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RAW MATERIAL — POLYMER INTERRELATIONS - TODAY'S CHOICE - TOMORROW'S OPTIONS

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<u>Abstract</u> - Against the backdrop of increasing demand and limited availability of fossil non-regenerative fuel reserves and resources guidelines are suggested by which to ensure future raw material supplies. The ambivalence of the fossil reserves in the energy and chemistry sectors is discussed and opportunities for separation of the two sectors are given. As regards the time factor, the necessary changes together with their impact on the raw material-polymer relationship are critically analysed.

In no branch of industry is the interrelationship between fossil fuels and organic raw materials as intimate as in the chemical industry, for more than 90 % of the energy and organic raw materials consumed throughout the world are based on petroleum, natural gas and coal.

It is foreseeable that the fossil reserves petroleum and natural gas will already be exhausted in the not too distant future, and coal in the longer term, unless their double function as sources of energy and raw materials can be disentangled in good time or eliminated step by step.

According to past experience with coal, petroleum and natural gas, and also with nuclear energy, the introduction of a new energy system or changeover to a new raw material basis, from the time of its technical availability to a large market share, takes at least 25-30 years.

From this it follows that long-term strategies cannot be derived from considerations based on short-term requirements. However, to be in a position to develop a strategy for safeguarding energy and raw material supplies in the long term, it is necessary first of all to analyze the present situation with great care.

<u>Primary energy consumption</u> - Due to the rapid economic growth since 1950 there has not only been a drastic increase in the quantities of primary energy consumed, but great changes have also taken place in respect of the proportions of the individual energy sources involved. This development is demonstrated in fig. 1.

Fig. 1 shows the changeover from coal to petroleum and natural gas; this happened because both the latter sources of energy were offered in the world markets at prices far below their value as energy and raw material sources. Considerable differences exist on a national and a regional level in regard to meeting energy consumption from fossil sources of energy (Fig. 2).

If the present pattern of energy consumption is compared with the available reserves of fossil raw materials it becomes obvious that there is a crass disproportion between the reserves and the consumption of petroleum and coal. This is shown in fig. 3 (1).

By definition, reserves are proven supplies which can be recovered economically. Resources include geologically detected deposits which will be recoverable at considerably greater expense sometime in the future. They include the reserves.

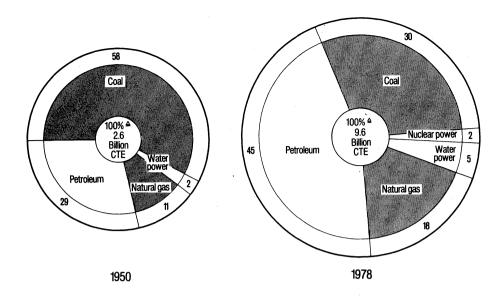
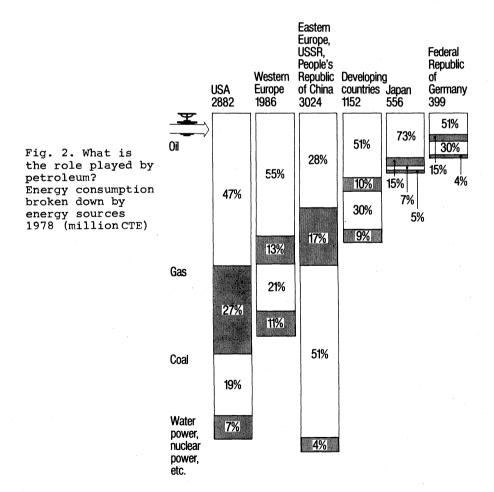


Fig. 1. Primary energy consumption throughout the world 1950 and 1978  $\,$ 



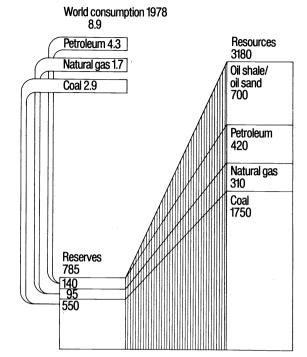


Fig. 3. Recoverable fossil fuels from reserves and resources (billion CTE)

The boundaries between reserves and resources will shift and are an expression of technological progress in opening up and exploiting the deposits. Whether a deposit is worth recovering is decided in the final analysis by the price too. The total world deposits of fossil energy sources are estimated at 12,000 billion CTE (coal-tonne equivalents), whilst the recoverable proportion is only some 3,200 billion CTE (2).

If the energy potential provided by the utilization of nuclear energy and the so-called inexhaustible energy sources is taken into account in these considerations, it should be sufficient for any growth rate.

Future development of primary energy consumption in the world All prognoses have in common that they are based on a large number of more or less reliable assumptions. Nevertheless, a qualitative statement on the trend is possible. The main question is: for how many people when and in which region do we expect what demand? Fig. 4 provides information on the current per capita consumption of primary energy and the breakdown by countries and regions (3).

Currently some 4 billion people have to be supplied with energy and raw materials - at the turn of the millennium the number will have reached 6 billion and in 50 years the 8 billion mark will have been reached or surpassed (4). According to studies of Keyfitz (5) an increase in primary energy consumption from 2 CTE to 3-5 CTE per person per year is to be expected during the next 50 years. This means a total consumption of 24-40 billion CTE/year compared to 9.6 billion CTE in 1978. In any case we shall have to expect a doubling of energy consumption within a few decades.

The situation in fig. 5 emerges if one attempts to produce a graphic representation of the estimated development of primary energy demand and supply, broken down by energy sources (6). Fig. 5 shows that the time the fossil reserves will last is decisively influenced by our capability to open up new energy sources and to develop their utilization to technical maturity early enough.

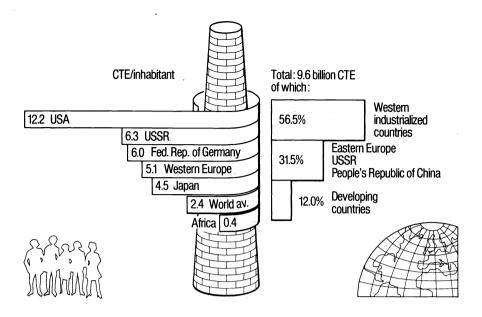


Fig. 4. World consumption of primary energy 1978

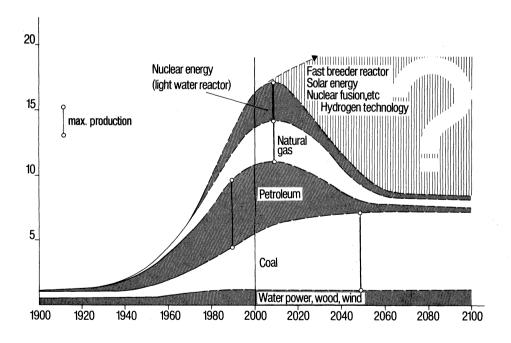


Fig. 5. Development of the world consumption of primary energy (billion CTE)

## Alternative energy sources with which to meet the world demand for primary energy

Utilization of nuclear energy currently is the only possible alternative for the nineteen-eighties and nineties. Nuclear energy, if consistently expanded, could already make a considerable contribution in the medium term towards extending the time which fossil, non-regenerative raw materials will last. Following thirty years of development this source of energy has reached industrial maturity, is preferable to coal and petroleum (which are environmentally detrimental) and is economically superior to fossil energy production (7).

Coal, too, in the form of its conversion products will have to make a greater contribution towards meeting the demand for energy and easing the pressure on petroleum.

An energy industry based both on hydrogen and electricity, utilizing in-exhaustible energy sources, would be a desirable long-term objective from which we are still far removed.

## Safeguarding raw materials through structural changes

Compared to the world consumption of petroleum amounting to 3 billion tonnes in 1978, the share of petroleum-based raw materials for the chemical industry in the order of 5-6 % appears to be insignificant (8). This is shown in fig.6.

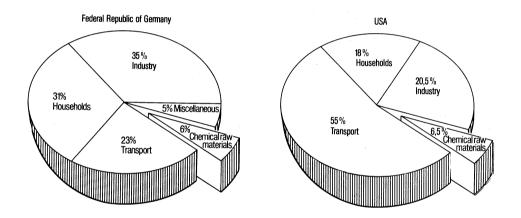


Fig. 6. Petroleum consumption by major consuming sectors (Fed. Rep. of Germany 1976, USA 1975)

This dependence only becomes really evident by the fact that the primary chemicals of organic chemistry and consequently also the starting products of polymer chemistry are currently based preponderantly on liquefied gas and crude naphtha from which the olefins ethylene, propylene, butene and butadiene as well as the aromatics benzene, toluene and xylene are obtained by pyrolysis. However, the proportion of crude naphtha produced during petroleum distillation is only some 23 % and is at the same time the starting product for carburettor fuel. Thus two large sectors of consumption are competitors for the same raw material. The importance of petroleum for the world production of primary organic chemicals and the steep increase in production during the last three decades can be seen from fig. 7 (9). Petroleum has developed into the most important raw material for organic chemistry because, in contrast to coal, it already contains the hydrocarbon units in the form they are required.

There are several possibilities of safeguarding energy supplies; for safeguarding supplies of organic chemicals there is no substitute for petroleum.

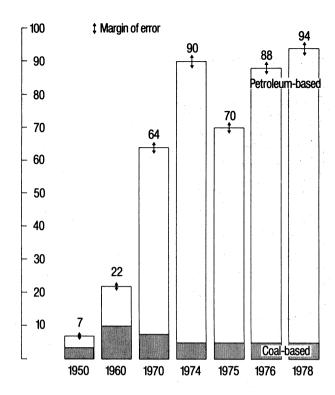


Fig. 7. World production of organic primary chemicals in millions of tonnes (without Eastern Europe, USSR, and People's Republic of China)

Under the present economic conditions and the state of the art of conversion, coal cannot compete with petroleum as a raw material of the chemical industry. Exceptions, for example, methanol and acetic acid from synthesis gas should, however, be mentioned. Nor will the exploitation of oil shale and oil sand deposits have any appreciable effect on raw material supplies during this century, but may be of importance for long-term considerations. The production of primary chemicals from natural products which grow again will be restricted to a small number and will hardly have a global effect. All factors considered realistically, we are still far removed from a "post-petroleum economy", which will begin by way of more intimate interrelations between petroleum and coal, while taking into account the possibilities of upgrading that are specific to both raw materials.

<u>Safequarding supplies of primary chemicals</u>
What developments for safeguarding supplies of primary chemicals stand out from today's aspect?

- 1. What appears to be of prime importance for western Europe, and is also realizable in the short term, is optimization of crude oil upgrading by restructuring conventional refineries into petrochemical refineries. This enables an increase from 23 % to a maximum of 60 % in the yield of naphtha, a feedstock that is of great importance for the chemical industry and the motor fuel sector. Through this measure alone the specific crude oil demand for petrochemical prime chemicals is reduced to one-third. Fig. 8 demonstrates this (9). The increase in yield outlined in fig. 8 is attained by operating crackers with naphtha and gas oil and, furthermore, by the use of plants for converting heavy mineral oil fractions into lighter fractions and also by resorting increasingly to heavy oil for the production by partial oxidation of synthesis gases rich in hydrogen.
- 2. The exploration and production techniques for petroleum must be further developed, with the objective of raising exploition of the deposits from the current 30 % on average to 50 % and more by secondary and tertiary methods.

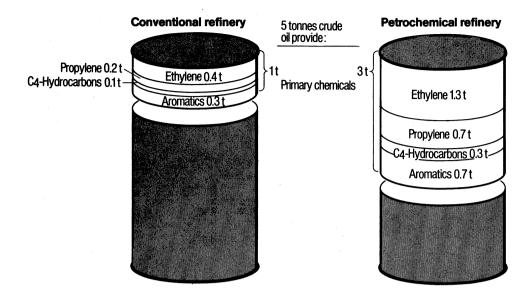


Fig. 8. Primary chemicals from petroleum Influence of the refinery structure

3. The upgrading of coal will gain importance already in the medium term. The first step in this technology is by way of coal gasification which must therefore be given top priority.

From the aspect of the availability of a suitable technology, coal chemistry should be directed to the production of liquid secondary energy sources (naphtha, motor fuel, heating fuel), that is to say sectors in which shortages are to be expected.

Further development of coal liquefaction by the method of "Bergius/Pier" in two directions suggests itself for this purpose. First, low-sulfur and low-ash fuels for power stations and industrial heating could be produced from coal by reduced hydrogenation and extraction by hydrogenation. On the other hand, the route of catalytic high-pressure hydrogenation of coal results in a coal oil with a higher content of aromatics which could be converted into gasoline, naphtha and primary chemicals in a refinery designed for the production of coal chemicals (10). The advantages of the direct conversion of coal into liquefied coal products are partly offset by the high consumption of hydrogen and the elaborate technique.

According to our present knowledge the specific coal consumption for the production of 1 tonne of coal chemicals by direct hydrogenation of coal is 3.6 tonnes of hard coal (11). Of this, 1 tonne alone is used for energy production and 1.36 tonnes for obtaining the hydrogen for hydrogenation. The corresponding consumption figures for the Fischer-Tropsch process are 4 tonnes of hard coal for every tonne of upgraded coal products which consist exclusively of aliphatic hydrocarbons.

An interesting alternative of the Fischer-Tropsch synthesis is represented by the Mobil Oil process (12), in which synthesis gas is first converted into methanol. This is converted in the presence of zeolite-containing catalysts with concomitant dehydration via dimethyl ether into hydrocarbons with a high aromatics content. If one assumes a specific coal consumption of 1.3-1.5 tonne of hard coal per tonne of methanol, a total coal consumption of about 3.4 tonnes can be calculated for the production of 1 tonne of coal chemicals.

In all these processes it would be possible to save the specific coal consumption for the synthesis gas production or hydrogen production by introducing and utilizing nuclear process heat from high-temperature reactors. The

decisive advantage of this future-oriented technology is that the coal is only used as a raw material, with a coal efficiency of 0.8 and more possibly being attainable (4).

This shows that substitution of petroleum by coal as the base product for chemical raw materials is possible in the long term. This is shown in simplified form in fig. 9 (13).

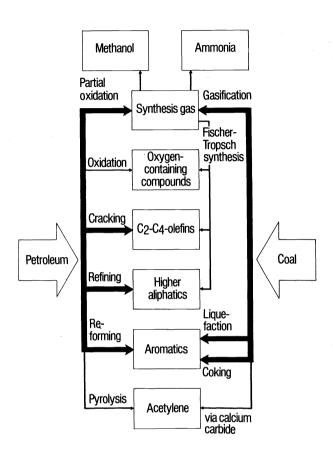


Fig. 9. Upgrading of petroleum and coal

If the possibilities of substitution are realistically assessed, the transitions to new supply patterns which also result from the symbosis of petroleum and coal will be gradual and will partially overlap. Changes in the pattern and availability of raw materials based on petroleum and coal, as they are to be expected in the medium and long term, are not without an influence on the interlinked system of starting products and intermediates of the chemical industry. These are problems which can be solved if they are recognized and tackled in good time. They will involve increasing capital expenditure and greatly influence the price structure of all chemical products in the future and, depending on the situation, will also cause processes to be changed.

Is resubstitution of plastics foreseeable? The increase in the price of raw materials will undoubtedly make itself felt most of all in respect of the products with the least number of upgrading stages. A large number of polymers are involved. This raises the question of resubstitution by alternative materials of inorganic or organic origin such as glass, wood and metal, since the introduction of a new material is normally prompted for price reasons. Under the pressure of costs, non-utilized properties of materials are not appreciated. The regulating mechanism in the resubstitution of plastics, however, is not determined by the price characteristics of the raw materials alone, but by the final costs of the finished products. Thus the extent of a possible substitution depends

on several cost factors which result among other things from the processing, shaping and finishing.

From the present-day viewpoint no substantial resubstitution is to be expected, as the cost advantages of plastics products in regard to capital expenditure and labour and energy costs preponderate as compared to finished goods made from natural products. The multiplicity of properties and combinations of properties have thrown open large markets and opened new fields of activity for plastics, synthetic resins, elastomers and man-made fibres. In their range of application they are far superior to all natural products. This explains the steep increase in the consumption of all polymer products throughout the world, which is shown in fig. 10.

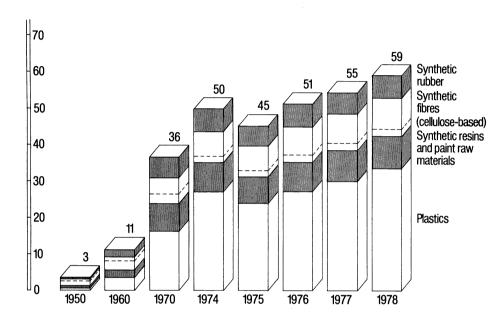


Fig. 10. World consumption of organic polymers 1950 to 1978 in millions of tonnes (without Eastern Europe, USSR and People's Republic of China)

In the area of thermoplastics the situation is marked by the commodity resins, namely the polyolefins, polyvinyl chloride and polystyrene. If one traces the development of the consumption of commodity resins back to 1970, it is evident that pronounced shifts in the proportions accounted for by the individual types of plastics have taken place, as demonstrated in fig. 11. This development is an expression of the fact that the incentive to substitute commodity resins for one another is determined to a great extent also by the relationship between price and properties, providing that processability and shaping characterists are equal. The possibilities of varying the property profiles have considerably extended the application spectrum of plastics and thus facilitated their substitutability for one another. This trend will continue and is a mark of the dynamism of the market and creativity.

Fundamentally new commodity resins are not to be expected. Further development of these classes of plastics by specific combination and variation of the mechanical and physical properties, tailored to the application in each case, will take pride of place. Predictions about possible changes in the consumption pattern are difficult. In most cases the price-cost gap referred to earlier on will be decisive in the large fields of application.

Commodity resins are appropriately complemented by a large number of high-quality engineering plastics. They are gaining increasing importance as polymer materials and are marked by a high development potential. There are narrow limits to substitution for each other because very specific property

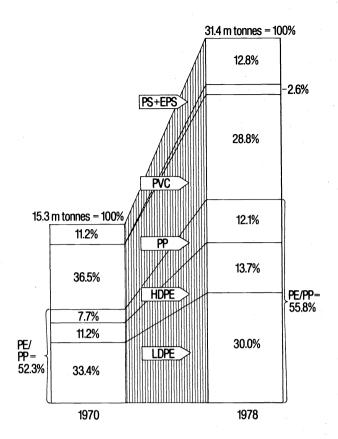


Fig. 11. Development of the world consumption of commodity resins 1970 and 1978 (without Eastern Europe, USSR and People's Republic of China)

combinations are demanded for polymer materials, which for reasons of safety do not permit compromises. In contrast, the substitution process of metals such as zinc, aluminium, copper and iron by polymer materials will continue apace, especially in the housing sector and vehicle and machinery production. This process of substitution was triggered by the high energy consumption in metal production and processing as compared to the polymer materials, see fig. 12 (14,15).

Designs of plastics mouldings, that take into account the properties of the material, result in savings in finishing and assembly costs as compared to mass-produced metal parts. These savings are also reflected in the processing costs, particularly the labour costs. In the face of rising costs there is an increasing economic incentive to substitute polymer materials for conventional materials. This is demonstrated with the aid of three examples in fig. 13 (15).

With the objective of producing more sophisticated products in mind, reinforced thermoplastics and thermosets will continue to gain ground as structural materials. Since the development of an injection moulding process for thermosetting moulding compounds and the surmounting of further problems of processing, the substitution of thermoplastics for thermosets is no longer so very important. In their profile of properties, moreover, they differ markedly from the thermoplastic materials. For reasons of saving raw materials and energy, the applications for highly filled plastics, that is to say combinations of polymers with inorganic fillers, will be extended. This applies also to plastics foams, especially those based on polystyrene and polyurethane. They are being increasingly used in the construction of housing for heat insulation and in the form of structural foam as materials for lightweight constructions.

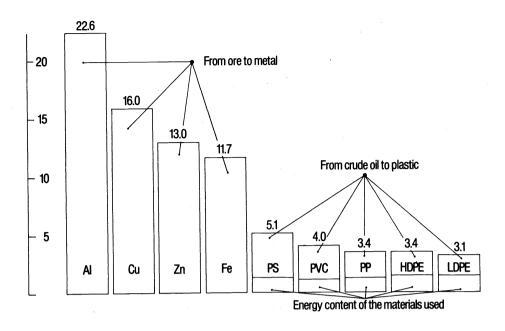


Fig. 12. Materials and energy consumption (CTE/ $m^3$ )

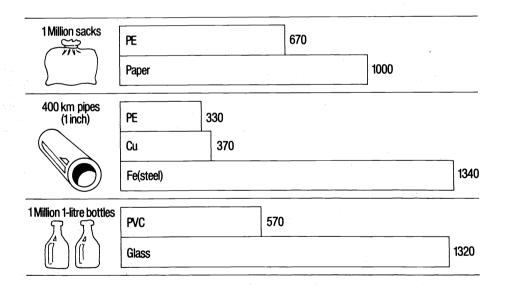


Fig. 13. Finished products and energy consumption (CTE)

In the wide and manysided field of packing the process of substitution in favour of plastics film based on petrochemicals is making further progress. This applies mainly to polypropylene because of its inexpensiveness, its higher dimensional stability under heat and its low water vapour permeability. The incentive to re-use plastics and recover waste will be stimulated in respect of all types of plastics. Several technically and economically feasible methods are appearing in outline both for re-use and the indirect utilization of plastics waste by pyrolysis or hydrolysis to obtain low molecular weight hydrocarbon compounds.

The potential for innovations is, however, not exhausted therewith. I have merely cited examples in order to underscore the statement that the polymer field will continue to gain in scope and importance.

Rising raw material and energy costs will hardly influence the resubstitution process with natural products but will tend to accelerate the substitution of polymer materials for metals.

Temporary bottlenecks in the supply of raw materials can never be excluded. The great variability of plastics is a characteristic of this area of production which has already proved in the past that it can rapidly adjust itself to changed raw material situations.

Let us return to the starting point of our reflections about raw materialpolymer interrelations - presence and future. What is the upshot? Under no circumstances must we continue in the future in the way we started. If we do, supplies of energy and raw materials will not be safeguarded even in the medium term. Consequently we must follow new paths which will result in radical structural changes. Above all, we must not lose any time if we want to win the race against tomorrow's problems.

## REFERENCES

- F. Barthel, P. Kehrer, J. Koch, F. K. Mixius and D. Weigel, 1. "Die zukünftige Entwicklung der Energie-Nachfrage und deren Deckung", Studie der Bundesanstalt für Geowissenschaften und Rohstoffe, Hannover, 1976
- 2. A. Ziegler and R. Holighaus, Umschau 79, 367 (1979)
- 3. Die Zeit, July 20, 1979
- 4. W. Häfele, lecture delivered at Achema 79, Frankfurt/Main, June 19, 1979
- 5. N. Keyfitz: Population of the World and its Regions 1975-2030 International Institute for Applied Systems Analysis, Laxenburg, Austria, 1977
- According to E. Edye, <u>Erdöl und Kohle</u> 31, 68 (1978) W. Schüller, <u>Umschau</u> 77, 41 (1977) 6.
- 7.
- BASF-intern 2/1978; R. L. Loftness, Energy Handbook 1978, 147 8.
- According to K. Stork, M. A. Abrahams and A. Rhoe, Hydrocarbon 9. Processing, November 1974, page 157
- H. G. Franck, <u>Chem. Ind.</u> XXXI, 377 (1979) H. Jüntgen, <u>Glückauf</u> <u>115</u>, 329 (1979) 10.
- 11.
- S. L. Meisel, J. P. McCullough, C. H. Lechthaler and P. B. Weisz, Chem. techn. 6, 86 (1976) 12.
- Nachrichten aus Chemie, Technik und Laboratorium 25, 228 (1977) 13.
- A. H. Smolders, Kunststoffe 69, 419 (1979) 14.
- 15.
- <u>Chemical Week</u>, March 28, 1979, page 20 P. J. Bakker, lecture delivered at the meeting of the Association 16. of Plastics Manufacturers in Europe, June 19, 1979 in Amsterdam

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