1
Introduction

Process Development. From the Initial Idea to the Chemical Production Plant. G. Herbert Vogel

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1.1
The Goal of Industrial Research and Development

In the chemical industry (Figure 1-1) about 7% of turnover is spent on research and development [Jarhbuch 1991, VCI 2000, VCI 2001] (Table 1.1 and Appendix 8.16). This sum is of the same order of magnitude as the company profit or capital investment. The goal of research management is to use these resources to achieve competitive advantages [Meyer-Galow 2000]. After all, the market has changed, from a national sellers' market (demand > supply) to a world market with ever-increasing compe-tion. This in turn has affected the structure of the major chemical companies. In the 1990s integrated, highly diversified companies (e.g., Hoechst, ICI, Rhone-Poulenc) developed into specialists for bulk chemicals (Dow/UCC, Celanese), fine and specialty chemicals (Clariant, Ciba SC), and agrochemical and pharmaceutical formulations (Aventis, Novartis) [Felcht 2000, Perlitz 2000].

Unlike consumer goods such as cars and clothes, most commercial chemical products are "faceless" (e.g., hydrochloric acid, polyethylene), and as a rule the customer is therefore only interested in sales incentives such as price, quality, and availability. All the research activities of an industrial enterprise must therefore ultimately boil down to three basic competitive advantages, namely, being *cheaper* and/or *better* and/or *faster* than the competitor. The AND combination offers the greatest competive advantage and is thus known as the world-champion strategy. However, more often one must settle for the OR combination. The qualitive term *cheaper* can be quantified by means of a *production cost analysis*. Initially, it is sufficient to examine the coarse structure of the production costs. Thus, each item in Table 1-2 can be analysed individually and the

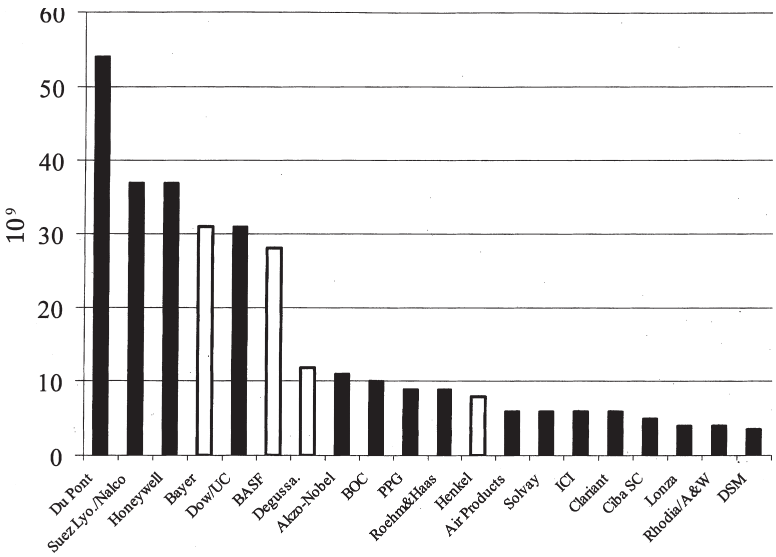

Fig. 1-1 Market capital of major chemical companies [Mayer-Galow 2000].

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Tab. 1-1 Growth of the German chemical industry [VCI 2001].

	1990	1995	1996	1997	1998	1999	2000
Turnover (10^9 EURO)	83.5	92.1	89.5	96.6	95.8	97.1	108.6
Employees in thousands	592	536	518	501	485	478	470
Investment in material goods	6.5	5.8	6.4	6.4	6.9	6.9	7.2
R&D experditure (10^9 EURO)	5.4	5.3	5.8	6.1	7.0	7.3	7.9

Tab. 1-2 Coarse structure of production costs.

	Materials costs	
	Energy costs	variable costs (production-dependent)
	Disposol costs	
	Personnel costs	
	Workshop costs	fixed costs (production-independent)
	Depreciation	
	Other costs	
Σ	Production costs	

total system optimized. The competive advantage *better* now refers not only to availability and product quality, but also to the environmental compatibility of the process [Gärtner 2000], and the quality assurance concept, delivery time, and exclusivity of the supplier, etc.

1.2 The Production Structure of the Chemical Industry

If the production structure of the chemical industry is examined [Petrochemie 1990, BASF 1999, Petzny 1999], it is seen that there are only a few hundred major basic products and intermediates that are produced on a scale of at least a few thousand to several million tonnes per annum worldwide.This relatively small group of key products, which are in turn produced from only about ten raw materials, are the stable foundation on which the many branches of refining chemistry (dyes, pharmaceuticals, etc.), with their many thousands of often only short-lived end products, are based [Amecke 1987]. This has resulted in the well-known chemical family tree (Figure 1-2), which can also be regarded as being synonymous with an intelligent integrated production system, with synergies that are often of critical importance for success.

A special characteristic of the major basic products and intermediates is their longevity. They are statistically so well protected by their large number of secondary products

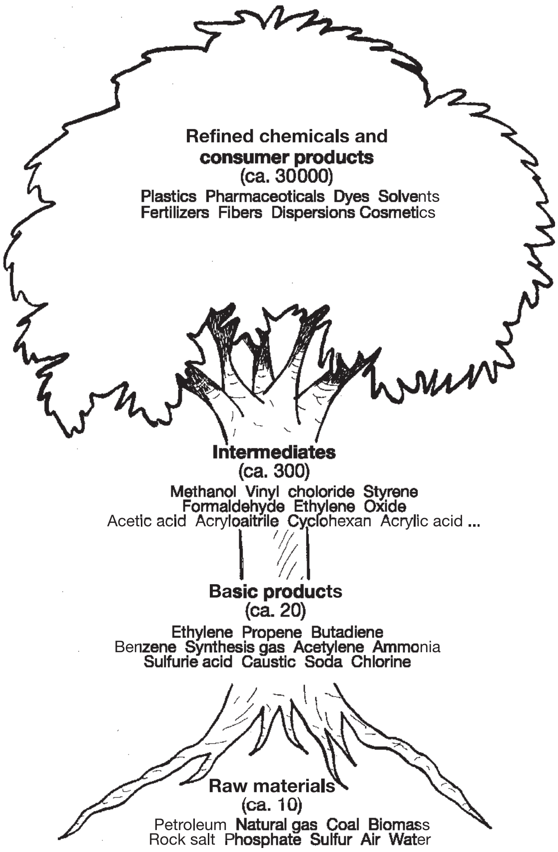

Fig. 1-2 Product family tree of the chemical industry: starting from raw materials and progressing through the basic products and intermediates, to the refined chemicals and final consumer products, as well as specialty chemicals and materials [Quadbeck 1990, Jentzsch 1990, Chemie Manager 1998, Raichle 2001].

and their wide range of possible uses that they are hardly affected by the continuous changes in the range of products on sale. Unlike many end products, which are replaced by better ones in the course of time, they do not themselves have a life cycle. However, the processes for producing them are subject to change. This is initiated by new technical possibilities and advances opened up by research, but is also dictated by the current raw material situation (Figure 1.3, Table 1.3).

In the longer term, an oil shortage can be expected in 40 to 50 years, and this will result in increased use of natural gas. The fossil fuel with the longest future is coal, with reserves for more than 500 years. The question whether natural gas reserves in the form of methane hydrate, in which more carbon is stored than in other fossil raw materials, will be recoverable in the future cannot be answered at present, since these lie in geographically unfavorable areas (permafrost regions, continental shelves of the oceans, deep sea).

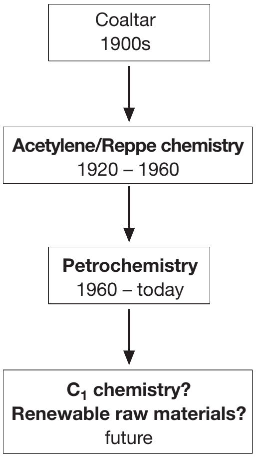

Fig. 1-3 How the raw material base of the chemical industry has changed with time [Graeser 1995, Petzny 1997, Plotkin 1999, Van Heek 1999].

In the case of *basic products* and *intermediates* it is not the individual chemical product but the production process or technology which has a life cycle. For example, Figure 1-4 shows the life cycles of the acrylic acid and ethylene oxide processes [Jentzsch 1990, Ozero 1984]. To remain competetive here the producer must be the price leader for his process. Therefore, strategic factors for success are [Felcht 2000]:

- Efficient process technology
- Exploiting economy of scale by means of world-scale plants

Tab. 1-3 World production (in 10^6 t/a) of the most important energy and raw materials sources.

	1994	1997
Fossil raw materials		
Coal	3568	3834
Oil	3200	3475
Lignite	950	914
Natural gas [10^9 m^3]	*2162***)*	*2300***)*
Renewable raw materials		
Cereals	1946	1983
Potatoes	275	295
Pulses	57	55
Meat	199	221
Sugar	111	124
Fats (animal and plant)	/	ca. 100

*) 1 t SKE (German coal unit) = 882 m^3 Natural gas = 0.7 t oil equivalent = 29.3×10^6 kJ

- Employing a flexible integrated system at the production site
- Professional logistics for large product streams.

The demands made on process development for *fine chemicals* differ considerably from those of basic products and intermediates (Figures 1-5 and 1-6). In addition to the

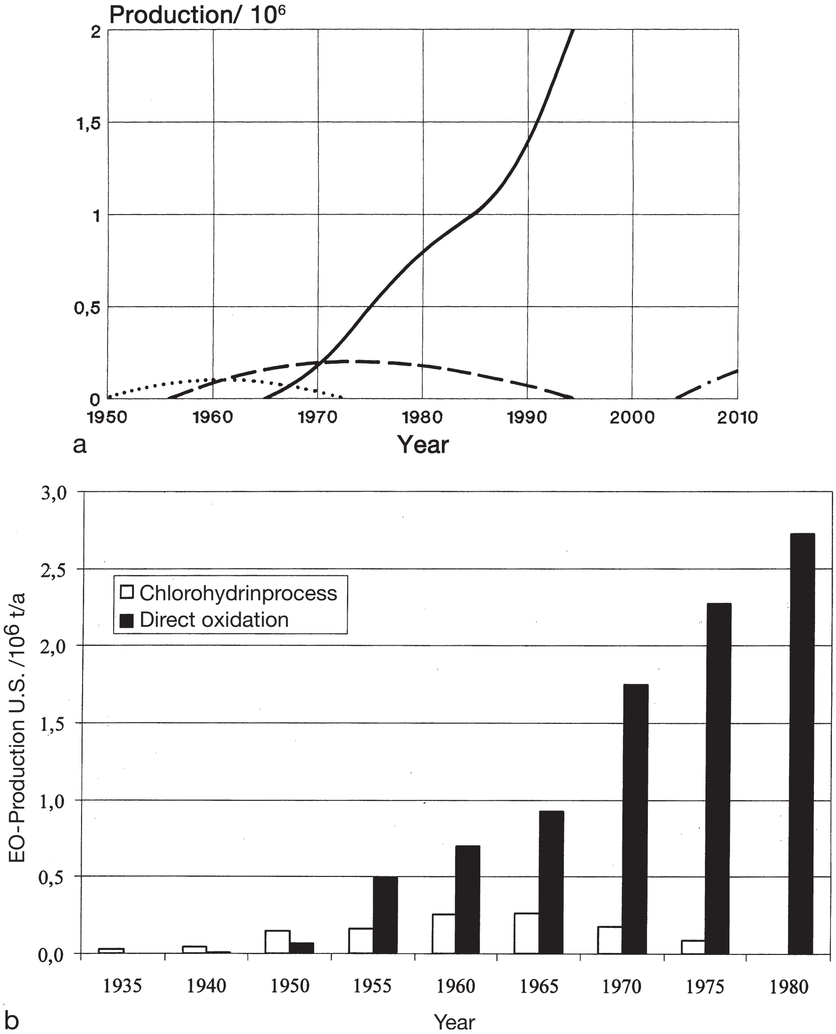

Fig. 1-4 Life cycles of production processes
a) Acrylic acid processes
. . . . Cyanohydrin and propiolactone processes
Reppe process
– – – – – – Heterogeneously catalyzed propylene oxidation
(2000: 3.456 × 10^6 t, 2003 (estimated): 4.8 × 10^6 t [Vogel 2001])
–·–·–·–·– New process ?
b) Ethylene oxide process.

above-mentione boundary conditions of better and/or cheaper, *time to market* (production of the product at the right time for a limited period) and *focused R & D effort* are of importance here. Only a few fine chemicals, such as vanillin, menthol, and ibuprofen, reach the scale of production and lifetime of bulk chemicals. Futher strategic factors for success are [Felcht 2000]:

- Strategic development partnerships with important customers
- The potential to develop complex multistep organic syntheses
- A broad technology portfolio for the decisive synthetic methods
- Certified pilot and production plants
- Repuatation as a competent and reliable supplier.

Specialty chemicals are complex mixtures whose value lies in the synergistic action of their ingredients. Here the application technology is decisive for market success. The manufacturer can no longer produce all ingredients, which can lead to a certain state of dependence. Strategic factors for successful manufacturers are [Felcht 2000, Willers 2000]:

- Good market knowledge of customer requirements.
- A portfolio containing numerous *magic ingredients*
- Good technical understanding of the customer systems
- Technological breadth and flexibility.

Active substances such as pharmaceuticals and agrochemicals can only be economically marketed while they are under patent protection, before suppliers of generic products enter the market. Therefore, producers of such products cannot simply concentrate on costly research. As soon as possible after clinical trials and marketing approval, worldwide sales of the product must begin so that the remaining patent time can be used for

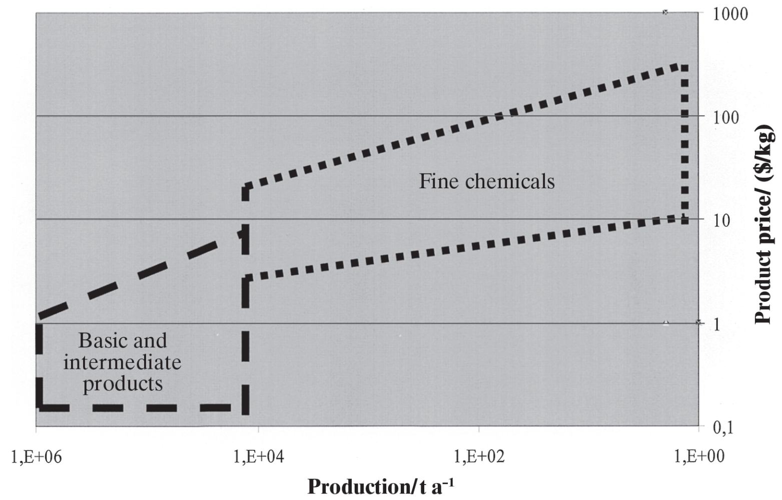

Fig. 1-5 Order of magnitude of product prices as a function of production volume for basic products and intermediates and for fine chemicals [Metivier 2000].

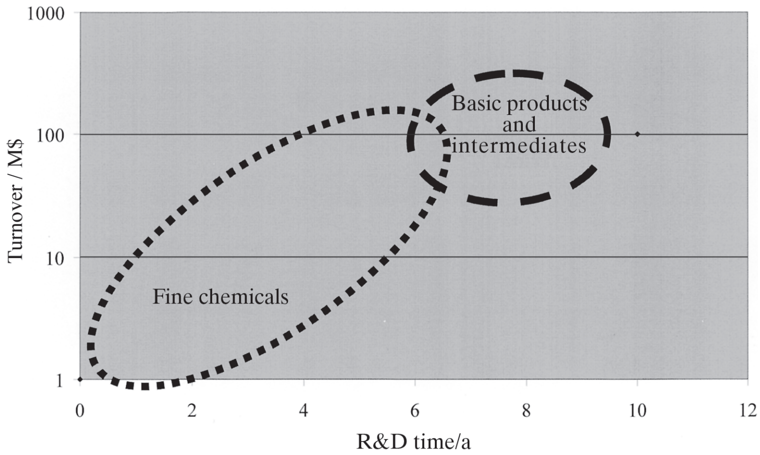

Fig. 1-6 Comparison between bulk and fine chemicals with regard to turnover and the development time of the corresponding process [Metivier 2000].

gaining customers. In contrast, the actual chemical production of the active substance is of only background importance. The required precursors can be purchased from suppliers, and the production of the active substance can be farmed out to other companies. Strategic factors for success of active substance manufacturers are [Felcht 2000]:

- Research into the biomolecular causes of disease and search for targets for pharmacological activities
- Efficient development of active substances (high-throughput screening, searching for and optimizing lead structures, clinical development)
- Patent protection
- High-performance market organization.

Enterprises which already have competitive advantages must take account of the *technology S curve* [Marchetti, 1982, Marquadt 1999] in their research and development strategy (Figure 1-7). The curve shows that as the research and development expenditure on a given technology increases, the productivity of this expenditure decreases with time [Krubasik 1984]. If enterprises are approaching the limits of a given technology, they must accept disproportionately high research and development expenditure, with the result that the contribution made by these efforts to the research objectives of *cheaper* and/or *better* becomes increasingly small, thereby always giving the competitor the opportunity of catching up on the technical advantage. On the other hand, it is difficult for a newcomer to penetrate an established market. But, as Japanese and Korean companies have shown in the past, it is not impossible. Figure 1-8 shows the so-called learning curve for a particular chemical process. It is a double-logarithmic plot (power law $y = x^n$) of the production cost as a function of the cumulative production quantity, which can be regarded as a measure for experience with the process. With increasing experience the production costs of a particular product drop. How-

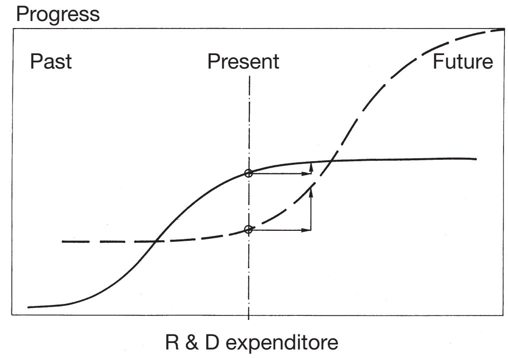

Fig. 1-7 The technology S curve [Specht 1988, Blumenberg 1994]: The productivity of the research and development expenditure increases considerably on switching from basic technology (——) to a new trend-setting technology (– – –).

ever, an overseas competitor who can manufacture the same product in a new plant with considerably lower initial cost can catch up with the inland producer who has produced 10×10^6 t after only about 100 000 t of production experience (Figure 1-8), and can then produce more cheaply.

Once an enterprise has reached the upper region of the product or technology S curve, the question arises whether it is necessary to switch from the standard technology to a new *pace-setting technology* in order to gain a new and sufficient competitive advantage [Perlitz 1985, Bönecke 2000]. Figure 1-7 depicts this switch to a new technology schematically and shows that on switching from a basic technology to a new pace-setting technology, the productivity of the research and development sector increases appreciably, and substantial competitive advantages can thus be achieved [Miller 1987, Wagemann 1997].

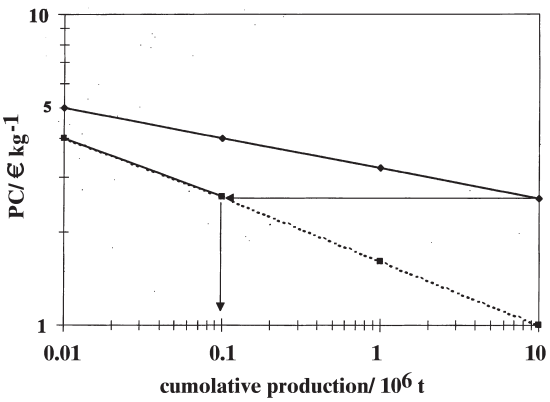

Fig. 1-8 Learning curve: production costs (PC) as a function of cumulative production, which can be regarded as measure of experience with the process, in a double-logarithmic plot [Semel 1997]: diamonds: inland producer, squares: overseas competitor (for discussion, see text).

The potential of old technologies for the development of cheaper and/or better is only small, whereas new technologies have major potential for achieving competitive advantages. It is precisely on this innovative activity that the prosperity of highly developed countries with limited raw material sources such as Germany and Japan is based, since research represents an investment in the future with calculable risks [Mittelstraß 1994], whereas capital investments in the present are based on existing technology.

To assess whether a research and development strategy of better and/or cheaper is still acceptable in the long term for a given product or production process, the R & D management must develop an *early warning system* [Collin 1986, Jahrbuch 1991, Steinbach 1999, Fild 2001] that determines the optimum time for switching to a new product or a new technology [Porter 1980, Porter 1985]. Here it is decisive to have as much up-to-date infomation on competitors as possible. This information can be obtained not only from the patent literature but also from external lectures, conferences, company publications, and publicly accessible documents submitted to the authorities by competitors (Section 3.5). Since industrial research is very expensive, instruments for controlling the research budget are required [Christ 2000, Börnecke 2000, Kraus 2001], for example:

- A cost/benefit analysis for a particular product area, whereby the benefit is determined by the corresponding user company sector.
- A portfolio analysis (Section 3.8) to answer the questions:
  - Where are we now?
  - Where do we want to be in 5 or 10 years?
  - What do we have to do to now to get there?
- An ABC analysis for controlling the R&D resources, based on the rule of thumb that
  - 20% of all products account for 80% of turnover, or
  - 20% of all new developments acccount for 80% of the development costs.

It is therefore important to recognize which 20% these are in order to set the appropriate priorities (A = important, profitable, high chance of success; B = low profitability; C = less important tasks with low profitability).

The way in which chemical companies organize their research varies and depends on the product portfolio [Harrer 1999, Eidt 1997]. Mostly it involves a mixture of the two extremes: pure centralized research on the one hand, and decentralized research (research exclusivelyin the company sectors) on the other [Hänny 1984].

1.3 The Task of Process Development

The task of process development is to extrapolate a chemical reaction discovered and researched in the laboratory to an industrial scale, taking into consideration the economic, safety, ecological, and juristic boundary conditions [Harnisch 1984, Semel 1997, Kussi 2000]. The starting point is the laboratory apparatus, and the outcome of development is the production plant; in between, process development is required. The following account shows how this task is generally handled. Although the sequence of steps in the development process described is typical, it is by no means obligatory, and it is only possible to outline the basic framework.

1.4 Creative Thinking

Numerous methods for creative thinking are described in the literature [Schlicksupp 1977, Börnecke 2000]. In the daily routine of work there simply is no time for important things such as coming up with ideas for new processes and products. Therefore, every year plans shoud be made in advance for:

- Visiting conferences, including ones that are outside of one's own specialist area
- Visiting research establishments (institutes, universities, etc.)
- Excursions to companies
- Regular discussions with planners and heads of department.

Here intensive discussions can lead to new ideas that can later be evaluated. Regular browsing in the literature can also be a source of inspiration.

Tab. 1-4 Creative methods for generating ideas [Schlicksupp 1977, Bornecke 2000, Kraus 2001].

Method group	Characteristics	Important representatives
Brainstorming its variations	Uninhibited discussion in which criticism is not permitted; fantastic ideas and spontaneous associations should be expressed	• Brainstorming • Discussion 66
Brainwriting Methods	Spontaneous writing down of ideas on forms or sheets; circulation of forms	• Features 635 • Brainwriting-pool • Ideas Delphi
Methods creative orientation	Following certain principles in the search for a solution	• Heuristic principles • Bionics
Methods of creative confrontation	Simulation of solution finding by confrontation with meaning contents that apparently have no correction to the problem	• Synectics • BBB methods • Semantic intuition
Methods of systematic structuring	Splitting the problem into partial problems; solving partial problems and combining to give a total solution; systematization of possible solutions	• Morphological box • Morphological Taublau? • Sequential morphology • Problem solving tree
Methods of systematic problem specification	Revealing the core questions of a problem by systematically and hierarchically structured approach	• Progressive abstraction • K-J-methods • Hypothese s matrix • Relevance tree