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Work flow in process development for energy efficient processes

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ABSTRACT

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 multi-objective optimization during process development. It will be shown how methods for increasing energy efficiency are integrated in the workflow of BASF's process development for new and existing processes. Special focus will be on the use of exergy analysis and its high relevance to industrial chemical processes. It will be shown how exergy analysis might be used for comparison of different process concepts. Additionally examples will emphasize how an increase of energy efficiency by change of operational conditions can be reached. Also these measures can be interpreted in terms of reduced exergy losses. For all examples the additional investment, if needed, is justified by the savings, which were altogether approximately 7 million euro per year.

1. Introduction

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. Usually a multi-objective optimization problem with sometimes conflicting objectives has to be solved. For example usually the increase in energy efficiency will result in higher investment costs, so it is essential to find the right compromise between those objectives. In the paper it will be shown how the incorporation of exergy analysis into the workflow of the chemical industry will help to identify potentials for reduced energy consumption. The specific measures have to be optimized in accordance with the other objectives.

The result of this optimization however is 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.

2. Work flow in process development

2.1. Development of new processes

For the development of new processes the phase gate process is used (Fig. 1). At the beginning, in the opportunity finding phase, different configurations will be evaluated by the aid of conceptual design tools. For example the ∞/∞ analysis (see e.g. Stichlmair and Fair [1], Ryll et al. [2]) or rectification body method (e.g. Bausa et al. [3], von Watzdorf et al. [4]) 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.

The heat and mass balances of the detailed simulation are then used for the basic design which is needed for 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 at gate 3.

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 pinch (e.g. Linnhoff et al. [5], Smith [6], Kemp [7]) or exergy analysis (e.g. Szargut [8]) will be done in the lab and pilot phase. At the end of the lab and pilot phase, scale-up and cost estimation will be finalized, the economic evaluation is used as decision guidance for a hand-over to the plant engineering and the launch.

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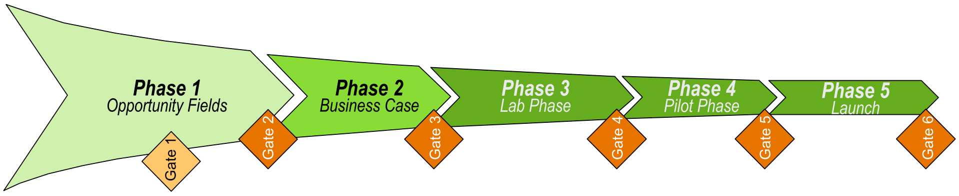

Fig. 1. Phase gate process for the development of new processes.

2.2. Re-evaluation of existing processes

The re-evaluation of existing processes follows the basic principles of 6σ (Fig. 2). First the process will be *defined*. For the defined process the actual operational conditions have to be *measured* and then *analyzed* with the help of process simulation. Pinch and exergy analysis will identify potentials for improvement of energy efficiency. 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. 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 those measures. After the implementation the expected improvement has to be *controlled*.

3. Exergy analysis

Exergy analysis has been investigated in many different applications (a review is given e.g. in Sciubba and Wall [9], for recent examples refer to Klemes and Friedler [10] or Friedler [11]). For example an early contribution in chemical engineering was the exergy analysis of rectification (cf. e.g. Wozny et al. [12,13]), recent applications of exergy analysis in distillation for example column sequencing can be found in Dejanovic et al. [14]. However exergy analysis today is not widely-used in the work flow in chemical industry. For example commercial process simulators like ASPEN do not offer exergy analysis. In the following it will be shown that 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 a 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.

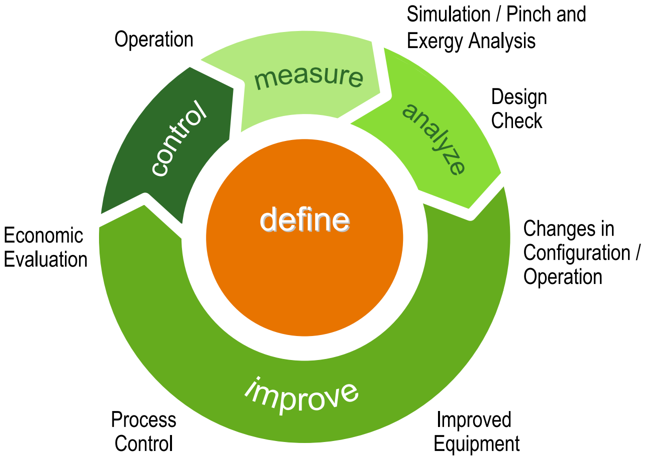

Fig. 2. Work flow for the re-evaluation of existing processes.

Exergy losses are caused by irreversibilities. Major reasons for exergy losses are:

- Pressure drop,
- mixing and
- heat transfer.

Exergy analysis can easily be integrated into a process simulation tool (e.g. Munsch et al. [15]) since all thermodynamic functions needed for the calculation of exergy are available and only one of the pre-defined sets for the environment has to be implemented additionally (Rivero and Garfias [16], Morris and Szargut [17], Szargut [18], Szargut et al. [19], Valero et al. [20]).

Exergy analysis can be used in an early stage in the development of new processes for example in the opportunity finding phase (see Section 2.1 and Fig. 1) for the comparison of different processes routes based on different feed stocks as well as for a detailed simulation, where for all operation units exergy losses can be determined. The requirements for using exergy analysis are the same as for a process simulation, which means a model for the enthalpy and entropy is necessary and in case of reaction the information about standard enthalpy and entropy of formation of the components will be needed.

There is one basic rule for the exergy: Exergy losses should be accepted only with an overall economic justification (Szargut [8]). This again emphasizes the multi-objective character of process development with conflicting objectives like for example investment and energy efficiency.

4. Results

In the following the use of exergy analysis in the work flow will be demonstrated for a few examples with different process concepts for existing and new processes and some with different operating conditions for existing unit operations.

4.1. Different process concepts

4.1.1. Pressure reduction

In this first example (Fig. 3) an existing process was investigated. Here a natural gas stream with 55 bar was released in a let-down valve to 6 bar. The estimated exergy loss in this case is 3.3 MW. Installing a turbine instead can reduce the exergy loss to 1.0 MW. Thereby it is possible to gain electrical power of 2.3 MW. The additional investment is paid back within 3 years.

4.1.2. Separation of an amine/ammonia mixture

For the development of a new amine production process different process concepts for the ammonia removal have been investigated. The conventional distillation for the separation of an amine/ammonia mixture is shown in Fig. 4. Here it is a wide boiling mixture as can be seen in the temperature profile: The temperature at the top and the bottom of the column show a large difference. Unfortunately the heat of 3.6 MW has to be provided at the highest

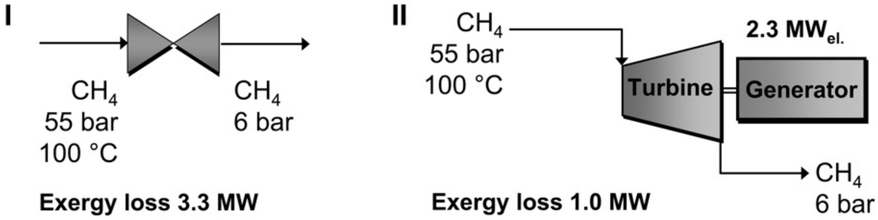

Fig. 3. Comparison of concepts for pressure reduction of natural gas: I) let-down valve, II) use of a turbine.

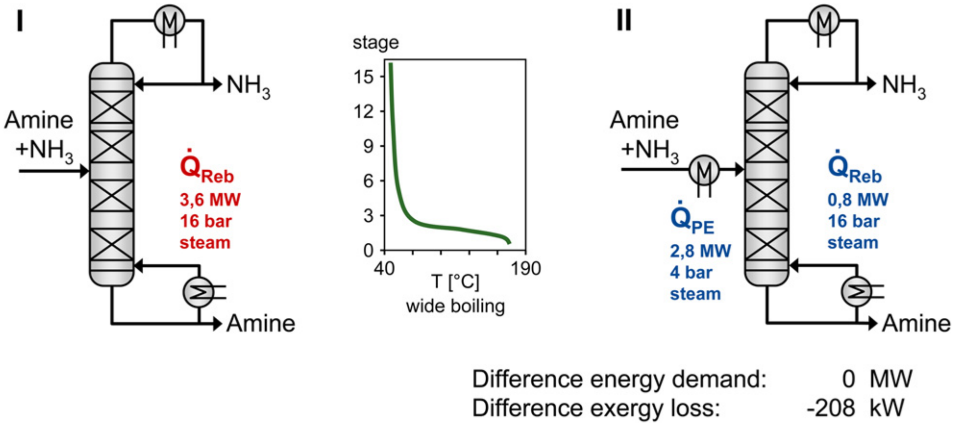

Fig. 4. Exergy losses in the columns of two different concepts for the separation of an amine and ammonia: I. conventional distillation, II. distillation with pre-evaporator.

temperature approx. 190 °C in the reboiler. This is the reason, why 16 bar steam for heating has to be used. When using a pre-evaporator instead, it is possible to provide 2.8 MW at a lower temperature by using only 4 bar steam. The reboiler duty is decreased to 0.8 MW. Comparing these two configurations shows that the total energy demand is the same but the exergy losses in the pre-evaporator case is reduced by approx. 200 kW. The pre-evaporator results in higher investment costs whereas investment cost for the reboiler is decreased. At the site, where this plant was designed for, steam was produced in a combined heat and power plant. The price for 16 bar steam is higher than for 4 bar steam, since 16 bar steam can be used (similar to the previous example) to produce power and 4 bar steam. The energy expenditure savings caused by the use of a lower steam quality allows a payback of the additional investment within 3 years.

4.1.3. Separation of methanol/water

In this example for a new plant a methanol/water mixture with 6 wt.% water has to be separated (Sirch et al. [21]). Fig. 5 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. One might think about using a pre-evaporator again like in the previous example, but since the feed is gaseous this is not possible.

Examining the exergy losses in the column of the conventional distillation (Fig. 6, 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 (Fig. 6, 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 overall energy demand for both concepts is the same.

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 overheads increases and therefore they can be used for heating. This leads to the concepts III and IV in Fig. 7.

In concept III a part of the vapor is compressed in one stage and used for the side reboiler. Concept IV shows the conventional vapor recompression for distillations. Here also only a part of the vapor 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

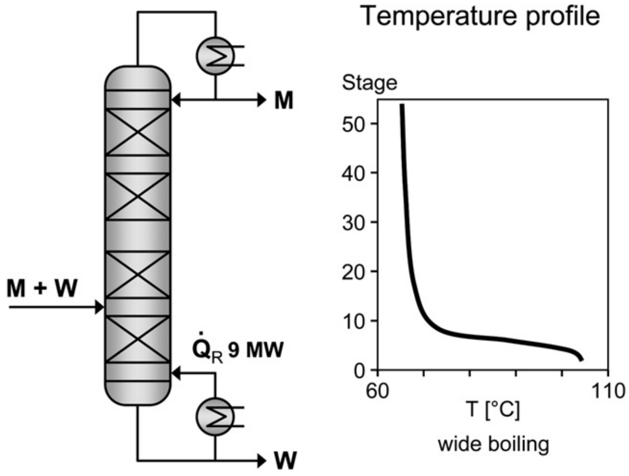

Fig. 5. Temperature profile of the wide boiling mixture methanol (M) + water (W).

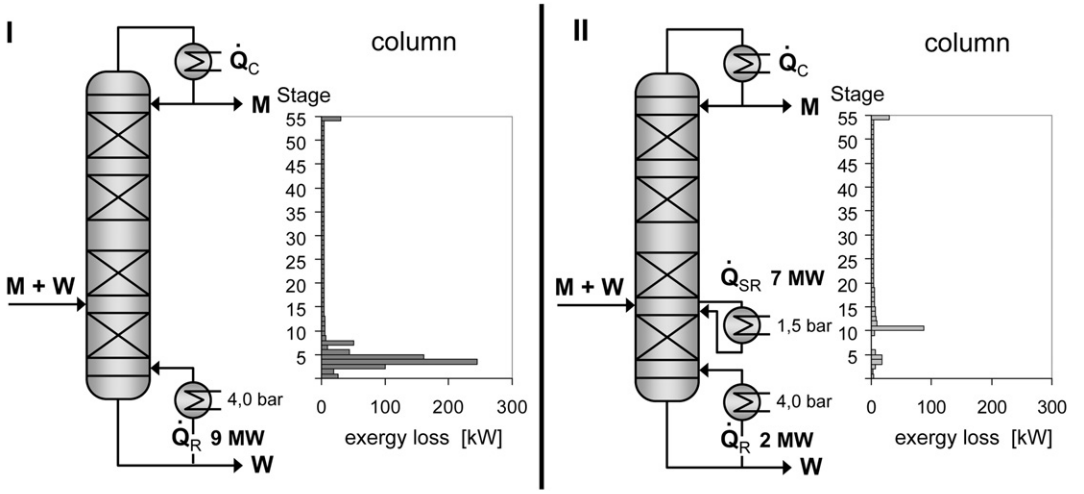

Fig. 6. Exergy losses in the columns of two different concepts for the separation of methanol (M) and water (W): I. conventional distillation, II. distillation with side reboiler.

Table 1
Exergy losses of different concepts for the separation of methanol and water (Fig. 7).

Unit	Exergy loss in kW			
	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

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 overall exergy loss (Table 1).

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.

4.2. Change in operation

4.2.1. Optimization of an incinerator

In Fig. 8 the incineration of a plant off-gas is shown. The off-gas is first pre-heated before it enters the incineration chamber. Here additional fuel and air have to be added. The off-gas of the incineration is used to produce steam and to pre-heat the off-gas from the plant. Optimization trials for the incineration have shown that it is possible to reduce the incineration temperature from 970 °C to 870 °C while staying within the CO emission limit of 5 ppmv. Major impact of this measure was a fuel saving of 800 m^3/h. Due to the reduction of the temperature the steam production decreased by 10 t/h. Since the temperature changes for the exergy are of minor importance compared to the chemical energy of the fuel, exergy losses can be estimated by comparing the exergy of 800 m^3/h fuel with the exergy of 10 t/h steam resulting in an exergy loss reduction of 5.8 MW. The reduced steam production was no problem for the plant. Here it was possible to generate a huge benefit due to the fuel savings without any investment.

4.2.2. Optimization of a calciner

In the last example, shown in Fig. 9, a zeolite powder is calcined in a rotary kiln. Here the existing facilities where not able to handle the full zeolite powder stream. For this reason a toll manufacturer was commissioned. The optimization of the operation of the rotary kiln (rotating speed and air make-up) leads to a capacity increase by a factor of 2.6, since also unscheduled down-time could be reduced. Assuming the same heat input in terms of electrical power (0.5 MW, see Fig. 9) for the toll manufacturer than for the own plant, electrical power of 1.6 times 0.5 MW is saved, therefore the exergy loss is reduced by 0.8 MW. Thus, the toll manufacturer was not necessary any more and there was a huge saving without investment.

Experiments have demonstrated that the implementation of internals might increase the capacity further to a factor of 4.5 of the

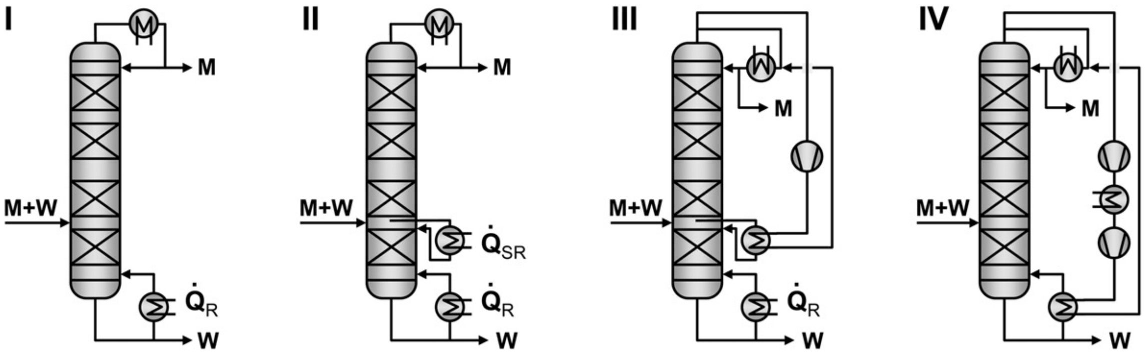

Fig. 7. Different concepts for the separation of methanol (M) and water (W).

Table 2
Exergy, energy expenditures and return on investment of different concepts for the separation of methanol and water (Fig. 7).

	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 years	~10 years

[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.

original capacity thereby reducing exergy losses by 1.8 MW. Here the payback time of the investment is approximately one month.

5. 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 a few examples. It was also shown how improvements in process operation can also be seen in the light of reduced exergy losses. The examples resulted in overall savings of about 7 million € per year for five plants. This shows the huge potential in the chemical industry by evaluating different process concepts for new plants and by improving existing plants. All examples shown (except the pre-evaporator example, see Section 4.1.2) have been or will be realized.

The exergy analysis of course has also some limitations, as it will not give hints how to reduce exergy losses. Here some experience is necessary and may be experienced users will not need exergy analysis to come to similar measures. But for inexperienced users the exergy analysis will help to identify units, where it is worthwhile to consider improvements. In all examples the operating costs and also the exergy losses were reduced. This shows that the integration of the exergy analysis in the workflow reflects in the right way energy efficiency. But usually only an economic evaluation will show if a measure to reduce exergy losses is appropriate. Therefore the incorporation of different objectives (like for example exergy losses and costs) in the simulation for a good optimization is a goal for future improvement of the workflow.

At the time being the multi-objective character of process optimization is not reflected in the work flow and the simulation tools for process simulation. Quite often different options will be simulated and subsequent a basic design and an economic evaluation will take place. So the optimization process is an iterative process with a lot of interfaces and usually different isolated software tools. One step forward is the concept of the intelligent total cost minimization approach (i-TCM) presented by Wiesel and Polt [22]. Here the different objectives are weighted with costs to a total cost function which can be minimized.

For the variable costs raw material costs, utility (like for steam or cooling water) costs and disposal costs have to be implemented into the simulation tool. For the fixed costs this method requires the integration of short-cut design tools to estimate the size of the different units e.g. heat exchangers or columns. With the equipment size it is than possible to estimate the project cost including investment with help of cost functions. These fixed costs are depreciated over a certain time range and will give together with the variable costs the total costs, which can be minimized. Here the subsequent steps are integrated in one tool, which performs an optimization without interim user action. One drawback of the method is that other, not cost related objectives (like for example exergy or safety aspects) can not be included. Furthermore the typical drawbacks (Miettinen [23]) of a weight-based multi-objective optimization have to be expected.

Next step in improving the process development work flow would be the integration of a real multi-objective optimization into simulation and to estimate the Pareto front. The Pareto front describes a set of solutions where no improvement in one objective can be reached without at least getting worse in another objective. The Pareto front allows to investigate the trade-offs between

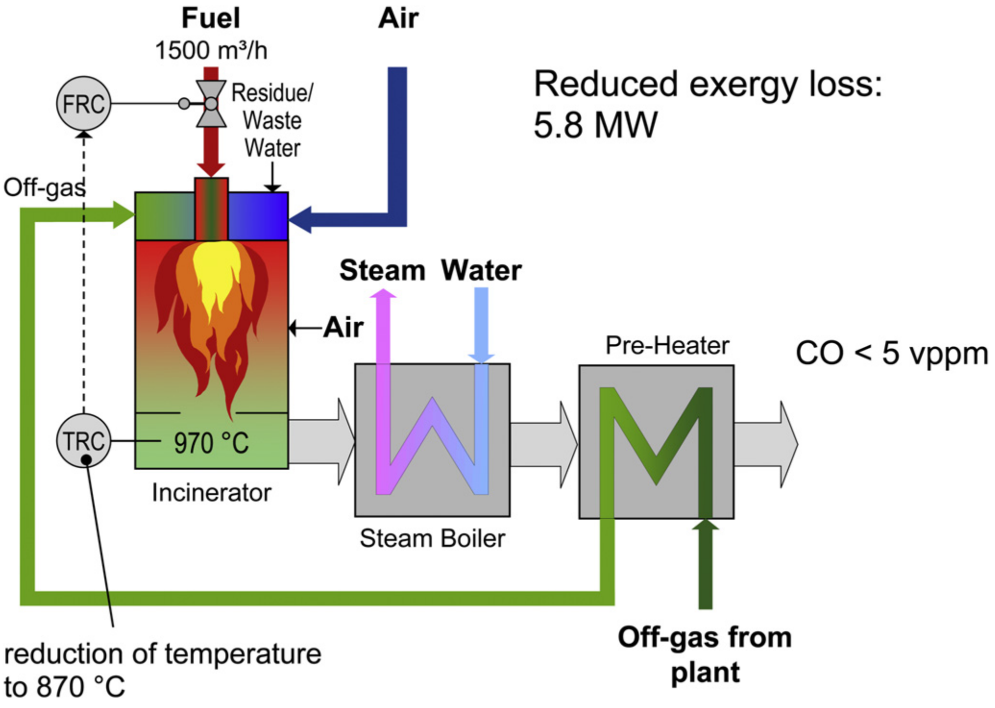

Fig. 8. Optimization of the operating conditions of an incinerator.

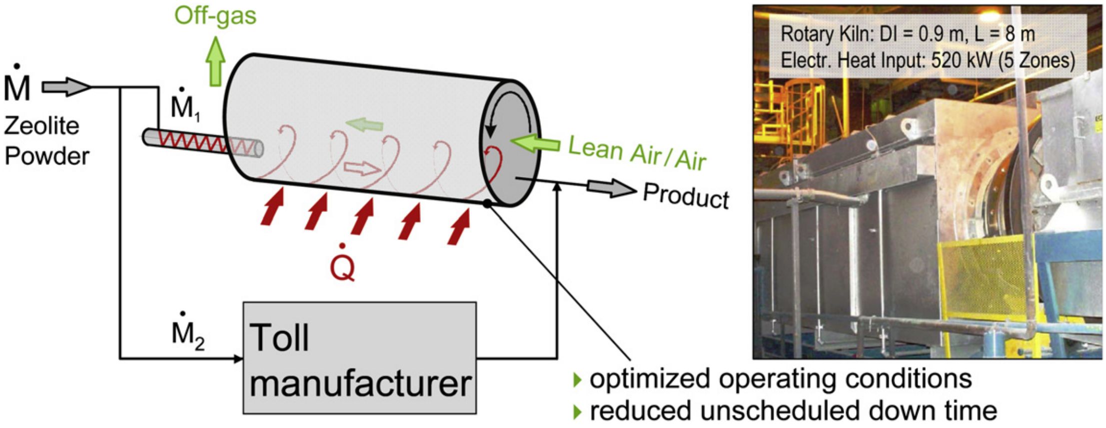

Fig. 9. Optimization of operating conditions of a calciner.

different objectives. Therefore it make sense to use the multi-objective optimization together with a decision support system which allows to navigate within the Pareto front and to choose the best compromise between the objectives (e.g. Monz [24], Welke et al. [25,26]). This will help the process developer to find a process design with balanced objectives for example accounting for energy efficiency, costs and other relevant objectives.

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