products obtained by processing crude oil as well as other fossils, and would sell some by-products which could be used for the fuel sector. As a result, the demands of the chemical industry would be assured by specific, optimal, case-to-case investments and realization would be time-market dependent. Independent and profitable production would result, with appropriate linkage to the fuel sector.

Figure 5 is an example of a typical case showing that "7%" can solve its own problems better than is foreseen in general solutions.

In standard practice, the synthesis of ammonia is based on the transformation of natural gas. The process consists of 5 (sometimes 6) typical elementary technological units. The integrated parameters describing efficiency of the process are  $E_1$  (total energy consumption in m.t.c.e.), and  $I_1$  (total investment expenditures). The method proposed by the "generalists" for ammonia synthesis from coal has two production processes:

- (1) preparation of synthetic natural gas (technological process, line 2 in Figure 5) in five technological units;
- (2) preparation of ammonia in the standard unit.

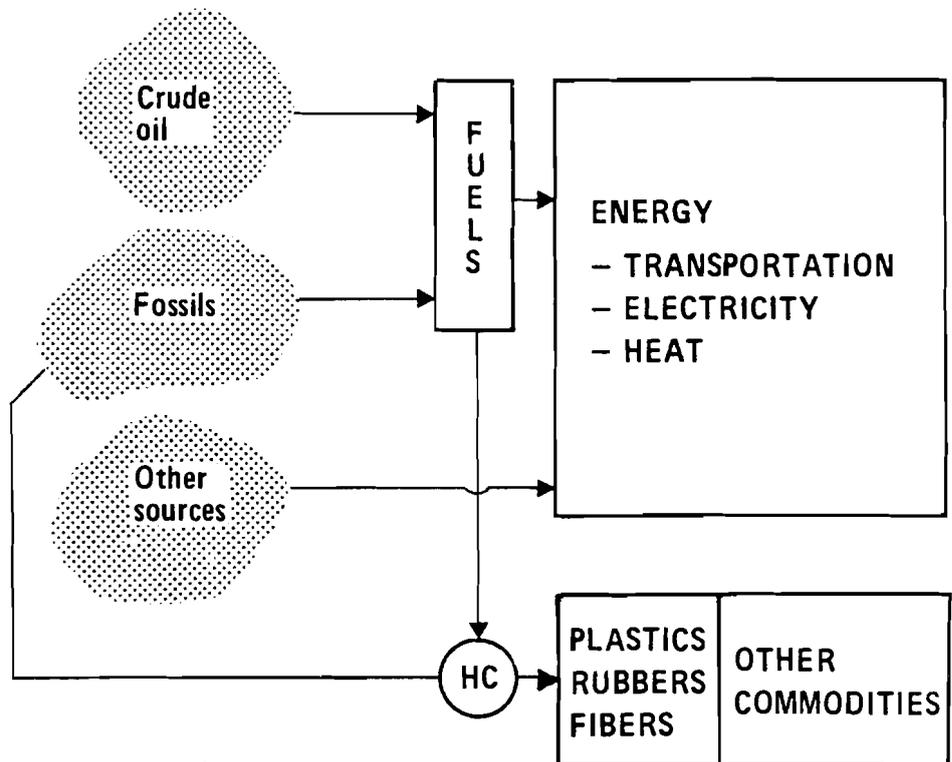
The integrated parameters describing efficiency will be the sum of the two sets  $E_1 I_1 + E_2 I_2$ , and one can claim that coal-derived ammonia is much more expensive than that obtained from natural gas.

When utilizing new raw materials, application of standard methods of production design would not be optimal. An appropriate combination of existing processes would solve the problem better. The extreme case is given in line 3, where, in a process with 6 technological units, one can produce ammonia. The energy  $E_3$ , and investment  $I_3$ , will be substantially smaller than in the previous case--this is expressed by the equation at the bottom of the figure. Only through a detailed investigation of the different possibilities can one choose the proper solution for ammonia production in a given environment.

#### WHAT IS TO BE SOLVED AND OPTIMIZED?

The research program concerning the above should include the analysis of different possibilities for providing chemical feedstock and synfuels as by-products from hard coals and lignites, using various technological schemes and demand-supply cases:

- to cover present and future demands from crude oil (extreme case)



- Specific optimal case-to-case solutions
- Realization step by step

**Result:**  
Independent and profitable production  
Cooperation with fuel sector

Figure 4. Case C: The robust solution.

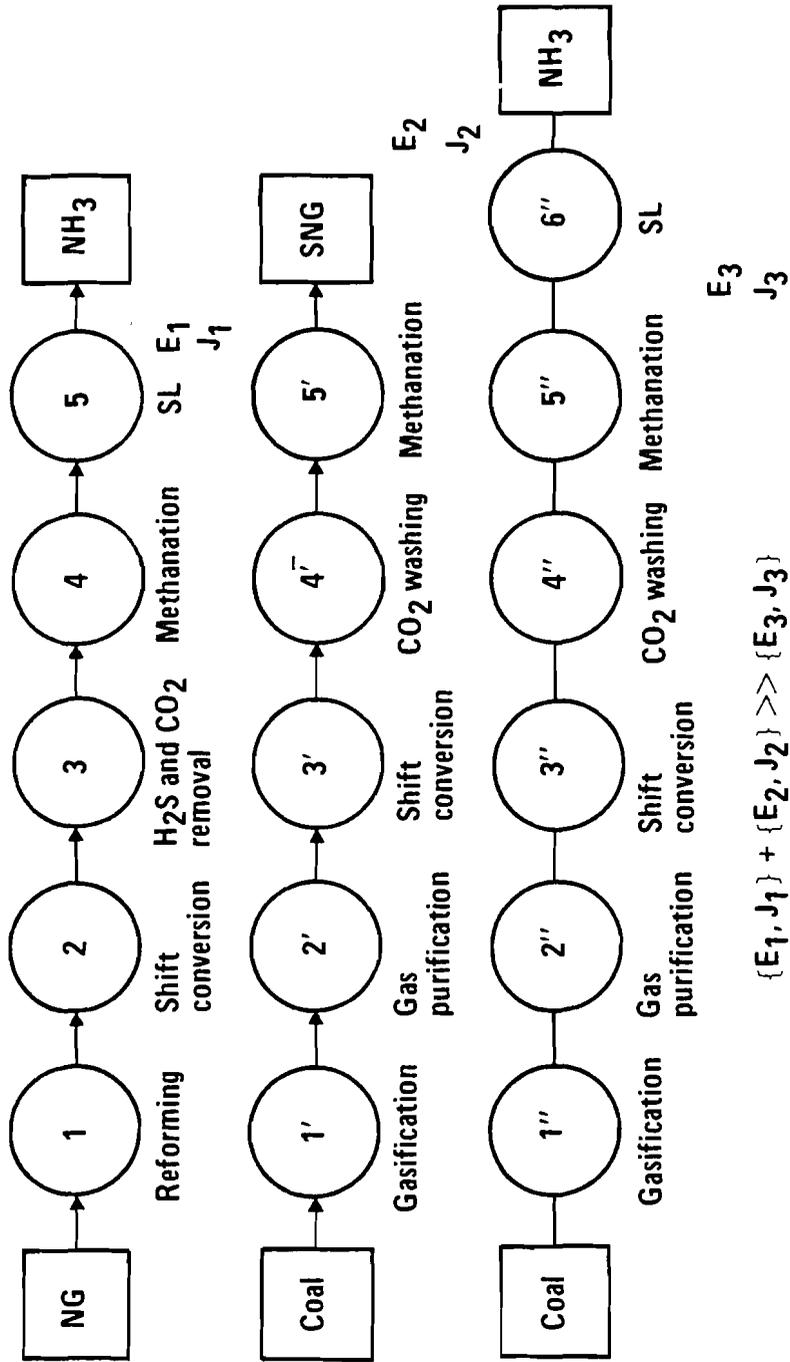


Figure 5. 7% can solve its own problems better.

- to provide an actual supply of hydrocarbons from crude oil and to cover the growing demand for hydrocarbons from fossil-derived products
- mixed scenarios.

The problems of power generation should be taken into consideration only for a comparison of the efficiency of energy consumption and to establish possible trade-offs between different industrial sectors. Coal mining should also be treated as an external system, and the necessary data included as exogenous from the existing WELMM sets of information.

In order to limit the scope of the program, at the first stage it should only cover the basic demand vector:

- basic monomers
- basic aromatics
- methane
- methanol and higher alcohols
- naphtha
- ammonia.

Because of the non-uniformity of the demand vector in different countries and economic regions, one ultimate solution obviously does not exist. The availability of the given array of fossils also varies from place to place. Therefore, selection of the method for transforming fossils into hydrocarbons in different countries and/or regions may require a different industrial structure.

Let us discuss the situation shown in Figure 6. In a given economic region, the specific consumption demand may either exist or be modeled for a given scenario. Taking into account that it is necessary to exclude wasteful consumption and include some recycling of ready-made products, the commodities production structure (II) could be defined. From simple material balance and knowledge of necessary transformations (technological lines) or foreseen improvements and possible innovations, the production structure of polymers and additives (I) can be derived. This means that it is not necessary to foresee drastic changes in large, investment-intensive areas of the industrial structure. On the other hand, the fossil resources are known, and appropriate technological and technical conditions for their utilization have to be applied. The importance of environmental impacts is well-known and it does not have to be stressed at this point.

Therefore, if the demand vector  $Y$  is known and vector  $X$  of available resources can be defined, then the problem rests with such a structuralization of the set  $t_j$ , as to obtain optimal transformation  $T$ . Now we have to try to disclose what the transformations  $t_j$  and their components are.

Hydrocarbons can be obtained from any substance containing carbon. The higher the hydrogen content, the lower the cost of

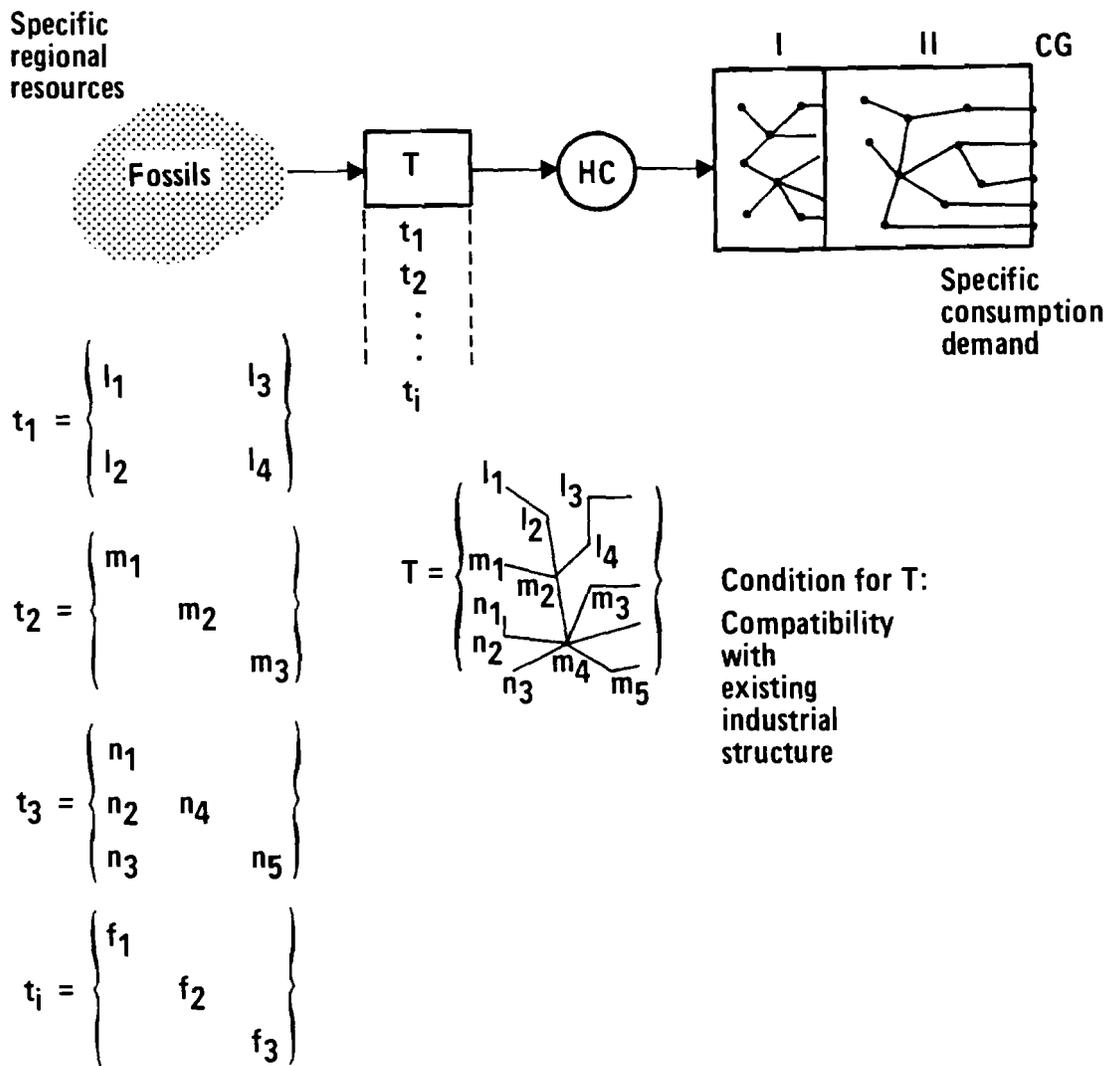


Figure 6. What is to be optimized?

its transformation to a specific molecular structure. Unfortunately, in the available fossils, the hydrogen content is not higher than 4-5%, and natural hydrocarbons used as feedstock for the chemical industry contain between 10-12% of hydrogen. To ensure transformations, several technological processes have been developed (see Figure 7). Then, to describe every production process  $t_i$ , it is necessary to collect and store the information concerning the function and structure of the process, and a set of its respective parameters. This would be a rather complicated task. Some of the technological processes are under development, some are very old; therefore, it is necessary to find a uniform way of describing different parameters of these processes.

The research program foresees the collection of numerical values which are necessary to perform the calculations of the integrated parameters and carry out simulation and optimization analysis. Some engineering studies for the particular processes will be indispensable.

Another specific aspect of different production processes used to extract hydrocarbons from fossils is their complexity. Every process is composed of several elementary technological units:  $l_i$ ,  $m_i$ ,  $n_i$ , etc. We define an elementary technological unit as that part of the industrial structure which transforms the flow of the materials and energy into specific products, or mix of products. The following cases can be identified:

- the product as a pure saleable substance;
- the product as a mixture of saleable substances;
- the product as a mixture of substances which are used at least twice in a given production/distribution area.

Therefore, we aim at composing a specific transformation  $T$ , having at our disposal definite process data sets for every elementary technological unit and utilizing specific properties of production dendrites (or process routes), from a given array of fossils. The algorithm necessary for optimization of technological structures composed in this way are currently being developed.

Parallel to the description of different structures by integrated parameters, it would be possible to carry out an analysis of various alternatives to select the one minimizing the consumption of basic natural resources (WELMM). Because several criteria have to be taken into account, the multi-objective optimization procedures developed at IIASA (Wierzbicki 1979) could be applied.

Generally, two methods of investigation have to be checked:

- (1) Simulation of several (sometimes 20-30) different production processes composed of different technological units, and transformation of all possible grades of fossils. In computing every case, all WELMM parameters will have to be established. Comparison and choice of the most feasible solution will be found on an interactive basis.

GROWING DEGREE OF DESTRUCTION OF THE ORIGINAL COAL STRUCTURE →						
<b>PROCESSES</b>	Extraction of coal and lignite by gases in super-critical conditions	Hydrogenation of coal extracts	Flush pyrolysis of coal and heavy oil mixtures	Coking	Carbide	Gasification of coal (oxidation)
	Extraction of coal by liquid solvents	Hydrotreatment of coal suspensions	Flush pyrolysis of coal			
<b>PRODUCTS</b>	From light to heavy oils (Syncrude)	From light to heavy oils (Syncrude)	Syncrude and coke	Tars and coke	Acetylene	Synthesis gas

Figure 7. Coal processing.

- (2) Simulation of all possible compositions will be attempted, but the optimization module will choose several close-to optimal solutions to be analyzed in a multiobjective optimization module in order to choose the optimal WELMM solution.

The first approach will require more work preceding computerized analysis, but the system would be more flexible and could become feasible under varied conditions.

An automated system would require prior development of a large number of different technological models, and possibly, some of them will be found useless or irrelevant for the next step of analysis. Therefore, rather typical cases, like the production of naphtha should be investigated with this type of methodology.

#### MODEL OF THE PROPOSED SYSTEM

The pragmatic model to investigate all aspects of the problem presented herein is in preparation. IIASA's experience in the application of the WELMM approach as well as ICSE-AMM's in simulation and optimization of industrial structures make a good starting point for the program which has already been initiated.

Most effort should be concentrated on the definition, description, and processing of the following sets of data and modules of the system (Figure 8):

##### Sets of data:

- Fossils information file (data sheet compiled information), including available raw materials, quantities, forecasts and limitations of development, description of qualitative parameters, integrated economic parameters (E,I).
- Encyclopedia of production processes (data sheet compiled information), including identification of elementary technological units, description of the process and structural features and parameters, physical and economic properties of the WELMM indicators.
- Hydrocarbons information file (data sheet compiled information) including final destination, consumption coefficients, constraints for application, qualitative description, physical and economic parameters.

##### Operational modules:

- Macro-balance modules, M1.  
Function: To define the upper and lower limits of the use of fossils for different production programs. Control of constraints and definition of logistics.
- Master file module, M2.  
Function: To define principles of the sequence of coupling of the elementary technological units to assure defined transformation T into a certain product.

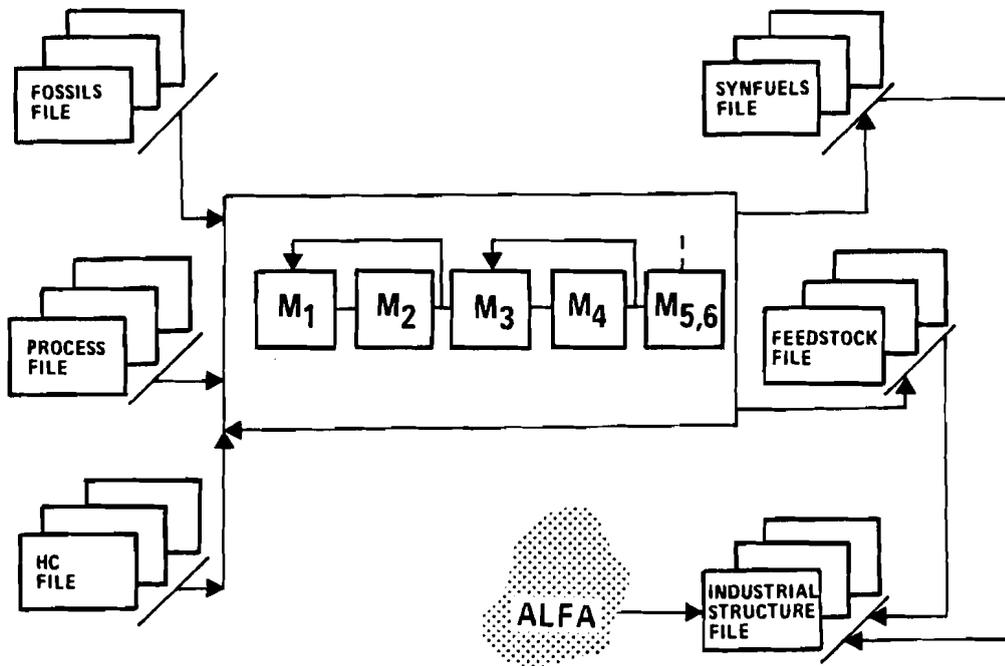


Figure 8. Under investigation (optimization system).

- Micro-balance module, M3.  
Function: To define properties of every production process (consumption figures for materials and energy, other resources utilization).
- Simulation and optimization module, M4.  
Function: To define different production lines and their arrangement into a more complex network; static and dynamic optimization of a multiobjective character.
- Module of adaptation to regional constraints, M5.  
Function: To control the ability of the environment to absorb the proposed technological solution. Additional input-output analysis.
- Decision modules, M6.  
Function: To define a feasible solution; further analysis of exogenous constraints.

The systems analysis approach presented above would not replace the classical economic analysis indispensable in making decisions for implementation of a single investment project, but would only be a guideline of great importance, enabling rejection of infeasible solutions. Due to this approach, it would be possible to make a selection from many different models on the basis of uniform, sensible, and objective criteria. Thus, only the models selected by such means would be further analyzed using traditional methods of investment decision making. The set of models from which one is to be selected for realization would be enlarged, and the selection itself would be more objective and rational.

It is also important that at present, information on individual process lines and, even more, on various models describing them, is scattered. To gather all the information takes more time than is available in many cases, not only for carrying out analysis, but also for taking a decision. The system proposed in the present study would gather the information in a place such as IIASA and make it easily accessible. Actually, to a certain extent, the selection would still be based on experience. At this stage, also the model developer's intuition would play a very important creative role in addition to his knowledge. Moreover, in comparison with the present state of the art, the difference would lie in the fact that more diverse models could be analyzed in a shorter time.

The number of process lines included in the program, taking into account alternatives bound up with different production rates, raw materials as well as process technology, total 241. This is a preliminary estimation. As a result of a thorough examination of the individual process lines, it is quite probable that the total number of process lines will be reduced. It should also be emphasized that several units, or even sets or complexes, contained in the individual process lines will be repeated.

Table 1 shows the basis for estimation of the number of process lines to be analyzed.

Table 1. Number of process lines included in the system.

Process line definition, type of production, raw materials, process, production rate	Number of alternatives:				Total
	Production rate	Feed-stock	Process Technology		
1. Gasoline, motor and fuel oils from crude oil: 2 types of refinery, 3 production rates	3	1	2		6
2. Gasoline, motor and fuel oils from coal: 3 production rates, 2 coal types (brown and hard). Types of process: gasification + F-T synthesis, gasification-methanol-Mobil, LTC + hydrotreatment, flush pyrolysis hydrogasification, 2 liquefaction processes, 2 complex processes (ADL, COGAS)	3	2	9		54
3. Ammonia from natural gas: 3 production rates, 2 processes (reforming, partial oxidation)	3	1	2		6
4. Ammonia from heavy residue: 3 production rates	3	1	1		3
5. Ammonia from coal: 3 production rates, 2 grades of coal, 4 gasification processes	3	2	4		24
6. Olefins from crude oil: 2 production rates, 3 types of feedstocks (naphtha, heavy residue, LPG)	2	3	1		6
7. Olefins from coal: 2 production rates, 2 grades of coal. Types of process: gasification + F-T synthesis, gasification + Mobil, LTC, flush pyrolysis, hydrogasification and 2 complex processes	2	2	7		28
8. BTX from crude oil: 3 production rates, 2 processes (steam cracking, reforming)	3	1	2		6

Continued overleaf.

Table 1. Number of process lines included in the system, continued.

Process line definition, type of production, raw materials, process, production rate	Number of alternatives:			
	Production rate	Feed-stock	Process Technology	Total
9. BTX from coal: 3 production rates, 2 grades of coal. Types of process: LTC, flush pyrolysis, hydrogasification, coal liquefaction--2 processes, 2 complex processes and gasification + Mobil	3	2	8	48
10. Methanol from crude oil: 3 production rates, 2 kinds of feedstocks (natural gas and heavy residue). Methane reforming and partial oxidation of heavy residue	3	2	1	6
11. Methanol from coal: 3 production rates, 2 grades of coal, 4 gasification processes	3	2	4	24
12. Methane from coal: 3 production rates, 2 grades of coal, 4 gasification processes and hydrogasification	3	2	5	30
TOTAL NUMBER OF DIFFERENT PROCESS LINES				241

## CONCLUSIONS

It is very difficult at this stage of research to attempt to present final conclusions. The problem is of great importance to the world economy, and, from the point of view of the methodology, there are at least as many approaches as the number of engineering and scientific organizations seeking the solution.

None of the existing or proposed methodologies has been proved to be appropriate in general analysis. The program proposed here provides a chance, because it uses an example of a rather limited industrial structure which may help not only to solve a problem (the answer lies in the development of an industrial structure for the production of hydrocarbons), but it can also provide valuable results which could find practical and methodological applications in a wider context, e.g., in synfuels production as well as in other industrial development programs.

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