Development of a Pressure-Driven Dynamic Model to Study the Start-up of a Flexible Tray Column

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Abstract. The flexible operation of unit operations and chemical processes was gaining increased attention in the past. Flexible operation includes steady-state operation over a broad range of operating points as well as the dynamic transition between operating points, including the start-up of unit operation and processes. In particular, the start-up of distillation columns is a time consuming task. Start-up can be accelerated by tailored start-up strategies or by appropriate design measures. The latter approach was pursued here as we investigated the start-up of a flexible column design. Therefore, we developed and extended a dynamic modelling approach to describe the start-up operation of a segmented tray column. We especially paid attention to the influence of heat transfer between the segments that are integrated in one single column shell during start-up operation. Results showed a significant influence of the heat transfer on the start-up duration depending on the chosen start-up strategy.

Keywords Pressure-Driven Modeling, Flexible Operation, Start-up Operation, Distillation

Introduction

Start-up of distillation columns is a time consuming and complex task. During start-up, the column is far from equilibrium conditions and the product cannot be withdrawn with sufficient quality. Therefore, it is essential to minimize the start-up duration.
Besides operational decision making during the start-up process, new technical design approaches provide an alternative path towards reduced downtimes in flexible operation.
In one of our previous publication [1], we presented a flexible tray column design, which aims from the scratch to maximize capacity flexibility and provide accelerated dynamics during the start-up and between operating points. A division of the active area into area-equal segments characterizes the developed tray column. By installing vertical walls within the column shell, the segments are separated from each other and each segment can be operated, started-up or shut-down independently.
In addition, the design allows for a coupling of the segments next to each other via the downcomer of each tray. The aim of this coupling is to use a share of the downcomer liquid holdup of each tray in the segment operated at a steady-state to assist the start-up of a new segment. Coupling each tray via the downcomer allows for a start-up with a predefined concentration and temperature profile, by that potentially reducing start-up durations. The segmented column, the vapor and liquid flows in the segments and the coupling of the segments via liquid transfer between the downcomer are illustrated in Fig. 1.
Fasel *et al.* [2] presented a first experimental setup of the column. Experimental results showed that a sufficient amount of liquid can be transferred between the segments while at the same time stable operation of the column was ensured from a hydrodynamic perspective.
Bruns *et al.* [3] developed a first suitable modeling approach and analyzed the start-up behavior of the column by dynamic simulation studies. Results show that the start-up duration for individual segments can be reduced significantly when coupling segments via the downcomer liquid hold-up compared to a conventional start-up strategy. In addition to exploiting the coupling between the segments, start-up could be further accelerated by manipulating the timing at which feed is introduced into the segments and heat is supplied to the reboiler.
In this contribution, we extend our previously developed dynamic modeling approach to describe inter-segment heat transfer to incorporate and analyze the phenomenon of preheating inactive segments into the start-up simulations. The aspect of heat transfer between different segments within a single column shell is for example interesting for the operation of dividing wall columns but was studied by only few authors, e.g. [4-5] focusing on overall energy-efficiency.
The remainder of this contribution is structured as follows: first, we briefly present the modeling approach derived for the simulation of start-up for the flexible tray column. We then perform start-up simulations taking a closer look on

the influence of heat transfer from a segment operated at a steady-state operating point to an adjacent segment and the influence of the resulting preheating of the segment on the start-up process. Finally, we present and discuss the results of the simulation study followed by conclusions.

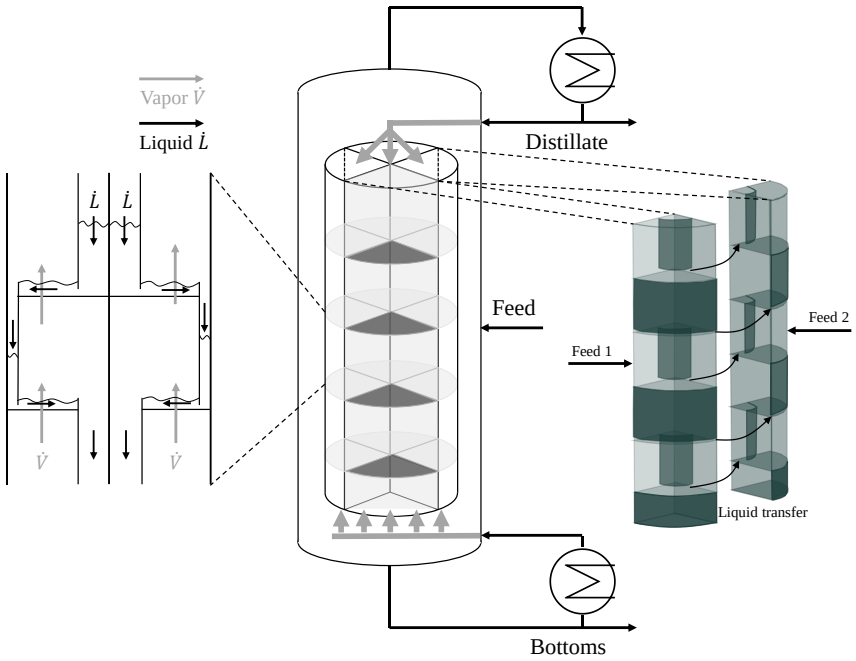

Fig. 1 Schematic representation of the column with flow directions in the segments (left) and schematic illustration of liquid transfer for start-up operation (right).

Modeling approach

We developed a modeling approach that is able to describe the start-up of a single segment of the flexible column based on the coupling of two adjacent segments. When considering the unique structure of the segmented column, it becomes apparent that the model needs to account for the following dynamic phenomena to represent the start-up of inactive segments:

- hydrodynamic description from an empty stage and downcomer to steady-state holdups,
- thermodynamic description from ambient to equilibrium conditions,
- coupling of the downcomer and the stage as well as
- coupling of segments via adjacent downcomers.

Fig. 2 shows the resulting control volumes for the downcomer and the stage with all relevant flows.

From previous studies on the start-up of distillation columns, it was shown that equilibrium stage models are indeed suitable to adequately describe the phenomena occurring on single trays and that they are able to sufficiently cover the dynamic behavior between a dry column at ambient conditions and at steady-state operation. These models describe each equilibrium stage by the MESH equations. For the developed model, we solely assume heat and liquid accumulation on the trays until bubble-point temperature is reached. At bubble-point temperature, equilibrium conditions between liquid and vapor phase are calculated. Moreover, below bubble-point temperature, we assume that all vapor instantly condenses on the trays. Due to the nature of the equipped sieve trays in the flexible column, we account for weeping using a correlation derived by Staak *et al.* [6] and an equation presented by Wunderlich *et al.* [7] to avoid numerical instabilities. Pressure drop on each stage is described as function of tray geometry, physical properties, vapor flow rate and tray hydraulics, represented by an equation from Zuiderweg [8]. Liquid holdup is calculated based on tray geometry, physical properties and tray hydraulics, and the liquid flow rate over the weir is determined using the Francis Weir equation.

For the downcomer, we assumed that no mass transfer is occurring and only the liquid phase is considered for balancing the downcomer. The vapor holdup present in the downcomer is attributed to the vapor in the control volume of the equilibrium stage. The downcomer submodel consists of component balances, an energy balance and summation condition in the liquid phase, as represented by eq. (1) – (3).

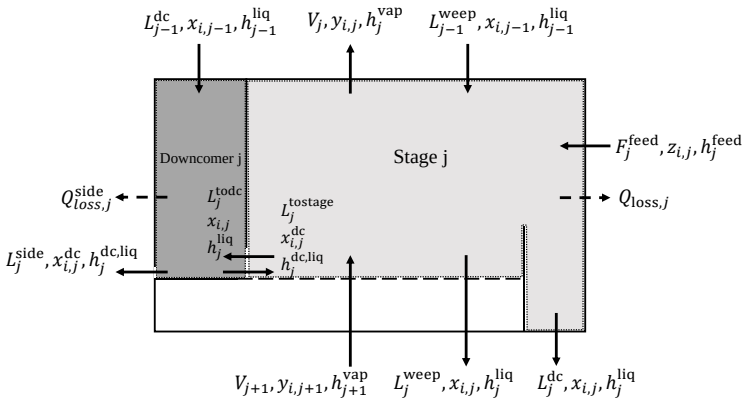

Fig. 2 Representation of control volumes for downcomer and stage and corresponding flows.

$$\frac{d\left(HU_j^{\mathrm{dc,liq}} \cdot x_{i,j}^{\mathrm{dc}}\right)}{dt} = L_{j-1}^{\mathrm{dc}} \cdot x_{i,j-1} + L_j^{\mathrm{todc}} \cdot x_{i,j} - L_j^{\mathrm{tostage}} \cdot x_{i,j}^{\mathrm{dc}} \pm L_j^{\mathrm{side}} \cdot x_{i,j}^{\mathrm{dc}} \tag{1}$$

$$\frac{d\left(HU_j^{\mathrm{dc,liq}} \cdot h_j^{\mathrm{dc,liq}}\right)}{dt} = L_{j-1}^{\mathrm{dc}} \cdot h_{j-1}^{\mathrm{liq}} + L_j^{\mathrm{todc}} \cdot h_j^{\mathrm{liq}} - L_j^{\mathrm{tostage}} \cdot h_j^{\mathrm{dc,liq}} \pm L_j^{\mathrm{side}} \cdot h_j^{\mathrm{dc,liq}} \tag{2}$$

$$\sum_{i=1}^{\mathrm{NC}} x_{i,j}^{\mathrm{dc}} = 1 \tag{3}$$

Here, HU represents the liquid hold-up in the downcomer j, L is the liquid flow from and to the downcomer j according to Fig. 1, x is the mole fraction for each component i, and h is the corresponding enthalpy of the flows.
Coupling of the stage and the downcomer was established by means of Toricelli's law and the derived discharge equation of a submerged rectangular orifice. The discharge of liquid from the downcomer to the stage is described as follows:

$$L_j^{\mathrm{tostage}} = \xi_{res,j}^{\mathrm{tostage}} \cdot A_{da} \cdot \rho_{m,j}^{\mathrm{dc,liq}} \cdot \sqrt{2 \cdot g \cdot \left(h_{\mathrm{cl},j}^{\mathrm{dc}} - h_{\mathrm{cl},j}\right)} \tag{4}$$

$\xi_{res,j}^{\mathrm{tostage}}$ represents the resistance to the liquid flow from the downcomer to the stage, A_{da} is the available area under the downcomer apron, $\rho_{m,j}^{\mathrm{dc,liq}}$ is the mass density of the liquid in the downcomer, and $h_{\mathrm{cl},j}^{\mathrm{dc}}$ and $h_{\mathrm{cl},j}$ are the actual clear liquid heights of the liquid in the downcomer and on the stage. If $h_{\mathrm{cl},j} > h_{\mathrm{cl},j}^{\mathrm{dc}}$ liquid flows from the stage to the downcomer and must be considered adequately by rearranging eq. (4). The resistance coefficient is calculated using a steady-state momentum balance.
The coupling of the segments is implemented using the same approach based on Toricelli's law. Therefore, the driving force term in eq. (4) was adapted to account for the clear liquid heights in the adjacent downcomers. For this study, the segments are additionally coupled via an equation describing the heat transfer from the segment operated at steady-state conditions to the adjacent one (cf. eq. (5)).

$$Q_{loss,j}^{\mathrm{side}} = \alpha \cdot A_{seg} \cdot \left(T_j^{\mathrm{steady-state}} - T_j^{\mathrm{adj}}\right) \tag{5}$$

The heat transfer coefficient is set to $\alpha = 0.025\ \mathrm{kW \cdot m^{-2} \cdot K}$, according to [9] and A_{seg} represents the lateral area between the segments.
When a segment is started-up, heat flows from that segment to the adjacent one, which is initially at ambient temperatures, resulting in two effects: a slightly higher reboiler duty is required to operate the active segment when compared to adiabatic conditions during start-up and steady-state operation; the adjacent segment exhibits higher temperatures at the beginning of its start-up procedure, because the temperatures in both segments will converge over

time. The overall column is assumed to be adiabatic so that no heat loss to the environment ($Q_{\text{loss},j} = 0$) is considered in the model.
The duration of the start-up process is quantified by the MX-function presented by Yasuoka *et al.* [10].

$$MX_{\text{total}} = \sum_{i}^{\text{NC}} \sum_{j}^{n} \left| x_{i,j} - x_{i,j}^{\text{steady-state}} \right| < 0.01 \quad (6)$$

For any additional information regarding modeling and control of the single segment as well as model implementation during start-up, we refer the interested reader to our previous publication [6]. The overall dynamic column model was implemented in Aspen Custom Modeler.

Simulation study

Start-up simulations were performed using an equimolar mixture of water and methanol as a case study. Physical properties for the binary mixture are calculated by the NRTL method. At steady-state operation, a nominal feed of 15 kmol·h^{-1} is fed to each single segment. We assumed that the column is operating at atmospheric pressure.
The column and tray geometry was adapted from the experimental setup presented in [2] and is summarized in Table 1. The number of stages is 10 and the feed stage is set to stage 5. A reflux ratio of 3 and a reboiler duty of 333 kW is necessary to achieve sufficient purity of the methanol.

Table 1. Design parameter for the segmented column**.**

Parameter	Value	Unit
Tray spacing	0.5	m
Sump height	1	m
Area factor	0.8	–
Column diameter	0.85	m
Outer weir length	0.632	m
Inner weir length	0.208	m
Outer weir height	0.029	m
Inner weir height	0.046	m

For all start-up simulations, we used a conventional start-up scheme, as, e.g., described by [11]: the reflux ratio remains constant at the steady-state value during start-up; heat is supplied to the reboiler as soon as the set-point of the liquid level is reached, which was set to 50% of the sump height; reboiler duty is increased step-wise before set to the steady-state value. The segment is controlled using a standard LV-configuration [12] and all controllers are active during start-up except the temperature controller that is activated as soon as the segment is at steady-state conditions.

Results

Accounting for heat transfer between the segment operated at steady-state conditions and the adjacent one, while the overall column is assumed adiabatic, leads to a pre-defined temperature profile in the empty segment. Over time, the empty segment reaches a similar temperature profile. In the following, the influence of this effect on the start-up of an empty segment is assessed.
Based on the previously described start-up strategy, two cases were derived to adapt the conventional strategy to the requirements of the flexible column:

- Case 1: On each tray, the segment to be started-up is supplied with liquid from each downcomer of the adjacent segment operated at steady-state conditions. This enables a start-up of an individual segment with pre-defined concentration and temperature profiles. In this case, a feed flow is introduced to the segment to

be started-up from the very beginning of start-up operation ($t = 0$). The remaining relevant variables are treated as described in the previous section.

- Case 2: At the beginning of the start-up operation ($t = 0$), the segment to be activated is supplied with liquid from each downcomer of the adjacent segment operated at steady-state conditions on each tray. In this case, a feed flow is introduced as soon as liquid accumulates at all stages ($\forall L_j > 0$). The feed introduction is delayed to reduce any negative mixing effects due to different concentrations of the components in the feed. Additionally, the set-point to start supplying heat to the reboiler is set to ¼ of the original set-point, thus the heat supply to the segment starts earlier.

Results are summarized in Fig. 3 in the form of temperature profiles over time. The left side shows the temperature profiles for both cases without heat transfer and the right side shows the results when heat transfer is considered. It can be seen that temperatures differ significantly at $t = 0$ depending on whether the heat transfer is considered or not. If heat transfer is neglected between the segments, temperatures on all stages are at ambient temperature at the beginning and experience steep gradients during the first minutes of start-up before approaching steady-state temperatures. Steady-state temperatures are reached faster for Case 2 than for Case 1. This can be attributed to the fact that in Case 2, a more accelerating start-up procedure is chosen.

On the contrary, if heat transfer is considered, the initial temperatures of all stages are at the steady-state temperatures of the adjacent segment at $t = 0$ and all temperature profiles pass through a minimum during the first minutes of start-up. This minimum is less pronounced for Case 2 than for Case 1. For the distillate, this minimum is almost inexistent in Case 2 and temperature remains constant at the desired steady-state value during start-up.

The main difference between Case 1 and Case 2 is the point in time, at which the fresh feed is introduced into the segment to be activated. The cold feed disturbs the temperature and, more importantly, the concentration profiles within the segment and delays the approach to a steady-state. This mixing effect is responsible for the minimum that the temperature profiles pass through when heat transfer is considered during start-up. The aim of the adjusted start-up procedure in Case 2 was to minimize this effect. As can be seen in the lower right diagram, the influence of the feed temperature on the temperature profiles on the stages is reduced by delaying the introduction of the feed until a liquid profile is established in the segment. Moreover, the results show that the earlier heat supply reduces the inertia of the column as this decreases the total mass in form of liquid in the column during the start-up process.

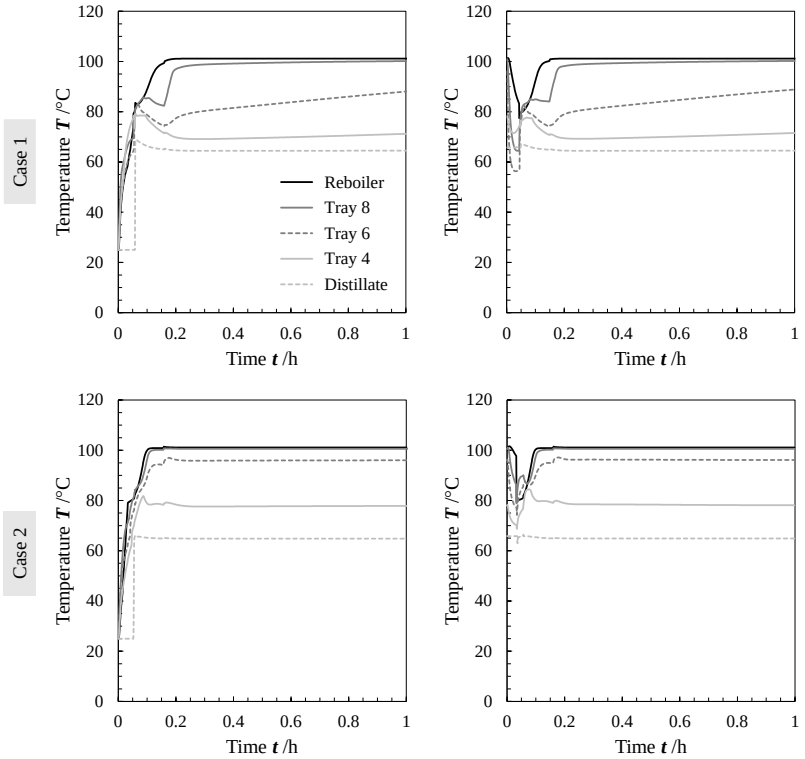

Fig. 3 Evolution of temperature profiles during start-up for different scenarios without (left) and with (right) heat transfer between adjacent segments.

Quantifying the effect of heat transfer between the segments is possible by using the previously defined MX-function (cf. eq. (6)). For Case 1, the start-up duration is reduced by only 1.5%, which is due to the supply of large amounts of cold, fresh feed at $t = 0$ that severely disturbs not only the temperature profiles but also the concentration profiles. In contrast, for Case 2 with an adapted start-up strategy, the start-up duration is further reduced by 65% if accounting for heat transfer to the empty segment.
In conclusion, considering heat transfer between the segments during the operation of the column is an important phenomenon that needs to be considered for adequate modeling. The additional heat that is required to operate single segments in comparison to a conventional column is indeed compensated by reducing the start-up time when additional segments need to be activated.

Conclusions

In this work, we presented the extension of a dynamic modeling approach to describe the start-up of a flexible distillation column. The column consists of unique segments within a single column shell that can be operated and started-up independently. The extension of the pressure-driven model aimed at implementing a description of the heat transfer between the segments to identify the effect of different temperature profiles at the beginning of the start-up operation.
Results showed that considering the heat transfer between the segments before and during start-up significantly influences the evolution of the temperature profiles. Depending on the chosen start-up strategy, start-up duration was affected differently. For a start-up strategy that aims on reducing mixing effects due to the introduction of fresh feed, the consideration of heat transfer between the segments was more important than for a less tailored start-up strategy.
In future work, we want to extend the dynamic, pressure-driven model aiming on the determination of optimal switching points for the start-up of single segments. Therefore, a thorough reformulation using sigmoid functions is necessary to describe the overall range of possible operating points.

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