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INTRODUCTION

The chemical industry is an economic sector which is facing a challenge regarding its innovative activities. Innovation is usually related to R&D expenditures and therefore these expenditures have an important influence on the long term competitiveness of a chemical company. In Germany R&D expenditure in the chemical industry dropped by more than 500 million DM from 10 950 million DM in 1991 to about 10 439 million marks in 1995, but regained a level of 11 300 million marks in 1997 [BMBF 1997]. In general three main factors influencing innovation can be identified:

- The first of these is continuous technological development, due to a better understanding of reaction mechanisms, the availability of more exact or new physical properties for new components and owing to more powerful techniques for the simulation and model-based optimisation of chemical processes. All these aspects make an important contribution to the continuous innovation activities referred to as the technology push.
- The second factor in innovation is market pull. This is based on the desire of customers to obtain higher-quality products at a lower price, or products with a new functionality or improved properties. Thus product and process innovations are required to fulfill customer demand.
- The third driving force of innovation is society itself, as the production of a chemical is linked to the consumption of natural resources, and the production of necessary products also results in unwanted by-products and waste, which may be toxic and harmful to humans and nature. There is therefore a constant pressure from society to reduce the consumption of natural resources (material and energy use), to replace toxic and harmful materials, such as chlorine or hydrogen cyanide, by alternatives, and to avoid emissions responsible for climate change, such as CO₂.

Depending on the chemical product a different innovation strategy is required: For bulk chemicals, innovation is mainly focused on the *processes*, for highly sophisticated chemicals, innovative activities are primarily directed towards *process* developments and *product* innovation, whereas for the fine chemicals, which are sophisticated products with a low output, the focus is on *product* innovations. Examples of recent *product* innovations are the reduced wall thickness of plastic bottles, plastics liners for packaging systems, roofing tiles made of plastic instead of clay, and automobile headlights and windscreens made from polycarbonate. Examples of *process* innovations are the development of improved catalysts, membrane separation and membrane reactors, material and heat integration, and the combination of conventional production procedures with biological processes. In the chemical industry, the main targets of innovation are to

- (1) develop new products for new markets
- (2) adapt products to meet new demands
- (3) improve product quality
- (4) reduce the input of resources (material, energy)
- (5) reduce the amounts of by-products and waste
- (6) substitute or eliminate toxic and hazardous materials
- (7) make more use of renewables as energy and feedstock resources, and to
- (8) develop and implement recycling technologies which prevent downgrading.

This paper focusses on technical innovations in *production processes* and not on product-related innovations. We study the possibilities of reducing the material and energy consumption related to the production of organic intermediates. The technologies covered are either well-known and have already been implemented to some extent or they are newly commercialised processes which might become important in the future. On the other hand, innovations which are at the laboratory or pilot plant stage have been excluded. By combining current production figures with the respective saving potentials in specific terms, the importance of innovation can be determined.

Process innovation can contribute in two ways to the improvement of production processes. One path is the development of new process routes starting with different feedstocks but resulting in the same product; the other is the continuous improvement of existing process routes, e.g. by new catalysts or better energy integration. Large improvement possibilities are often identified when using systematic methods, e.g. Pinch Analysis for heat integration studies, a method dating back to 1979. As about two-thirds of the energy consumed in the chemical industry is used for thermal separation processes, a good thermal integration of distillation columns is very important in order to ensure a high energy efficiency of the sector. New developments have even extended Pinch Analysis to the analysis of mass transfer processes.

Technical Analysis

In the following, the energy saving potential related to advanced processes is studied for a selection of chemical intermediates, most of which are usually derived from ethylene and propylene feedstock, are taken. *Table 1* lists the production figures of the selected intermediates in Germany in 1995. The **Gross primary energy consumption to produce these intermediates amounted to about 423 PJ**. To estimate the potential savings, different existing processes and innovative alternatives were analysed. As the main sources for process data, we used our own compilation for 50 chemical intermediates /Patel, Eichhammer et al. 1998/ and the results of a subcontract placed with Chem Systems /Chem Systems 1998/. Gross primary energies for precursors were taken from a number of sources, including /APME-Ecoprofiles/, /BUWAL 1995/, /Kindler, Nikles 1980/ or are based on own calculations.

For five of the twelve products included in *Table 1* high saving potentials have been determined. For these products a short description of the production processes is given in the following. A more detailed discussion on these products and on the other intermediates can be found in /Patel et. al., 1999/.

Table 1: *Production of intermediate products (selection) in Germany, 1995 /StaBu 1996/*

Product	Formula	Production in kt
Vinyl chloride (VC)	C ₂ H ₃ Cl	1380
Propylene oxide (PO)	C ₃ H ₆ O	684
Phenol	C ₆ H ₆ O	587
Ethylene oxide (EO)	C ₂ H ₄ O	698
Ethylene glycol (EG)	C ₂ H ₆ O ₂	278
Ethyl alcohol (Ethanol)	C ₂ H ₆ O	166
Acrylonitrile	C ₃ H ₃ N	427
Styrene	C ₈ H ₈	1081
Acetaldehyde	C ₂ H ₄ O	386
Hexamethylenediamine (HMDA) ¹	C ₆ H ₁₆ N ₂	0
Acetic acid	C ₂ H ₄ O ₂	474
Cumene ²	C ₉ H ₁₂	450

Propylene oxide (PO)

For the production of propylene oxide three main production schemes are analysed. In Germany all propylene oxide is produced by the chlorohydrin process. Two other process routes to propylene oxide are available on an industrial scale. In both processes large amounts of by-products are formed. Starting from ethylbenzene, about 2.5 t of styrene are produced per tonne of propylene oxide. If isobutane is used as feedstock, 2.5 t of t-butyl alcohol is produced as a by-product. To compare the different processes, it is therefore necessary to take the Gross primary energy of the by-products into account. A comparison of the manufacture via the chlorohydrin and the styrene process shows that the Gross primary energy of propylene oxide is about 30% lower for the styrene process. Therefore a large improvement potential exists in Germany, as all propylene oxide is produced via the chlorohydrin process route. Considering the ratio of the amounts of styrene and propylene oxide consumed in Germany (1081 kt / 684 kt = 1.6 in 1995), it might be not sensible to convert the total production capacity to the co-product process, as in this case too much styrene would be produced at present consumption levels. Further obstacles to the implementation of the styrene process are the large area requirements and equipment size and the risk of explosion.

The process starting from isobutane requires higher Gross primary energy values in comparison to the other two processes. In addition, it entails large investments, and it is only economically viable if integrated into a refinery complex.

Two further processes, which are not yet available on an industrial scale, are the direct oxidation of propylene and the manufacture from propionic acid and hydrogen peroxide. For the latter which is still under development the economics will depend strongly on the price of hydrogen peroxide. The direct oxidation process, which is also used for the production of ethylene oxide, is close to commercialisation. For both processes no detailed plant data are available. Therefore, the calculation of the Gross primary energy is not possible.

Phenol

In Western Europe (1989) about 95% of the phenol is produced from cumene using the Hock process. The remaining 5% is mainly produced by the oxidation of toluene. The Gross primary energy for phenol obtained via the oxidation of toluene (106.7 GJ/t_{phenol}) is about two times higher than for the cumene oxidation process. An important advantage of the toluene process is that only minor quantities of by-products are produced. The relation of by-product acetone and main product phenol in the Hock process is about 0.61. Comparing the relation between the total production figures of the two chemicals in Germany (383 kt_{acetone} / 587 kt_{phenol} = 0.65) it is obvious that the production of by-product acetone could in principle be absorbed by the market.

¹ Consumption of HMDA was about 161 kt (1995) but all HMDA was produced outside of Germany.

² Estimated production based on cumene consumption and foreign trade.

To determine the potentials of process innovation, we compared different process data sets for the Hock process. According to our calculations, Gross primary energy improvements of about 12.1 GJ/t of phenol are possible. This is mainly due to better energy integration which can lower the Gross primary energy of the process energy by about 40% (cf. *Table 2*). By reducing the amount of light and heavy hydrocarbons produced as unwanted by-products, the required feedstock material can be reduced accordingly, but this will have only a small effect on the Gross primary energy of phenol, as the hydrocarbons can be used to supply the process with energy.

Table 2: Gross primary energy for the production of phenol

Process	Gross primary energy [GJ/t Phenol]		
	Cumene-Oxidation (Hock-process)	Cumene-Oxidation (Hock-process; advanced)	Toluene-Oxidation
raw materials	77.0	81.5	65.6
process energy	18.2	29.4	41.6
by-products	-37.7	-41.3	-0.5
Total	57.5	69.6	106.7

Ethylene glycol (EG)

Ethylene glycol is mainly produced from ethylene oxide by hydration, and production is usually linked to the production of ethylene oxide. As the reaction of ethylene oxide to ethylene glycol shows a high product yield, only small differences in the Gross primary energy of the *feedstock* can be identified when comparing existing processes. The main difference in the Gross primary energy of ethylene glycol is caused by the large differences in *process energy consumption* of the hydration step, which can be in the range of 10 GJ/t_{EG}. This is caused by the large excess of water (about 20 times the quantity as needed for the reaction) to avoid the unwanted by-products di- and tri-ethylene glycol. Depending mostly on the energy consumption for the separation of water and ethylene glycol, the Gross primary energy for the production can be reduced from 53.0 to 42.9 GJ/t_{EG} (19%). Therefore innovation is required for low energy separation processes, e.g. by using membranes or by the development of highly integrated distillation systems. Savings can also be achieved, if higher concentrations of di-ethylene glycol can be accepted as it may be marketed as a second product.

Due to the high energy intensity of the process, a lot of new routes to ethylene glycol are being discussed. At the end of the seventies, the production by direct oxidation of ethylene was discussed, but was abandoned due to corrosion problems. Given the progress in materials science, it may be interesting to reconsider this process. A second alternative might be the production of ethylene glycol from carbon monoxide and hydrogen (synthesis gas). The disadvantage of this reaction is the high operating pressure required to reach acceptable reaction rates. To reduce the water excess for the production process, the use of ethylene carbonate as a feedstock (synthesised from carbon dioxide and ethylene oxide) is also being discussed. This would allow to cut the water excess by half.

Styrene

The production of styrene by dehydrogenation of ethylbenzene is an endothermic reaction taking place at temperatures of about 600°C. The second route which is being applied commercially is the production of styrene with the co-product propylene oxide (see above). The co-product process has a share of about 10% in the world market. Process temperatures are in the range between 130 and 250 °C and therefore lower than for the dehydrogenation of ethylbenzene. The capital investment for the co-product process is about 3.5 times larger than for the dehydrogenation process. A comparison based on the available data for the co-product process /Overtoom, 1998/ shows that the Gross primary energy consumption of this process is about 10.8 to 17.3 GJ/t_{Styrene} lower than for the dehydrogenation process. Compared to the dehydrogenation of ethylbenzene, a reduction potential for Gross primary energy of 6.51 GJ/t_{Styrene} is identified for the co-product process. 72% or 4.7 GJ/t_{Styrene} of this reduction are related to more efficient use of energy in the process. As the level of energy consumption is still very high, further improvements are realistic in the near future /Meili,

1998/. To reduce costs, new process ideas focus mainly on the replacement of ethylbenzene as feedstock for the styrene production. The raw material ethylbenzene make up about 65 % of total production costs. Feedstocks being discussed are toluene and pyrolysis gasoline. As toluene has a Gross primary energy close to ethylbenzene, this will not influence the Gross primary energy of styrene significantly.

Cumene

Cumene is mainly produced from benzene and propylene via the alkylation of benzene. For confidentiality reasons production figures for Germany are not available from official statistics (only two producers in Germany). A first estimate of the production can be made by analysing the fields of application for cumene by taking into account foreign trade (for which data are available). This results in cumene consumption figures of 350 kt for the production of phenol resins, 170 kt for the production of epoxide resins and 270 kt for the production of polycarbonates. As these are the dominant uses, the total cumene consumption in Germany is about 800 kt. Imports (1.2 kt) and exports (8 kt) can be neglected.

Large differences in feedstock and energy consumption can be observed, when present process specifications are compared. The difference in the Gross primary energy between the CD process (ABB Lumus) and the UOP process is about 19.6% or 13.49 GJ/t_{Cumene}. The CD process has a lower feedstock consumption (56.34 compared to 64.67 GJ/t_{Cumene}) and generates small amounts of excess steam (-1.01 GJ/t_{Cumene}) whereas the UOP process is a net process energy consumer (4.15 GJ/t_{Cumene}). Other processes with higher excess steam rates seem to be possible (e.g. Mobil/Badger) but since no detailed data on feedstock consumption are available, it is not possible to calculate the Gross primary energy for these options. However, data are available for the process energy requirements (-2.12 GJ/t_{Cumene}) according to which the process produces much more excess steam which can be exported from the plant.

Results and Conclusions

Process innovations and their effect on the Gross primary energy of 12 intermediate products have been analysed. **Table 3** shows the saving potentials identified. To calculate the reduction potential based on production figures for 1995, we have assumed that only half of the calculated potential we identified can actually be realised, due to practical constraints and the distribution of consumption figures of existing plants. For the production of cumene we have used a corrected production figure to avoid the double accounting for the production of cumene. Part of the cumene production accounted for in the production statistics is further converted to phenol and the process data we used for phenol production already include this process step. Moreover, totally new process routes could not be taken into account, as detailed process data were not easily available. For these reasons, the calculated values represent a relatively low estimate of possible improvements.

In addition the calculated savings only reflect the potential in the last step of production, which however, is expressed as a fraction of the entire energy requirements including the feedstock and the whole process chain from cradle to product (Gross primary energy). As a consequence, a whole range of improvement options have not been taken into account, e.g. efficiency improvements in the supply of precursors and auxiliaries, of steam and electricity. The inclusion of the potentials in these areas would require a separate analysis. Based on the results of other studies (e.g. /IKARUS/), we would expect the total improvement potential, excluding feedstocks, to amount to at least 20%. If feedstocks are included in the calculations, an overall saving potential higher than 10% seems to be realistic.

Table 3: Saving potentials due to process innovations considering 50% of the theoretical savings.

Product	Production (StaBu, 1996) [kt]	Total [PJ/a]	Gross primary energy consumption Saving potential	
			[PJ/a]	[%]
Vinyl chloride (VC)	1380	71.2	4.2	5.9
Propylene oxide ¹⁾ (PO) + Styrene	684 +1081	145.8	10.0	(6.9)
Phenol ²⁾	587	37.3	3.6	9.5
Ethylene oxide (EO)	698	40.2	0.2	0.5
Ethylene glycol (EG)	278	13.3	1.4	10.5
Ethyl alcohol ³⁾ (Ethanol)	166	11.2	N/A.	N/A.
Acrylonitrile	427	39.1	1.2	3.1
(Styrene) ⁴⁾	(1081)	(74.6)	(3.5)	(4.7)
Acetaldehyde	386	18.2	0.4	2.1
Hexamethylenediamine (HMDA)	0	--	--	--
Acetic acid ⁵⁾	474	19.2	0.1	0.6
Cumene	450	27.9	3.0	10.9
Total ⁶⁾ (1995)	6611	423.4	24.1	5.7

¹⁾ The calculated saving potential is based on assuming the maximum use of the oxiran process. For a production of 684 kt PO and 1081 kt styrene a part of the PO (193 kt) has to be produced with the chlorohydrin process. The relative saving potential is therefore a function of the assumed mix of the two products.

²⁾ Phenol is typically produced from Cumene. To avoid double counting of potentials, the Cumene production was reduced by the Cumene used for Phenol production.

³⁾ Due to insufficient process data available the potential could not be calculated.

⁴⁾ The saving potentials linked to Styrene production are accounted for together with PO production.

⁵⁾ Potential if the production is shifted completely to the process route via Acetaldehyde.

⁶⁾ Without separate potential for Styrene production.

The production of intermediate products included in this analysis amounts to about 6.6 Mio. tonnes. Total Gross energy consumption for the production is about 424 PJ. Compared to the value of 1800 PJ (1000 PJ/yr for raw materials and 800 PJ/yr for process energy) for the total production of the chemical industry, including the non energy use, the products included in this analysis account for 24%. Based on the analysis (cf. **Table 3**) 24.1 PJ/yr or 5.7% of the Gross primary energy can be saved, if the process innovations for these products will be adopted more widely by industry. Based on these savings in Gross primary energy, the savings of CO₂ emissions can be calculated. The saving of 24.1 PJ/yr is equivalent to a reduction of emissions of 1.6 million tonnes of CO₂ per year.

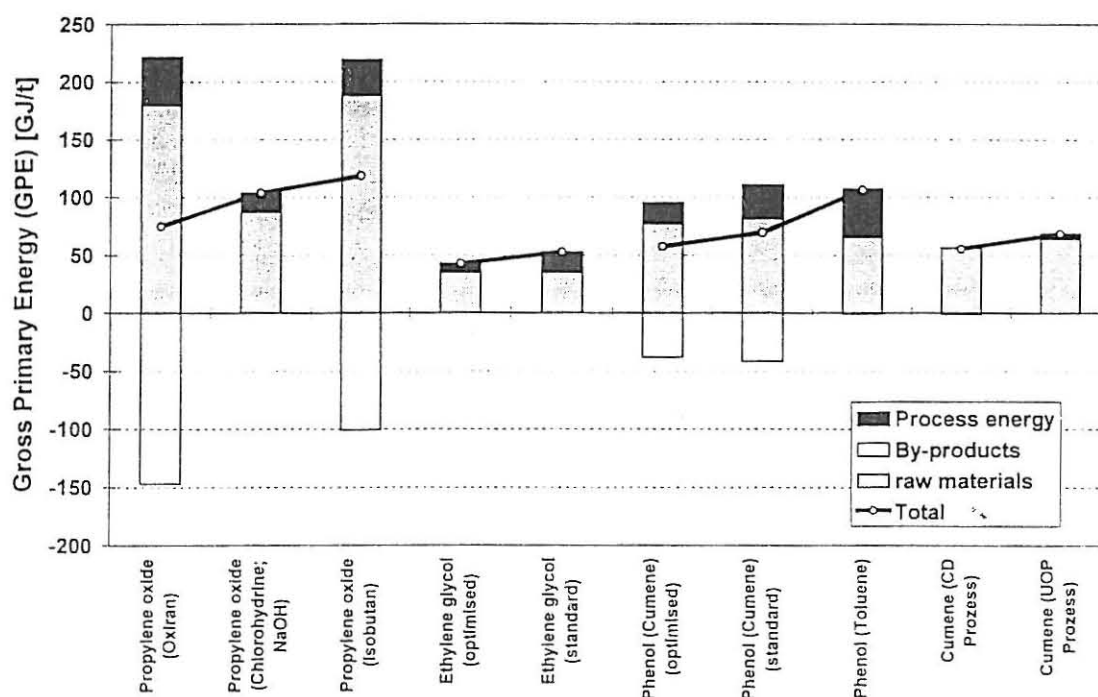


Figure 1: Comparison of Gross primary energy for processes with high improvement potential.

Figure 1 summarises the calculation results for the processes with high improvement potentials. For these processes, realistic saving potentials are in range of 10% or higher. Since the total production costs of most of these products are strongly related to energy costs, it seems obvious that the adoption of new or improved processes with lower Gross primary energy values will not only be advantageous in reducing CO₂ emissions, but will also be interesting from an economic point of view.

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