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# Work Flow in Process Development for Energy Efficient Processes

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Increasing expenditures for energy require an optimization of chemical processes with regard to energy efficiency. Energy efficiency is of course only one aspect of a multiobjective optimization during process development. In the paper the work flow in BASF's process development for new and existing processes will be presented. In the different phases of the development several methods are used to provide facts for a stop/go decision of the project. An overview about the different methods will be given. Special focus will be on the use of exergy analysis for comparison of different process concepts. A second focus of the presentation will be the increase of energy efficiency by change of operational conditions.

## 1. Work Flows in Process Development

In process development for the chemical industry energy efficiency is only one objective among others like for example raw material and investment cost, product quality, health, safety and environmental aspects. Examples for parameters of this optimization are feed stock, utilities, configuration, equipment, operational conditions and production site aspects.

The result of this optimization is however only a snapshot of the actual situation since feed stock, utilities and equipment costs are time-dependent boundary conditions and may change rapidly as the experience of the past has shown. So also for existing processes it is worthwhile to reconsider different options to improve the energy efficiency. The approaches for new and existing processes at BASF's process development are different. The work flows and the different methods used for both kinds of processes are briefly presented in the following.

### 1.1 Development of new processes

For the development of new processes the phase gate process is used (Figure 1). At the beginning, in the opportunity finding phase, different configurations will be evaluated by the aid of conceptual design tools. For example the $\infty/\infty$ analysis (see e.g. Stichlmair and Fair, 1998; Ryll et al., 2008) or rectification body method (e.g. Bausa et al., 1998; von Watzdorf et al., 1999) might be used to check the feasibility of different configurations. Heat and mass balances provided by these tools can be used as a starting point for a more detailed simulation.

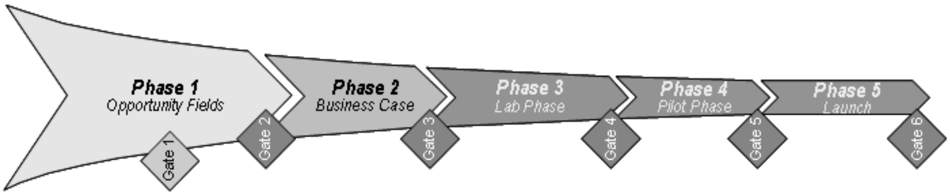


*Figure 1: Phase-gate process for the development of new processes*

The heat and mass balances of the detailed simulation are then used for the basic design which will be needed for the cost estimation and economic evaluation. In the business case phase the net present value and the expected commercial value will be estimated and will provide the basis for the stop/go decision for the project.

Next step in the phase gate process is the laboratory phase. The miniplant and/or pilot plant is an essential tool to confirm the process concept and to validate and improve the simulation model. With the validated model a further optimization using methods like Linnhoff (e.g. Linnhoff et al., 1982; Smith, 2005; Kemp, 2007 ) or exergy analysis (e.g. Szargut 2005) will be done. At the end of the lab and pilot phase, scale-up and cost estimation will be finalised, the economic evaluation is used as a decision guidance for a hand-over to the plant engineering and the launch.

**1.2 Re-evaluation of existing processes**

The re-evaluation of existing processes follows the basic principles of 6σ (Figure 2). First the process will be defined. For the defined process the actual operational conditions have to be measured and than analysed with the help of simulation. A design check helps to identify bottlenecks of the plant and to see which equipment has to be replaced in case of a capacity increase. Linnhoff and exergy analysis will identify potentials for improvement of energy efficiency. Last but not least the process may be improved by new configurations, different operational parameters, new equipment or advanced process control, if the economic evaluation justifies the measures. After the implementation the expected improvement has to be controlled.

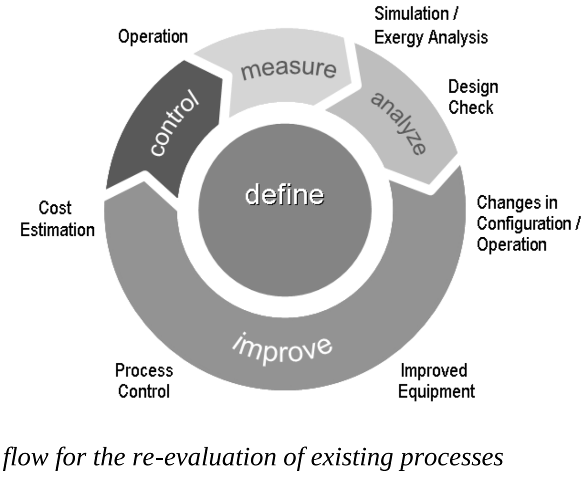


*Figure 2: Work flow for the re-evaluation of existing processes*

## 2. Exergy analysis

Exergy analysis is a helpful tool in the evaluation of energy efficiency, since it describes different energy qualities. Exergy is the maximum work attainable in the given natural environment. With exergy analysis it is possible to quantify the exergy losses in each process step, to identify units for improvement and to compare different process configurations. Exergy losses are caused by irreversibilities. Major reasons for exergy losses are: Pressure drop, mixing and heat transfer.

Exergy analysis can easily be integrated in a simulation tool (Munsch et al., 1990) since all thermodynamic functions needed for the estimation of exergy are available and only one of the pre-defined sets for the environment has to be implemented (Rivero and Garfias, 2004; Morris and Szargut, 1986; Szargut, 1989; Szargut et al., 2005; Valero et al., 2002). There is one basic rule for the exergy: Accept exergy losses only with an overall economic justification (Szargut, 2005).

In the following the use of exergy analysis will be demonstrated for the separation of water and methanol as an example.

## 3. Example: Separation of Methanol / Water

In this example a methanol/water mixture with 6 wt.% water has to be separated (Sirch et al., 2009). Figure 3 shows a conventional distillation column with 55 theoretical stages. The temperature profile shows that this is a separation of a wide boiling mixture, i.e. the boiling points of the components show a large difference. The gaseous feed enters the column at stage 7. In total a heat demand of 9 MW is required for the separation. Unfortunately in this concept the heat has to be provided at the highest temperature of the column.

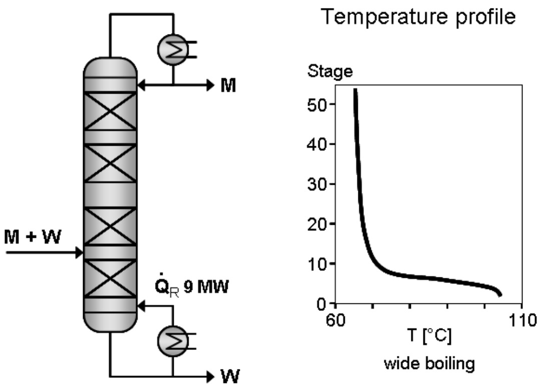


*Figure 3: Temperature profile of the wide boiling mixture methanol (M) + water (W)*

Examining the exergy losses in the column of the conventional distillation (Figure 4, concept I) it can be seen that especially below the feed stage high exergy losses are present. One possibility to reduce these exergy losses is the use of a side reboiler slightly above the feed stage (Figure 4, concept II). Also the total exergy losses can be reduced by 300 kW, if steam of a lower quality (1.5 bar instead of 4 bar steam) is available (Table 1). If a lower steam quality it is not available, there is no reduction of exergy losses since the energy demand in total for both concepts is the same.

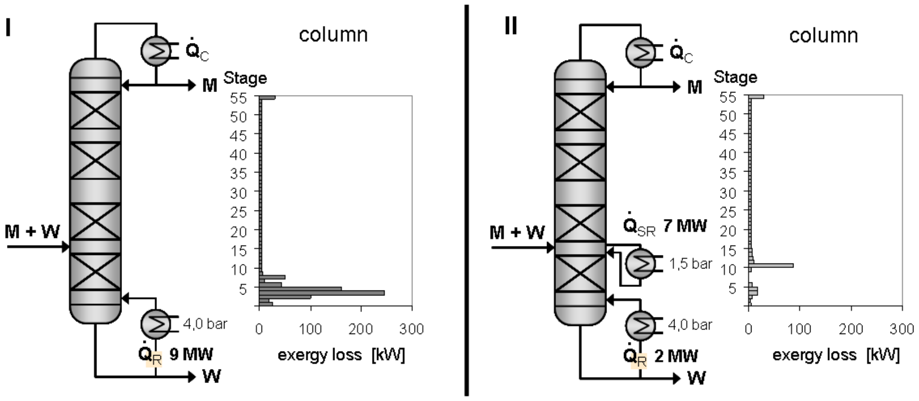


*Figure 4: Exergy losses in the columns of two different concepts for the separation of methanol (M) and water (W): I. Conventional distillation, II. Distillation with side reboiler*

Examining the exergy losses of all units, Table 1 shows that the major source of exergy loss is the condenser. Unfortunately the heat attainable in the condenser is only available at a low temperature. Vapor recompression is one option for using this heat. By increasing the pressure by compression the condensation temperature of the vapor increases and therefore it can be used for heating. This leads to the concepts III and IV in Figure 5.

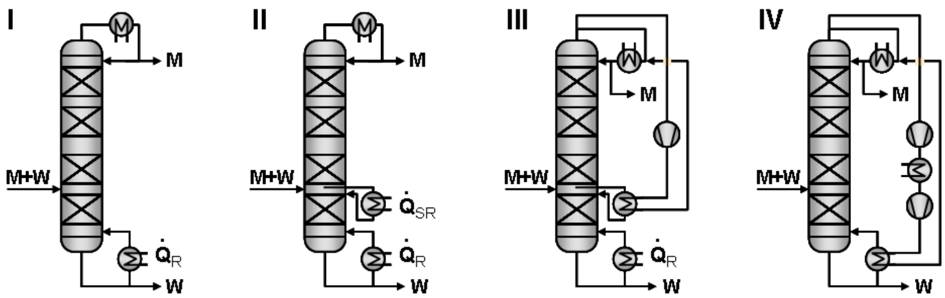


*Figure 5: Different concepts for the separation of methanol (M) and water (W)*

In concept III a part of the vapour is compressed in one stage and used for the side reboiler. Concept IV shows the conventional vapour recompression for distillations. Here also only a part of the vapour at the top is used. The reason, why only a part is used, is the gaseous feed, so much more has to be condensed than evaporated. In concept IV a two-stage compression unit with an intermediate chiller has to be used to raise the condensation temperature of the vapors for an use in the reboiler. Although the exergy loss of the condenser in concept IV is the lowest, concept III offers the lowest total exergy loss (Table 1).

*Table 1: Exergy losses of different concepts for the separation of methanol and water (Figure 5)*

| | *Exergy loss in kW* | | | |
|---|---|---|---|---|
| *Unit* | *Concept I* | *Concept II* | *Concept III* | *Concept IV* |
| Column | 875 | 371 | 371 | 875 |
| Condenser | 2366 | 2366 | 1637 | 1533 |
| Reboiler | 758 | 127 | 127 | 548 |
| Side reboiler | - | 832 | 471 | - |
| Compressor(s) | - | - | 200 | 466 |
| Intermediate chiller | - | - | - | 322 |
| Total | 4000 | 3697 | 2806 | 3742 |

Table 2 compares for all four configurations the total exergy loss, the relative energy expenditure and the return on investment for the case, when only 4 bar steam is available. Here the results for energy expenditure and the total exergy loss lead to similar considerations. In terms of return on investment the combination of the vapor recompression with the side reboiler (concept III) is the most economical and allows a payback of the investment within 3 years.

*Table 2: Exergy, energy expenditures and return on investment of different concepts for the separation of methanol and water (Figure 5)*

| | *Concept* | | | |
|---|---|---|---|---|
| | *I* | *II* | *III* | *IV* |
| Total exergy loss in MW | 4 | 4[a] | 2.8 | 3.7 |
| Relative energy expenditures | 100 % | 100 % | 54% | 65 % |
| Return of investment | - | never | ~3 y | ~10 y |

*[a]Here it assumed that only 4 bar steam is available. For this reason there is no reduction of exergy losses between concept I and II, since the energy demand in total for both concepts is the same.*

## 4. Conclusions and Outlook

Energy efficiency is one target of process development in the chemical industry which besides other objectives has to be taken into account in the workflow. To evaluate and optimize the different process alternatives several methods are necessary and have been briefly presented.

Exergy analysis is a powerful method to identify exergy losses and to compare different concepts as has been demonstrated for the separation of methanol and water. In the presentation additional examples will be given and it will be shown how improvements in process operation can also be seen in the light of reduced exergy losses.

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