COST ANALYSES OF CHEMICAL MICRO PROCESSING FOR HIGHLY INTENSIFIED AND HIGH-VALUE RAW MATERIAL PROCESSES - REAL BUSINESS AND VIRTUAL CASES

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Abstract

As a result of its rapid development within the last years an increasing commercial interest on micro process engineering is given. Process intensification effects of this novel technology were clearly demonstrated. In this context, a generic cost view needs to be developed. As a first investigation, two generic cost analyses investigate here the profitability for two edge cases. One refers to dominance by raw materials, the other by the operator's salary. Both shares dominate the operational costs of a micro-chemical process, but in a varying extent. The write-downs of the investment costs, mainly consistent of the micro-reaction plant itself and the plant engineering, are of minor relevance. The first case study considered here focused on the synthesis of a high-value fine-chemical intermediate where raw-material costs outpaced even the high operator costs. The process under investigation is an economically conducted fine chemical process of the customized chemical producer AzurChem GmbH, the formation of the 4-cyanophenylboronic acid, using the benefits of micro process technology supplied by IMM GmbH [5] among others. This process was chosen since it is representative for several of this company's manufacturing processes of fine and specialty chemicals.

The other study refers to a highly intensified process, the aqueous Kolbe-Schmitt synthesis with reaction times being reduced by three orders of magnitude, from some hours to some tens of seconds [24]. Correspondingly, space-time yield and productivity were increased using this so-called high pressure and high temperature (high-p,T) micro processing concept. For a given productivity, the operator costs are notably reduced for the micro-chemical process as compared to a batch process. A detailed view on the different cost portions will be given and demonstrate how the variable and the total costs change. For both case studies, the impact of process intensification (e.g. by scale-out) and parallel operation (e.g. by numbering-up) are pointed out.

Introduction

Microstructured reactors and micro process engineering are highly promising valuable novel tools and processing approaches to enable process intensification, shared with further reactor and process engineering advantages such as process safety, legislation, or modularity [1, 2]. This intrinsically implies that there are business drivers for doing so and that cost analyses were performed internally in the chemical industry. With two exceptions, however, such knowledge is not disclosed. One of these is a study from the fine chemical and pharmaceutical company Lonza, Visp/Switzerland detailing on capital (CAPEX) and operational (OPEX) costs for several pilot micro-chemical processes [3]. Merck Company, Darmstadt/Germany made together with Technical University Clausthal a four-staged potential analysis, which started with a technological evaluation to come finally to a business view [4]. For the latter, data on profitability and amortization time were given.

A German public funded project has been started to evaluate the potential of chemical micro process engineering based on BASF's widely developed eco-efficiency analysis [6]. Jena University has applied life-cycle assessment analysis (LCA, [7]) to a micro-chemical process at laboratory scale [8] and recently reported on an investigation alike for the production scale for the same process [9]. An exergy analysis (see [10-12]) was made for microstructured fuel processor technology [13] and a generic benchmarking of microstructured catalytic reactors [14] was given, with the catalyst and overall reactor volume as the figures of merit.

However, a generic view is still missing, i.e. which type of microstructured reactors and which type of plants are suited for which type of chemical processing and what are the key figures to optimize micro-chemical processes. The virtual case of a highly intensified process, refers to a generic cost analysis for the synthesis of 2,4-dihydroxy benzoic acid which was performed at IMM following the successful transfer from the batch to the continuously working and highly intensified process in a pilot-scale microreaction plant [24].

In addition, there is no detailed description about cost analysis for a real business case. This is based here on a commercial process and product using high-value raw materials, performed in this degree of detailedness for the first time. The enterprise AzurChem GmbH, a spin-off of the Institut für Mikrotechnik Mainz GmbH (IMM), produces and sells fine and specialty chemicals, for researchers, developers and producers in chemistry and biotechnology. The above mentioned studies instead refer to theoretical or pilot processes under further optimization, as far as information is disclosed [5].

Methodology of the Cost Analysis

The methodology used is based on the determination of the variable and the fixed costs, roughly corresponding to the CAPEX and OPEX costs, respectively. In a second step all variable costs have to be related to a certain amount of the manufactured product to get comparable values. Variables costs that have been taken into account are raw-material supply, waste disposal, operator's salaries, energy consumption and transport, but the latter could be neglected in our case.

The method used for the determination of the fixed costs is a simplified analysis of fixed cost absorption. Hereby the fixed costs are only divided into the product-related fixed costs and the remaining fixed costs. Normally, the remaining fixed costs are further divided depending on the level where they arise, e.g. product line, division or company related fixed costs. But in our case of a small start-up company (and a similar assumption in the virtual case) this was not useful.

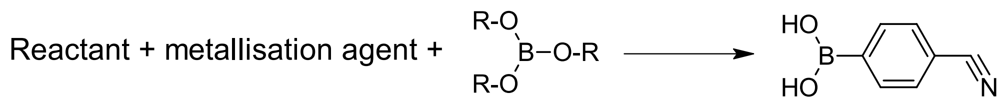
Product-related fixed costs are mainly the equipment costs which encompass as well the existing micro reaction plant including the microstructured reactor, pumps, valves and piping, measurement and control technology, thermostats/cryostats and installation costs as the necessary devices for the purification, e.g. a distillation unit. These costs have to be divided by the depreciable life and then they are summarized with the annual maintenance costs and the annual costs for premises.

After the cost analysis of the existing process was done a benchmarking by comparison with a conventional process which is a batch process was performed. In order to get information about potential improvements and their influence on the manufacturing costs some case scenarios were investigated. These scenarios base firstly on higher yield enabled by an optimized process, secondly on higher throughput by "smart dimensioning" alternatively to or combined with an internal numbering-up. The third possibility is the external numbering-up, e.g. several reactor lines operate in parallel.

Cost Analysis of the Commercial Manufacturing Process of 4-Cyanophenylboronic Acid

Process and Plant

Boronic acids are used as intermediates for the synthesis of pharmaceuticals and fine chemicals, e.g. for Suzuki couplings. High-value boronic acids are within the product portfolio of AzurChem GmbH besides other precious fine chemicals. As representative of this class of chemical intermediates, the manufacturing process of the 4-cyanophenylboronic acid was chosen to be investigated.



One key feature of the reaction is the high price of the raw materials and respectively of the chemical product 4-cyanophenylboronic acid; therefore the process is characterized in the following as dominated by the high-value raw materials

A basic flow sheet of the continuous working micro reaction plant used for the investigated manufacturing process is shown in Figure 1. The reactants and the quenching substance are pumped from reservoirs to the reactors. The first reaction step is performed in the microstructured reactor A, where the main reactant (primarily solved in a solvent) reacts with a metallisation agent. In the subsequent step (reactor B) a borate reacts with the resulting product mainly to the final product. The immersion of both reactors in a thermostatic bath guarantees a uniform tempering. Finally, the reaction is quenched in micro reactor C. The subsequent batch distillation purifies the crude product.

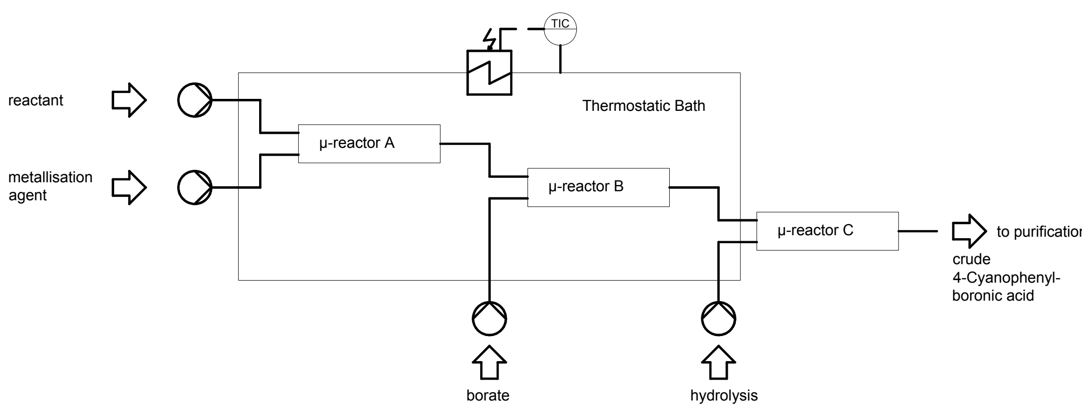


Figure 1. Simplified flow sheet of the reaction plant

Cost Analysis of the Realized Process

The following data were used for the determination of the variable costs: Costs for raw materials base on the purchase prices of AzurChem GmbH for one production period, in which 10 kg 4-cyanophenylboronic acid are manufactured and on an average yield of the process of 75% which could be achieved, including not only the reaction yield but also the loss of the product within the purification process. For the calculation of the operator's salary it is assumed that the supervision of the continuous working reaction plant can be done in parallel to the purification steps of the crude 4-cyanophenylboronic acid that takes place batch-wise. A daily working time of 8 hours, 5 days a week and 50 weeks per year is the base of the calculation. The energy costs are mainly limited to the electric power consumption of the thermostats and the pumps. Average energy costs of 0.25 €/kWh are used in the cost analysis.

With regard to the fixed costs an amortization period of 5 years was assumed in accordance with AzurChem GmbH's practice. Based on the fact that premises costs only have a marginal effect on the product related fixed costs they were obtained from estimated costs of 300 € for a laboratory per year and square meter multiplied with the required 3 m² floor space for micro reactor processing. In the case of a start-up company which is considered here the remaining fixed costs are unknown in detail, but as a realistic approach an overhead in terms of 50% of the variable and product related fixed costs was added.

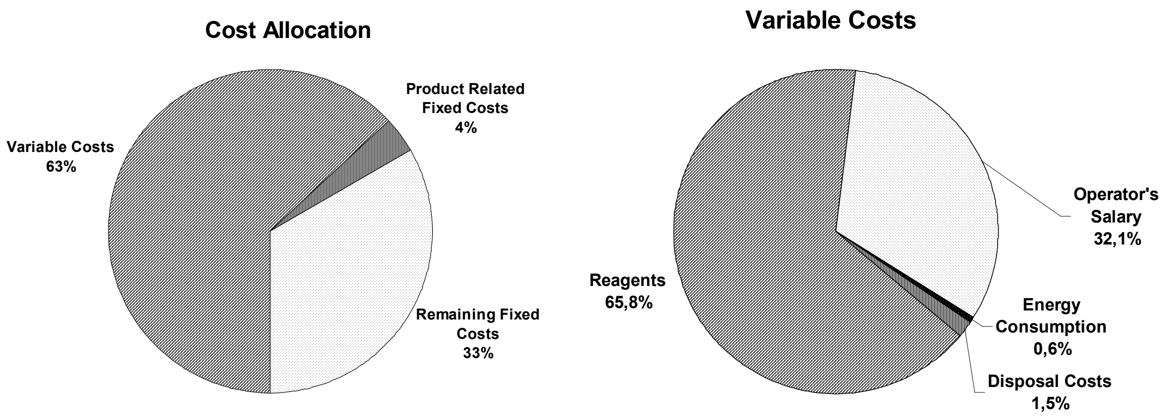


Figure 2. Total cost allocation of the realized process and shares of variable costs

Figure 2 points out the large portion of the variable costs amounting to 63% compared with the product related fixed costs of only 4%. The required high-value fine chemical raw materials and the large share of the operator's salary are therefore the reasons. Thus it is evident, that the investment costs for micro process equipment cannot be a major decision driver in this case, whereas suitable micro process engineering (also for future process optimization) directly affects the variable costs (Fig. 2 left).

The costs of the starting substances comprise 65.8% and the salary for the operator is 32.1%. Reaching together almost 98% they are the two major constituents of the variable costs The ratio between both is different compared with the afterwards considered Kolbe-Schmitt synthesis of 2,4-dihydroxy benzoic acid due to the high-cost starting substances used here (Fig. 2 right).

Comparison of the total costs and the influence of the plant scenarios for different case scenarios

When leveling the total costs of the real micro-chemical process to 100% (Fig. 3), the highest total costs arise from the virtual batch and amount to 133%. Three different scenarios with increased capacity show a dramatic decline in costs. Whereas the total costs for the micro-chemical process with fivefold capacity could be reduced to one third (33%) a further decline to 25% is enabled by tenfold higher capacity. Practicable ways to further increase profitability are provided both by process intensification and numbering-up.

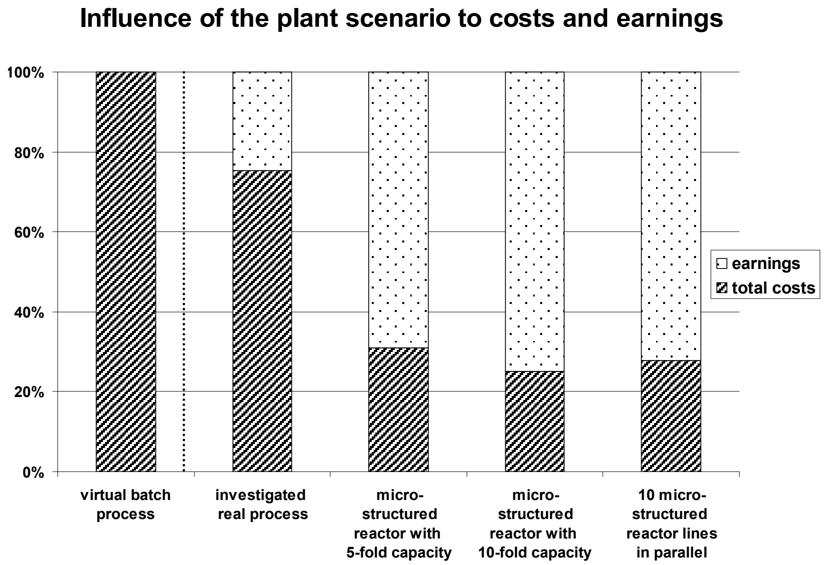


Figure 3. Comparison of total cost

A similar view is provided by the comparison of the ratios between manufacturing costs and earnings (Fig. 4). For all scenarios considered the theoretically attainable selling price was reduced in the same degree as the purchase prices were assumed. Under more realistic conditions of future competition, the selling price for such relatively large amounts of the product will probably even more fall. Nevertheless, these results also highlight possible cost advantages by using microstructured reactors with higher throughput, presumed the produced amounts can be sold on the market.

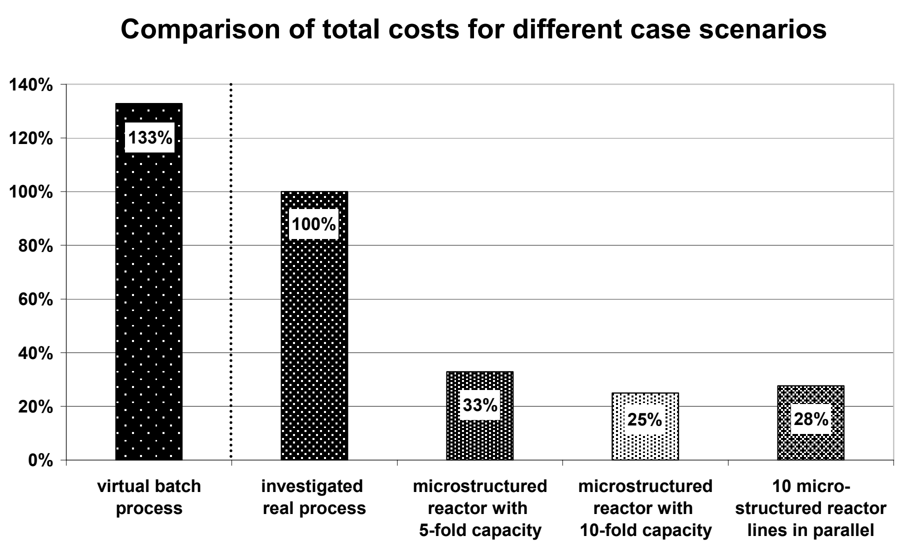
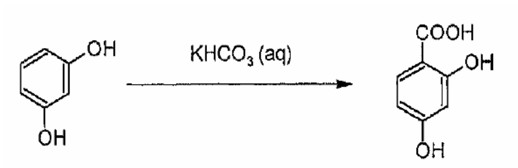


Figure 4. Influence of the plant scenarios

Cost Analysis of the Virtual Manufacturing Process of 2,4-dihydroxy benzoic acid

Process and Plant



The investigated process here is the aqueous Kolbe-Schmitt synthesis of 2,4-dihydroxy benzoic acid from resorcinol in an aqueous solution of potassium hydrogen carbonate under high temperature of 200 °C and high pressure of 40 bar in a continuous working microreaction plant (Fig. 5). The reaction times could be reduced by three orders of magnitude, from some hours for the batch process to some tens of seconds. The achieved selectivity was 45 % [24].

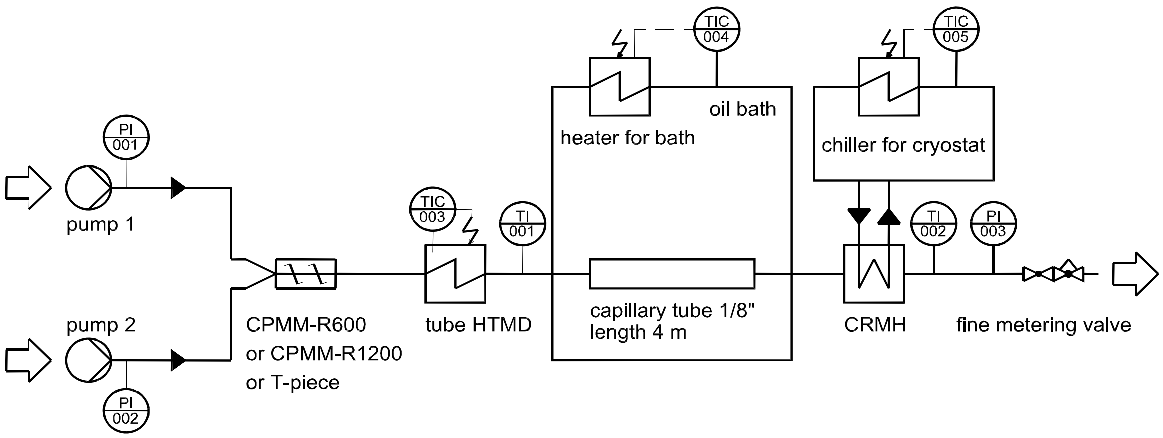


Figure 5. Flow sheet of the reaction plant

Cost Analysis of the Realized Process

The subsequent performed cost analysis should point out what the economic effects of this advanced technology are and highlight potential improvements. Since the aim of the investigations was not the manufacturing of a salable product it is only a "virtual" manufacturing process. For these reasons we considered the product related fixed costs only and disregarded the remaining fixed costs which depend from the company and not from the process itself. In contrast to the preceding cost analysis the purification costs of the rough product are not included here.

The base case is calculated with a five tube reactor allowing a theoretical production rate of 4.4 tons/year (assuming 8000 hours per year). The product related fixed cost of about 1 €/kg product, derived from the investment cost by dividing with the amortization time of 7 years, are very small compared with the operational costs of 91 €/kg product. The main and approximately equal portions of the operational costs are the raw material (prices for 25 kg units) and the operator's salary when a fourth manpower is assumed.

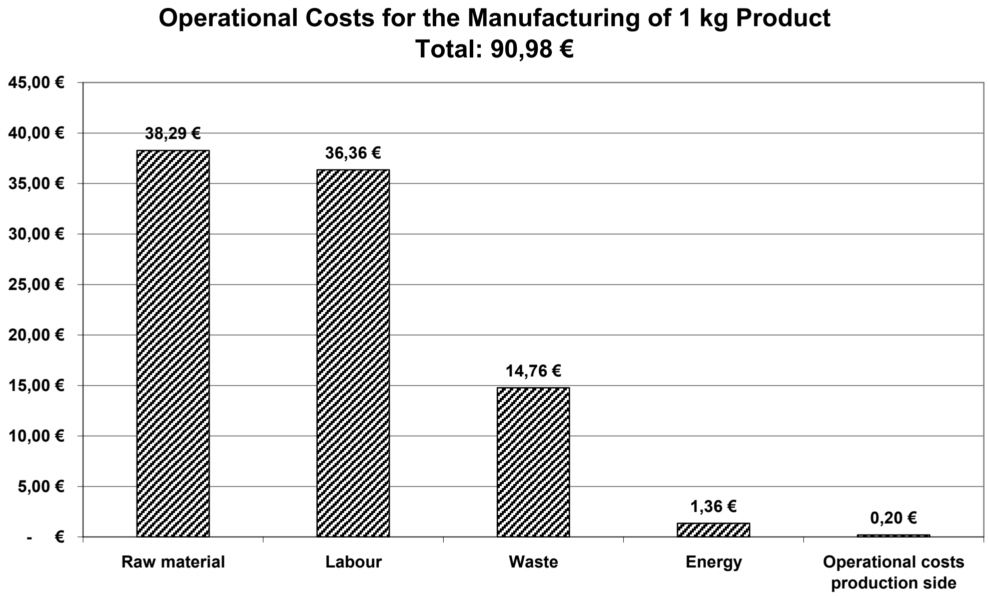


Figure 6. Shares of variable costs of the realized process

Cost Analysis of the Batch Reactor Plant

Whereas the manufacturing in a 1 l batch reactor at 100 °C and 1 bar and assuming the same selectivity of 45 % would lead to unacceptable high costs (more than fourfold higher) the manufacturing costs using a 10 l batch reactor are only slightly higher compared with the micro reaction plant.

Microstructured Reactors with a Tenfold Higher Throughput

Further process intensification which results in a tenfold higher throughput leads to dramatically decreasing operational costs and also decreasing fixed costs (Fig. 7). The main driver is the decline of the operator's salary. A similar result with only marginal higher costs could be obtained by external numbering-up, i.e. with ten reactors in parallel.

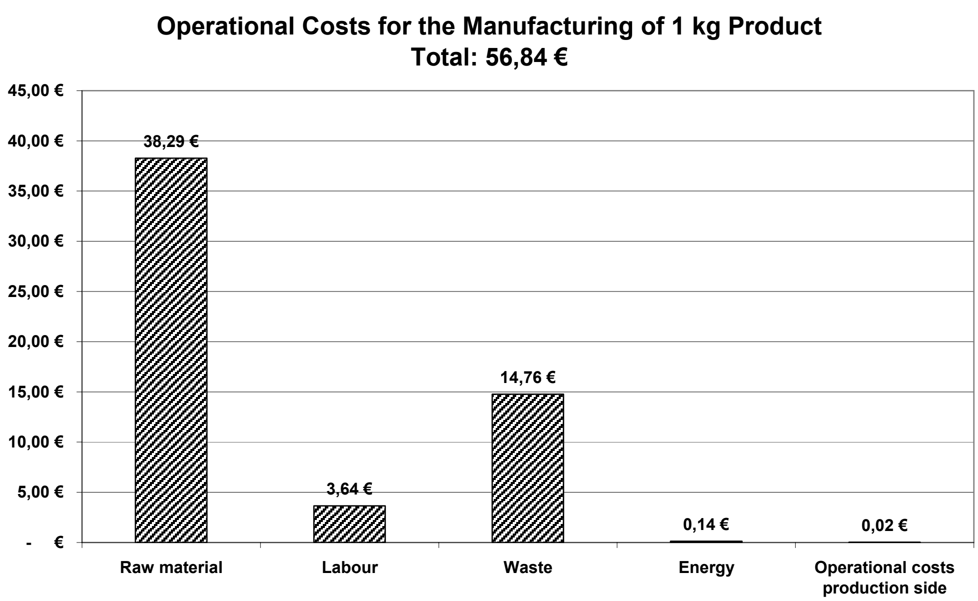


Figure 7. Shares of variable costs using Process Intensification

Conclusions

With our cost analyses the optimization of the operational (respectively variable) costs could be identified as the decisive point for a commercial profit of micro process engineering. This is in line with the quest to go from micro-reactor engineering to micro-reactor process engineering. It can be achieved in two ways: In the case of the synthesis of high-value products from expensive raw materials the high operator costs, which otherwise dominate, are of less relevance. On the other hand, process intensification through micro process engineering can reduce the operator costs compared to the batch. The equipment costs, consisting of the microstructured reactors and the balance-of-plant equipment, have a low share in both cases and thus should have minor influence on the decision for the implementation of this novel technology.

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