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MULTI OBJECTIVE OPTIMISATION FOR AN ECONOMICAL DIVIDING WALL COLUMN DESIGN

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Abstract
The dividing wall column is experiencing a growing interest in industry. The concern about difficult controllability vanishes further and this leads to growing demand of approved guidelines for the design which is indeed time consuming if no expert knowledge is available.
In this contribution the design task of a dividing wall column is treated as multi objective optimisation. Backbone of this optimised design method is a mathematical process model verified by an extensive experimental investigation. The optimisation itself allows to identify the best trade-off designs effectively regarding investment and operating costs as well as other constraints without any limitations for a fact based investment decision.

Keywords: dividing wall column, optimisation, multi objective, design

1. Introduction

Distillation units are still in focus of industry because of their importance for the purification of speciality and commodities. Despite all their advantages the purification of products by thermal separation in distillation columns requires the major energy demand of industry. Fulfilling the demands of the markets the aim of all companies is to gain economical advantages towards competitors by further research and development. The separation of a multi component mixture is a common task and dividing wall columns (DWC) are one opportunity to realise savings in investment and operation costs. This technology is favourable, especially for high purity products and an excess of the medium boiling product in the feed. So, high product quality and a high throughput at the same time move the DWC into the considerations during design or revamp of common distillation units. Figure 1 illustrates the principle set up of a dividing wall column.

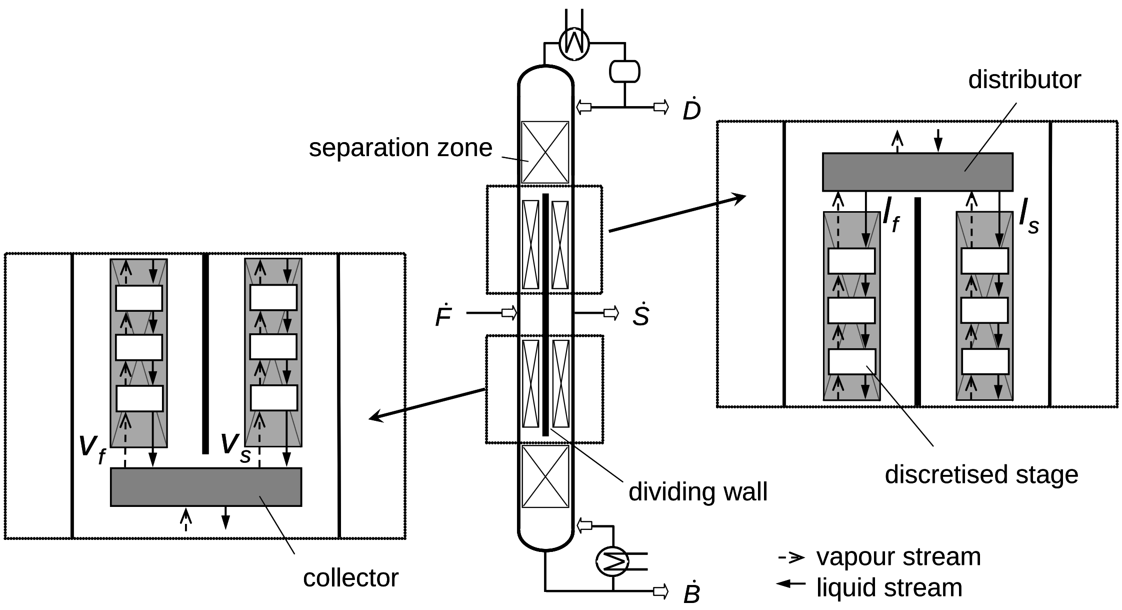

Figure 1. Sketch of a dividing wall column with three product streams and six separation zones as well as details of the dividing wall section indicating the internal streams

There have been a lot of investigations on novel distillation techniques. The DWC has already proven its superior functionality towards sequences of common distillation units or with side streams [1-3]. The design phase is challenging and if no expert knowledge is present, the development of optimal solution is time consuming. In this case 'optimal solution' means to exploit the maximum savings in investment and operation costs by applying the dividing wall technique. For these two goals the design of a new plant is a typical multi objective optimisation problem and is treated as single objective optimisation by combining both goals in one optimisation function by a priori chosen factors, classically. The advantage of solving a multi objective problem is mainly that the best trade-offs for the given objectives are found. From these results a direct evaluation of the different designs can be completed without any apriori reduction of the solution space[4]. Figure 2 shows the differences between a single and a multi objective approach for the minimisation of two functions. For the design of a new plant the two functions are investment and operating costs. This treatment of the design is fairly new although its advantages explain oneselves. The base of the proposed method is a multi objective optimisation using an evolutionary algorithm which is applied to the model based design of a DWC.

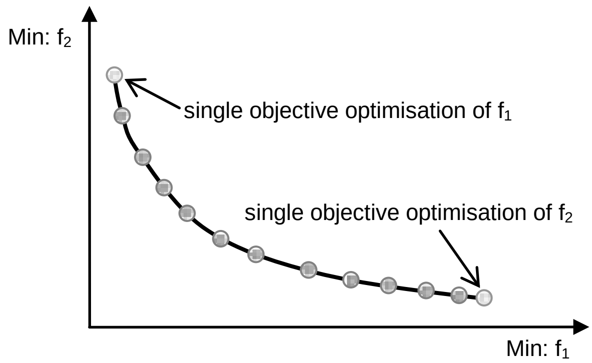

Figure 2. Single versus multi objective optimisation

2. Process modelling

Klatt and Marquardt[5] emphasise the inverse problem of model based process design. One precondition of the proposed optimal design is an existing accurate mathematical model. Several models for the simulation of DWC have been developed by academia and industry. Further the modelling is subdivided into steady state simulation or dynamic simulation. Both the equilibrium stage and nonequilibrium stage modelling are state of the art[6; 7]. Unfortunately, a lot of models suffer under a lack of proper verification by experimental data[8]. The first experimental data are published by Mutalib[9]. Wozny and Arellano-Garcia[10] indicate the importance of experimental knowledge explicitly. Niggemann et al. [6; 7] performed a huge set of experiments at a pilot plant located at Hamburg University of Technology. The experimental data consists of start up, steady state operation and transient operation which is unique. Additionally, the so gained experimental knowledge is extended by real production plant experience. The extensive experimental investigation allows a proper validation by pilot plant data and will ensures the significances of the modelling. In short the pilot plant has an inner diameter of 68 mm and a total height of approximately 11 m. The six separation sections are equipped with 0,98 m B1-500 packing of Montz GmbH. The dividing wall is welded at the diameter of the column. The pilot plant and the experimental data are the reference for the future evaluation and proof of the significance of the proposed approach. Design and operating parameters of this plant serve as references and the results are normalised to this design.

Several commercial software packages are available and offer steady state model libraries which include distillation columns. Fundamentally, these steady state models are suitable for a model based design and have proven their functionality. The program Aspen Plus® is taken as simulation environment. Because of the significance of the dividing wall technology AspenTech has already implemented the steady state model 'MultiFrac(Petlyuk)' which reflects a thermodynamic equivalent of the DWC. Since the first simulations indicate differences towards the experimental results of the pilot plant special attention has to be targeted at a detailed description of the dividing wall column with its special features. By comparison the 'MultiFrac(Petlyuk)' model hurts the condition of equal pressure drops along both sides of the dividing wall and leads to deceptive results/conclusion because the thermodynamic properties may change and influence the separation performance. Most important modification concerns the hydraulics since the pressure drops along both sides of the dividing wall adjust the vapour distribution below the dividing wall[11; 12]. In equation 1, the equality of the total pressure drops of the prefractionator and main column in the dividing wall section is considered. The vapour split ratio is defined by equation 2 and describes the vapour distribution below the dividing wall.

$$\Delta p_f = \Delta p_s \tag{1}$$

$$r_{dw,vap} = \frac{v_f}{v_f + v_s} \tag{2}$$

Accurate pressure drop correlations of all internals are necessary for determining this self adjusting parameter which additionally cannot be directly controlled. The vapour distribution is effected by the feed and side stream as well by the internal liquid distribution of the reflux flow above the dividing wall, as it is presented in figure 1. Consequently, disregarding this special feature of the DWC may lead to significant uncertainties of the design. Therefore on top of the standard model behaviour a self adjusting vapour split was realized since this ensures the significance of the model.

The presence of verified process models is the backbone of a design method which strongly relies on the quality of the mathematical model. With respect to model based design task, the process model has emphasised its validity for reflecting the operation of DWC. Now, it can be used for the model based design including optimisation.

3. Optimisation

Finally, the model based design is combined with an optimisation which guarantees that the so gained design proposal fulfils the optimisation problem[13]. Despite existing models optimal design of DWC is still challenging. Most currently used optimisation tools are just capable of single objective optimisation with a limited ability of global optimisation. Due to this constraint and the limited knowledge about the process good initial values are needed and several optimisation runs have usually to be done. On top all results are heavily dependent on constraints including the formulation of the objective function. This means any changes of the task would result in a complete recalculation of the optimisation. Eliminating the described limitations this contribution will present the design of DWC based on a multi objective optimisation approach which overcomes the problems mentioned before. The whole set-up will lead to a multi objective optimisation (MOO) of a mixed integer non-linear programming (MINLP) problem[14; 15]. The optimisations are conducted using the multi objective evolutionary algorithm *ncsMDE* by Leipold *et al.* [16]. In short, the task of the optimisation is defined below.

$$Min: \quad OC = f_1(\underline{u_O}) \wedge IC = f_2(\underline{u_D}) \tag{3}$$

$$g(\underline{x}, \underline{u_D}, \underline{u_O}) = 0 \tag{4}$$

$$h(\underline{x}, \underline{u_D}, \underline{u_O}) > 0 \tag{5}$$

At the same time the operating costs (OC) and the investment cost (IC) will be minimised. The costs are function of the operating and design parameters, respectively u_O and u_D. The formulation of the optimisation consists of equality and inequality constraints g and h. x is the vector of state variables and u is the vector of the parameters. The authors have developed a tool for the automatic solving of the optimisation problem. An interface realises the communication between AspenPlus and the optimiser. Although such automation decouples the definition of the design task and the execution of the optimisation, the utilisation of an automatic design approach is still rare.

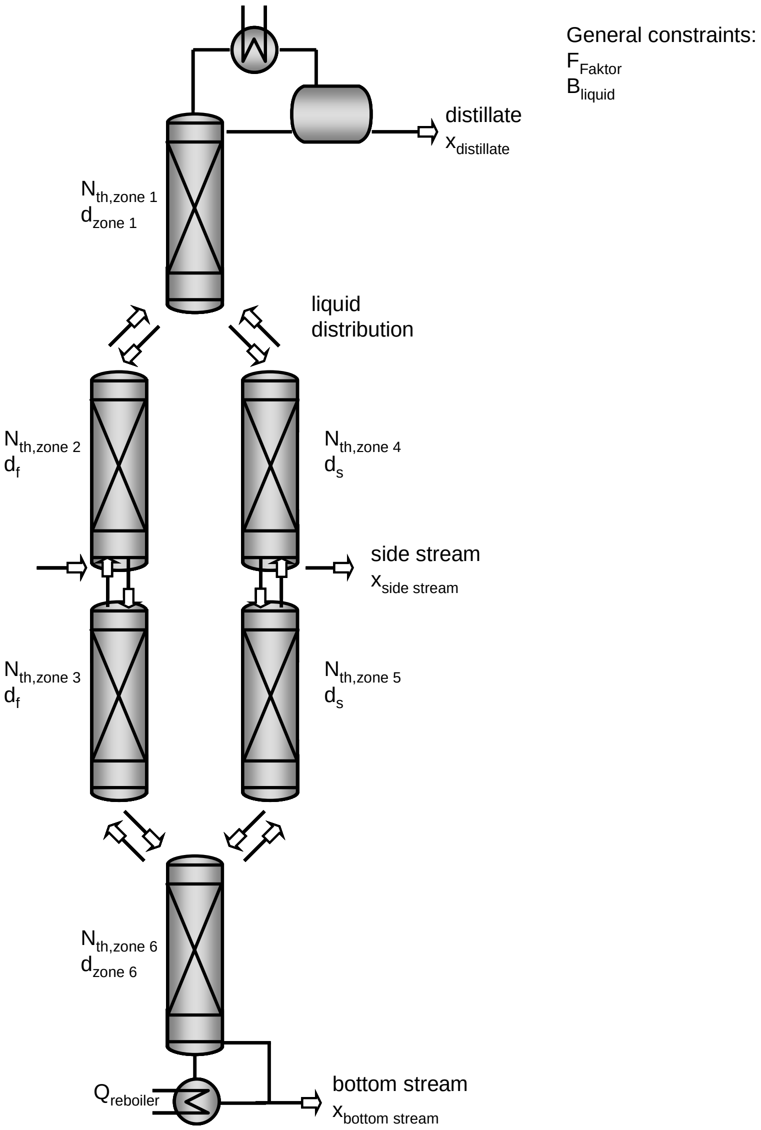

Figure 3. Graphical presentation of the optimisation problem

In the following the task of the design is described in more details. The mixture to be separated consists of three linear fatty alcohols hexanol, octanol and decanol which separation is of industrial interest[17]. Optimisation is done with respect to minimum investment and operation costs. Optimised design and operation parameters include reboiler heat duty, product streams, number of stages in each column section, feed stage and side stream stage as well as the diameters of the column sections, including the horizontal position of the dividing wall. In addition, the optimisation is subject to some extra inequality constraints. Those include purities of the products as well as maximum vapour, respectively minimum liquid load. According to the main advantages of DWC the mass fraction key component should be greater than 99,0 wt.-%. As a matter of course, the feed enters the column in the dividing wall section and the vertical position of the dividing wall is limited within the framework of the design. The liquid distribution above the dividing wall is also subject of the operating parameters. Other constraints can be considered if it is necessary e.g. construction limitations or constraints due to controllability.

Summarising the multi objective optimisation allows doing any evaluation or identification of solutions as a final step. In other words it is a posteriori choice of the best solution. The space of solutions can be screened completely in contrast to any other approach applying single objective optimisation or weighting several parameters within one optimisation run. The DWC is an ideal candidate for a multi objective optimisation due its degrees of freedom. Although this optimisation is a complex problem, the computing time of one simulation is done in around 5 seconds using a state of the art personal computer. Despite such a short computing time for one simulation a common optimisation which includes approx. 100.000 simulations could be quickly performed only by connecting several computers in parallel.

4. Results

In order to see clearly the influence of the different design cases the optimisation was performed for different feed compositions: equal mass fractions for all fatty alcohols as well as for mixtures with 80 wt.- % hexanol and 80 wt.-% octanol, respectively. The optimisations result in three different pareto optimal fronts. As shown in figure 4 the results of the study are normalised to the mentioned reference system. Each point in one pareto front refers to one optimal trade-off of the DWC design for the given optimization case, respectively the given objectives. All three fronts give a whole range of solutions for the different design cases (different constraints in optimisation). From these results investment decisions based on facts can be made by direct comparison of different design cases without an apriori decision for the trade-off between different objectives.

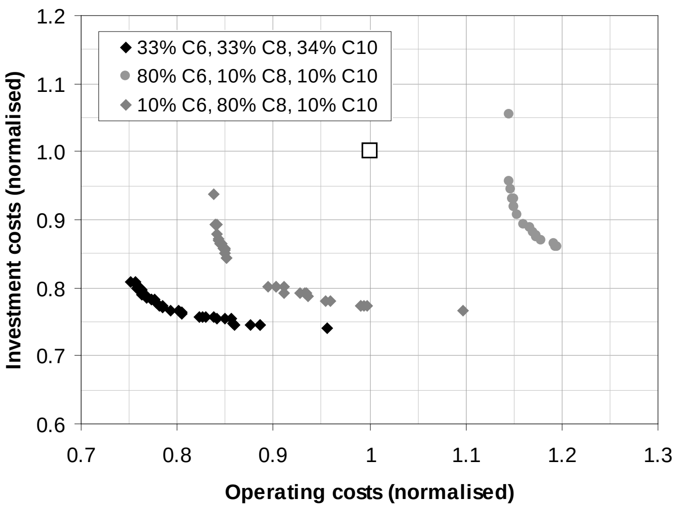

Figure 4. Optimisation result of three feed scenarios with 1000 generations of 100 individuals (normalised to reference system which is marked by a square)

Furthermore, figure 4 illustrates the sensitivity of the investment and operating costs depending on the feed composition. The reference is designed for the separation of a feed with equal fraction of the components. The results show that there exist several design alternatives which would realise reductions in both investment and operating costs of about 20 %. Comparing the three feed stocks among each other an excess of middle boilers results in a high influence on the operating costs while the investment costs may change less significantly. A feed stock with an excess of light boiler require higher investment and operating costs but the design has less influence on the operating cost in contrast to the other design cases. As a final remark it must kept in mind that the design alternative may vary strong. This requires extraordinary diligence during the design and supports the necessity of an automatic tool as it is presented here.

5. Conclusions

The DWC are under certain circumstances an excellent alternative for sequences of distillation units or conventional side stream columns. Their potential to save investment and operating costs at the same time led to realisation in industry. Dealing with DWC means to work with a quite complex system regarding design and operation.

This contribution presents a method for supporting the design of DWC. Due to their characteristics DWC design is a multi objective optimisation problem and should be solved as one. Applying automatic MOO tool enables with only a few multi objective optimisation runs to retrieve a wide spread knowledge base for decisions in DWC design problems. The method is efficient and based on facts a posteriori decision on the design can be done. However, the multi objective optimisation can also be used to compare the dividing wall technologies with conventional distillation sequences or side stream columns. Generally, this approach can be easily adjusted to any multi objective optimisation and thereby this one is capable to identify global optimal solutions.

Acknowledgements

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Nomenclature

Latin symbols:

B	liquid load, bottom stream
F	feed stream
d	diameter
D	distillate stream
g	equality constraint
h	inequality constraint
l	liquid flow
p	pressure
Δp	pressure drop
N_{th}	number of theoretical stages
r	ratio
S	side stream
u	vector of parameters
v	vapour flow
x	state variable, concentration
Q	heat

Subscript:

d	design
dw	dividing wall
f	feed stream sections
i	index
o	operating
s	side stream sections
vap	vapour

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