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Pareto optimal design and operation of multivessel batch distillation

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Abstract

Multivessel batch distillation (MBD) has been proposed and investigated to meet changing demands of the specialty and fine chemistry. This contribution addresses the multiobjective optimisation of a MBD with one intermediate vessel for the first time. The process is highly non-linear and inherent dynamic. Design and operating parameters has been considered simultaneously. The problem formulation results in a mixed integer dynamic optimisation (MIDO) problem. It is solved using a sophisticated framework based on a modified differential evolution algorithm (MDE). The challenging non-linear dynamic model is solved in Aspen Custom Modeler. The start-up phase, usually neglected, has been taken into account. Selected results of the multiobjective MIDO will be discussed.

Keywords: batch distillation, start-up, dynamic modelling, multiobjective optimisation, evolutionary algorithm

1. Introduction

Multivessel Batch Distillation (MBD) can be considered as a superstructure of all batch distillation configurations. It consists of a reboiler, a condenser, a distillate receiver, *N-1* thermally coupled column sections and *N-2* intermediate vessels where *N* indicates the number of components. It is generally recommended to operate the column with infinite reboil and reflux ratio to exploit the maximum separation efficiency. The products are simultaneously collected in associated vessels applying an appropriate process control strategy, so that no off-cuts have to be reprocessed. A MBD with one intermediate vessel, which is focus of this contribution, is illustrated in Fig. 1.

MBD has been subject to investigations over the last decade, whereas primarily process control strategies have been proposed. Only a few works can be found dealing with single objective global optimisation of a MBD with two intermediate vessels [1,2]. Global optimisation studies have been executed on the basis of evolutionary algorithms and dynamic optimisation. However, the weighting of the factors of the objective function is always difficult to handle in the design phase of a process. Moreover, the optimisation results in one single solution on which a decision has to be made. Using multiobjective optimisation, one can hold off on this decision to a later point of time. This guarantees more flexibility, since a posterior decision making can include superior information.

Our contribution addresses the multiobjective MIDO of a MBD with one intermediate vessel (Middle Vessel Batch Distillation). Since the process variables are inherently time-variant, an integrated complex dynamic optimisation has been performed.

2. Problem formulation

Multiobjective optimisation often leads to the problem to distinguish between investment costs (IC) and operational costs (OC). Both can be estimated using appropiate correlations from literature or in-house estimation methods. Then, OC is a function of the operating parameters $\underline{u}_o$ and the time t while IC depends on the design parameters u_d. Since the reboiler duty has been fixed during the optimisation runs of which the results are shown in this contribution IC is directly related to the number of theoretical stages in the upper and lower part of the column $N_{th,\mathrm{k}}$. The optimisation problem can be written as follows:

$$\text{Min OC} = f_1(\underline{u}_o, t) \wedge \text{IC} = f_2(\underline{u}_d) \tag{1}$$

subject to:

$$\underline{g}(\dot{\underline{x}}, \underline{x}, t, \underline{u}_d, \underline{u}_o) = 0 \tag{2}$$

$$w_i \geq 0{,}99 \quad \forall\, i = 1,2,3 \tag{3}$$

$$h(w_i) = \sum_{i=1}^{3} \Delta w_{i,j} \geq 0 \quad \forall\, i = 1,2,3 \wedge j = 1,\ldots N_{\Delta t} \tag{4}$$

where $\underline{g}$ indicates the dynamic process model, $\underline{x}$ the state variables, $\underline{u}_d$ the design variables and $\underline{u}_o$ the operation variables, i.e. the refluxes from *N-1* product vessels L_i. w_i denotes the mass fractions of the key components while h is an evaluation function that is used to improve the dynamic optimisation. $\Delta w_{i,j}$ indicates the difference of the mass fractions between two time intervalls during the dynamic optimisation. The indices i and j denote the number of components and the number of time intervalls $N_{\Delta t}$, respectively. The process has been discretised into six time intervalls. Design and operating parameters are, of course, constrained to reasonable ranges. However, the integrated approach of combining global optimisation and dynamic optimisation leads to a large number of possible combinations which demands a robust solver. In the next section, our optimisation approach is presented.

3. Multiobjective MIDO framework

The MIDO has been solved in MS Excel while the dynamic simulation has been executed in Aspen Custom Modeler. During the optimisation initial parameters are transferred from the optimisation framework to Aspen Custom Modeler to run the simulation. Afterwards, necessary values are transferred back to evaluate the objectives using the provided interface.

3.1. Multiobjective global optimisation using evolutionary algorithms

Compared to other methods, the class of evolutionary algorithms (EA) is the only method capable of finding a Pareto optimal set in a single optimisation run. Unfortunately, many special solution procedures exist, but no standard solver that can be easily applied to a given problem. Therefore, we developed the non-constrain-dominated sorting MDE (ncsMDE) on the basis of a MDE algorithm that will be presented in the following chapter.

Originally, the MDE algorithm, developed by Babu and Angira [3], was intended to solve single objective global optimisation problems. The main advantage of this algorithm is its robustness. The benefit can be explained by the facts that only a few solver parameters have to be specified and a bad solver tuning just prolong the time of an optimisation run. A solution is still guaranteed. The flowsheet of the algorithm is shown in Fig. 2. In the first step, m random individuals are generated to form the population (Initialisation). To evaluate the 0th generation, m dynamic simulation runs are executed in Aspen Custom Modeler. Afterwards, the fitness of each individual is determined. This is done using the characteristics of the non-dominated sorting genetic algorithm (NSGA) proposed by Srinivas et al. [4]. Violations of constraints are considered using the concepts of the *constrained tournament method* proposed by Deb [5].

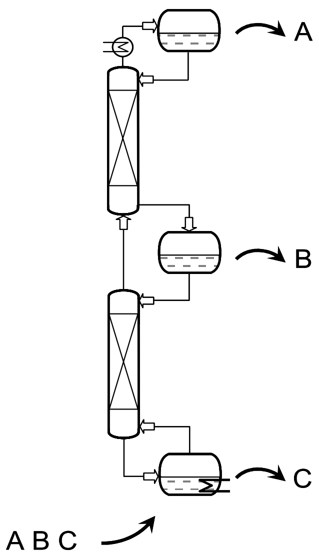

Fig. 1: Middle Vessel Batch Distillation

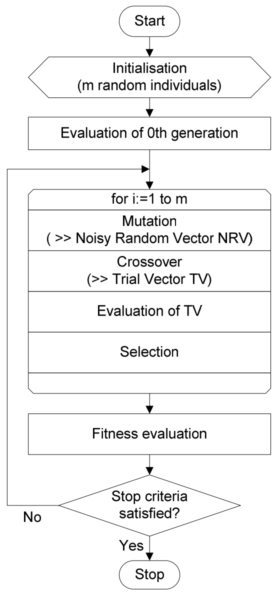

Fig. 2: ncsMDE flowsheet

The actual improvement of indivduals occurs by passing a series of genetic operators *m* times. In the *mutation* step, the MDE generates a new individual (noisy random vector NRV) by adding a weighted difference vector between two randomly chosen individuals to a third one. The target vector and the NRV are taken to create one new individual, the so-called trial vector TV.

The probability of preferring a genome of the target vector to the one of the NRV has to be set in advance (*Crossover*). The objective function values of the TV are determined after a dynamic simulation run (*Evaluation*). In the following *selection* step, the constrained tournament method is used to compare the TV to the target vector. If the TV perfoms better, it will be directly available in the next mutation step by replacing the target vector. This leads to a significant increase in velocity. At the end of the loop, the next generation is evaluated and the optimisation terminates if the stopping criteria are met.

The efficiency of the algorithm has been proven solving several problems of different level of complexity. Non-convexity has been taken into account as well as multiple inequality constraints. Two problems will be used in the presentation to introduce the concept of the algorithm in detail.

3.2. Modelling and simulation framework

Studies on batch distillation usually used a simplified approach to initialise the process, that is, the column trays are filled and contain liquid at feed concentration and boiling temperature. These assumptions lead to errors in the characterisation of thermodynamic and hydraulic profiles at the beginning of each optimisation run. The influence on the resulting optimal solution is still unknown and work is in progress. Since optimal switching of manipulated variables is expected to take place before the column reaches its hydraulic steady state, consideration of the start-up is strongly recommended. Therefore, we have developed and presented a dynamic tray-to-tray equilibrium model model that is capable of dealing with the physical phenomena occurring during this phase. Details can be found in [6,7]. For the first time, the start-up is encapsulated in the following investigations.

4. Pareto optimal design and control of multivessel batch distillation

4.1. Case study

The optimisation strategy has been applied to an industrial scale distillation column which aim was to separate a ternary mixture of hexanol, octanol and decanol subject to high product qualities (w_i > 0.99 kg/kg). The feed contains 400 kg of each component. In order to assure a reasonable vapour load, the reboiler duty has been set to 200 kW. The individuals are characterised by their genomes containing values of the number of theoretical stages in both column sections, two refluxes from the product vessels, and the length of six time intervalls. As a consequence of the available computational power, the population size was limited to 20. The optimisation has been terminated after 2000 generations. At this point of time, no further significant improvement of the Pareto-optimal front has been observed.

4.2. Results and discussion

Fig. 3 shows the the number of feasible individuals and the mean violation of constraints as a function of the number of generations. Two facts can be observed. The first feasible individuals have been found after 600 generations because of the large number of possible genomes. Despite the stochastic character of the solution method, the mean violation of constraints is rapidly decreased. This is a consequence of the constraint tournament method that has been adapted. Fig. 3 also illustrates the Pareto-optimal front and the first two dominated fronts after 2000 generations. The process time is displayed in relation to the batch time needed when conventional temperature control is

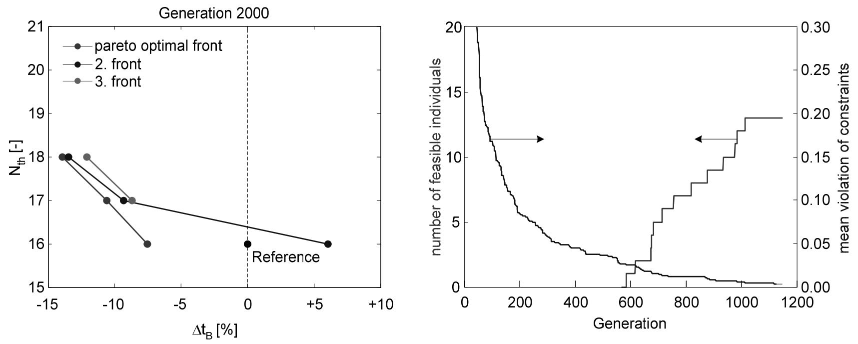

Fig. 3: Pareto-optimal solution and solver efficiency

applied (*reference*). It can be seen that the optimal solution perform better than temperature control. The trade-off between IC and OC can be clearly seen.

5. Summary and Conclusion

For the first time, an integrated approach to multiobjective MIDO of a MBD with one intermediate vessel has been presented. The optimisation problem has been solved using an efficient evolution strategy. Main advantage of the algorithm is its robustness that makes it possible to find the global optimum within a wide range of existing solutions and a much wider range of individuals. The dynamic optimisation permitted free time intervalls and included the startup phase. A convergent Pareto-set has been achieved after 2000 generations. The process time can be reduced compared to a conventional temperature control.

Acknowledgements

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