

Pressure-driven, Dynamic Modeling of Distillation Columns Using Smooth Reformulations to Describe Startup, Shutdown, and Flexible Operation

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Abstract. The dynamic modeling of plants at operating conditions far from the nominal operating point will become increasingly important because of the rising demand for flexibility of these plants. This contribution presents a dynamic, pressure-driven model of a distillation column with trays, which can describe the startup, the dynamic operation in range between nominal and low gas loads, and the shutdown of the column. The contribution discusses the core ideas of the modeling approach and then applies the model on two case studies: the startup of a binary distillation column for the separation of benzene and toluene, and the dynamic operation of a distillation column for the separation of 1,2-dichloroethane, an intermediate of the polyvinyl chloride production. The results obtained for both case studies are then critically discussed to derive recommendations for future experiments, which could improve the model's accuracy.

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Keywords Dynamic pressure-driven modeling, Distillation, Startup, Flexible operation, Demand response

Introduction

The continuing shift towards renewable energies, increasing costs, or variable production demands nowadays require a more flexible operation of chemical plants [1]. In addition, emerging incentives, such as balancing services to stabilize the electricity grid and trade at the energy exchange [2] as well as dynamic process intensification [3] encourage dynamic operation of these plants. However, these trends require more than ever that process models can accurately predict the process dynamics during startup or shutdown as well as in the case of significant load changes or safety-relevant events. As the deviation from the nominal operating point (for which the plant was originally designed) might be much more significant under these new operating conditions, conventional assumptions for dynamic models might not hold and new phenomena, such as the (dis)appearance of phases, weeping, or entrainment, must be considered in the model. Otherwise, the allowable operating window or the time constants for load changes under flexible operation cannot be accurately assessed. Consequently, several research groups have given attention to this topic in the recent years: Kender et al. [4] proposed a dynamic, pressure-driven model of a distillation column with packed bed and used this model to simulate the dynamic operation of air separation units. Bruns et al. [5] presented the innovative idea of a segmented distillation column, in which the number of used segments depends on the current load of the plant, and modeled this process dynamically. Finally, the authors proposed recently [6] a dynamic, pressure-driven model, which will be discussed in the following paragraphs. This model is used to (1) simulate the startup of a distillation column and (2) optimize flexible operation of a separator for 1,2-dichloroethane under demand response to demonstrate its fidelity for various applications.

Model formulation

The model consists of several sub-models, i.e., the condenser, the reflux drum, the trays, the downcomers, and the reboiler. The condenser is assumed to operate at steady-state and both a mole and an energy balance are considered. The dynamics are therefore completely shifted to the reflux drum whose holdup may change during operation. Two controllers control the level of the reflux drum (via the product flow) and the temperature at the top (via the reflux). The trays are modeled according to the UV flash [7], i.e., the tray is specified in terms of its internal energy and the available tray volume. Dynamic mole and energy balances are formulated that contain the streams visualized and explained in **Fig. 1**. Because there are no additional assumptions on vapor or liquid holdup, both vapor and liquid outlet flows must be expressed via algebraic equations to achieve an index-1 differential-algebraic equation (DAE) system. For the liquid flow over the weir, the Francis weir equation is used whereas the weeping liquid is modeled according to Staak et al. [8]. The vapor flow appears in the equation for the liquid pressure drop for which the expression derived by Bennett et al. [9] is applied. Thus, the vapor flow becomes pressure-driven because the flow between two trays is

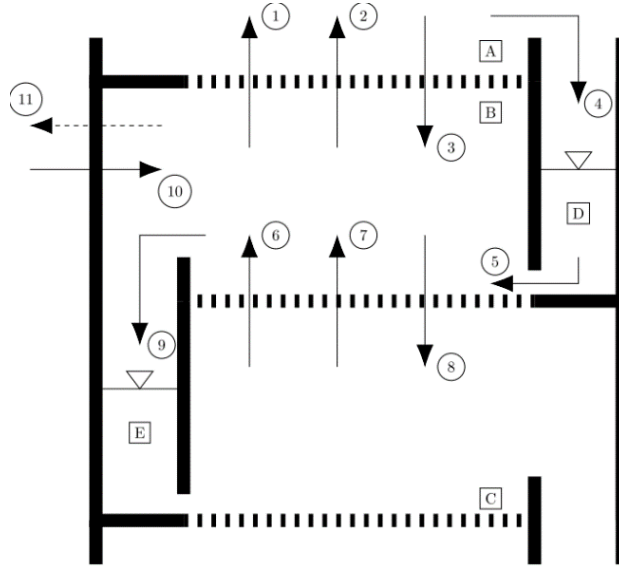


Fig. 1 Visualization of the modeled tray including the streams that are considered for the model formulation [6]. 1: vapor outlet from tray t ; 2: liquid outlet from tray t due to entrainment; liquid inlet 3: from the tray above due to weeping; 4: flow over the weir from tray $t - 1$; 5: liquid outlet from downcomer into tray t ; 6: vapor inlet from tray $t + 1$; 7: liquid inlet due to entrainment, 8: liquid outlet due to weeping; 9: liquid outlet from tray t over the weir into downcomer below; 10: feed; 11: heat loss.

determined by the respective pressure difference. In addition, liquid and vapor volume must be equal to the geometric tray volume. It is assumed that liquid and vapor phase are ideally mixed. Moreover, they can either be in equilibrium or the equilibrium can be corrected via Murphree efficiencies.

The downcomer sub-model consists of a dynamic mole balance that considers the flow over the weir from the tray above and the flow under the downcomer apron. The liquid level in the downcomer depends on the pressure difference between the trays, the hydrostatic pressure on the next tray, and the pressure drop due to the flow under the apron. Therefore, the model includes additional and independent holdups in the downcomer. At this point, the following assumption is made: if there is no vapor flow from the bottom, the levels of downcomer and tray strive to balance each other out, which is modeled via an expression equivalent to a proportional controller. Once the vapor flow is activated on the tray, the outlet flow of the downcomer is given by the pressure drop below the apron. To the authors knowledge, there are no experiments available that confirm or contradict this assumption. The choice of the proportionality constant might, however, have a significant effect on the process dynamics and is therefore of importance for modeling safety-relevant events.

Finally, the reboiler also features dynamic mole and energy balances. A controller sets the reboiler duty to achieve the desired temperature. This controller and the controllers at the top of the column can be turned on and off manually, e.g., to model shutdown.

The core feature of the model is its ability to model the (dis)appearance of the vapor phase, e.g., during startup or shutdown. This is realized via a smoothened sigmoidal function:

$$\theta = 0.5 + \left(1 + \frac{T_t - T_t^{VL}}{\sqrt{(T_t - T_t^{VL})^2 + (10)^{-10}}} \right). \quad (1)$$

This function takes the current tray temperature T_t and compares it to the boiling temperature T_t^{VL} for the current liquid composition. If both temperatures are equal, the function θ switches from zero to one. This activates thermodynamic equilibrium

$$y_{t,c} \cdot P_t = x_{t,c} \cdot P_{0,c}^{VL} \cdot \theta_t, \quad (2)$$

vapor flow

$$(T_t^{VL} - T_t) \cdot \psi_t + (1 - \psi_t) \cdot F_t^V = 0, \quad (3)$$

and vapor holdup

$$HU^{V,actual} = HU^V \cdot \theta_t. \quad (4)$$

The weeping model by Staak et al. uses a corrected Torricelli equation:

$$F_t^{weep} = \sqrt{2 \cdot g \cdot h_{cl,t}} \cdot A_{active} \cdot \varphi \cdot \Omega_t \quad (5)$$

in which the g is the gravitational acceleration, $h_{cl,t}$ is the height of clear liquid on tray t , A_{active} is the active tray area, and the weeping parameter Ω depends on the F factor and the free-area fraction φ . To obtain a differentiable expression, the min operator proposed by Staak et al. [8] was mathematically smoothened. A comparison between both expressions is shown in **Fig. 2**. A similar reformulation is used for cases in which the liquid level on a tray is smaller than the weir height. For these situations, a smoothened version of a max operator is applied, which ensures that all constraints hold even if the height above the weir is negative [10]. A much more extensive description of the model can be found in Hoffmann et al. [6; 10].

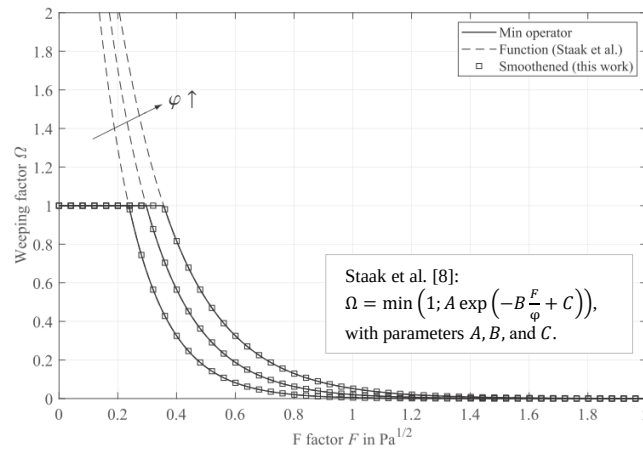


Fig. 2 Representation of the smoothened form of the weeping factor [10]. The parameters A , B , and C can be found in [8].

Case studies

The outlined model has been used in two case studies, i.e., the simulation of a column startup for the system benzene-toluene and the optimal operation of a 1,2-dichloroethane separator under demand response scenarios. **Table 1** shows the key parameters of both case studies. In case study 1, the column is initially empty. Once the feed has filled the bottom, the internal reboiler (volume of 0.8 m³) is started and the temperature increases tray-by-tray until a steady-state operation is achieved. As soon as the reflux drum (volume of 1.6 m³) is filled, level and temperature control at the top are activated. For the distillation column, 10 trays and a diameter of 1 m are chosen. The most sensitive tray temperatures in rectifying and stripping section are controlled via reflux ratio and reboiler duty, respectively.

In case study 2, the distillation column is located on top of a reactor in which chlorine and ethene react to 1,2-dichloroethane (DCE). DCE is a storable intermediate in the production of polyvinyl chloride. Unreacted chlorine or ethene leave the column whereas DCE is removed as a side stream. In addition, the high-boiling byproduct 1,2,3-trichloroethane (TCE) is removed at the bottom where an additional heat exchanger removes some of the heat generated by the reaction. The flowsheet is schematically shown in **Fig. 3**. The chlorine comes from a flexibly operated chloralkali electrolysis. Therefore, the chlorine feed varies over time between 70 and 105 % of the nominal load. To counteract the fluctuating chlorine feed, the ethene feed, the product flow, the reflux, and the heat removed in the additional heat exchanger at the bottom of the column can be manipulated.

The model has been formulated in MOSAICmodeling [11]. Case study 1 has been solved in gPROMS v5.1.1 [12] via the MOSAICmodeling export. For case study 2, the model has been fully discretized in time via orthogonal collocation and exported to AMPL [13] to optimize the trajectories of manipulated variables simultaneously on a time horizon of 45 minutes. The dynamic optimization for the fluctuating chlorine feed has been realized in a Python-AMPL framework in which IPOPT [14] is used to solve the optimization problem over a moving time horizon.

Table 1. Key data of both case studies.

Parameter	Case study 1	Case study 2
Feed	Benzene and toluene, equimolar	Chlorine and ethene, preferred ratio of 1:1.2
Pressure	1 bar	ca. 2 bar
Product purity	Top product > 85 % (molar), bottom product > 90 %	DCE > 99.85 % (molar)
Diameter	1 m	2.8 m
Number of trays	10 + reboiler	19

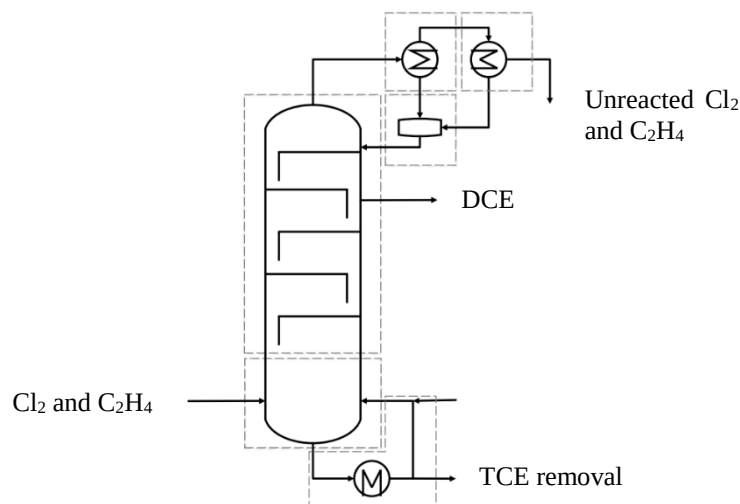


Fig. 3 Flowsheet of case study 2. The grey boxes mark the sub-models, i.e., the two partial condensers, the reflux drum, the trays, the reactor, and the bottom section with a heat exchanger.

Results and discussion

Fig. 4 shows the startup profiles of temperature and liquid mole fraction between the initial point and 1.5 hours for case study 1. The temperature remains constant as long as the feed fills up the bottom of the column. Once a certain level threshold is achieved, the reboiler heats up the bottom. The temperature slope during this heat-up time is almost linear according to the molar heat capacities of both components. The temperatures of the trays do not change during this period. This behavior can also be observed in real plants during startup. As soon as the boiling point in the bottom is reached, the sigmoidal of the bottom switches to one and the vapor flow begins to heat up the trays. This is typically much faster because of the smaller holdups on the trays. When the tray temperature reaches the respective boiling point on this tray, the sigmoidal on this tray also switches from zero to one and thus the temperature profile slowly forms until the vapor reaches the top of the column. At this point, the temperature remains almost constant and the reflux reaches its steady-state value and the remaining benzene in the bottom is evaporated. After approximately one hour, the steady-state operating point is reached. The results show that it is possible to formulate a differentiable equation system that allows the dynamic simulation of startup (and shutdown) of a distillation column. This would of course also apply to batch distillation columns. The obtained profiles seem realistic as they match quantitatively with experimental profiles obtained by our research group (e.g., [15]). Nevertheless, the profiles should be analyzed qualitatively as well. Many of the included assumptions and correlations were derived under steady-state conditions – transient profiles, e.g., for the weeping flow, are to the best of our knowledge still unavailable. They are, however, important to assess the expected vapor flow and pressure peak in a distillation column in case the reboiler malfunctions and a large amount of light-boiling component weeps through the column and is evaporated in the hot bottom. For this reason, experiments will be conducted in our lab to study these phenomena.

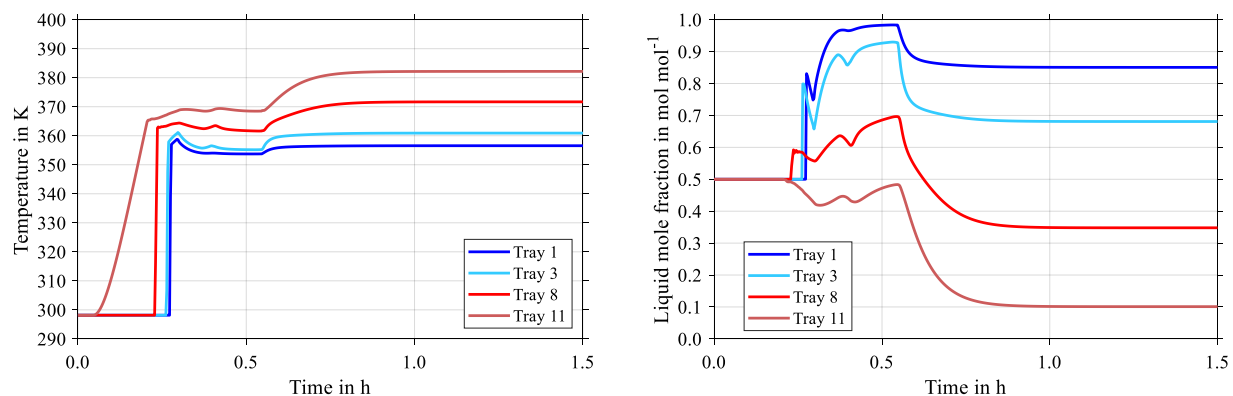


Fig. 4 Profiles of temperature (left) and liquid mole fraction of benzene (right) during startup on four different trays (case study 1). Trays are counted from top to bottom.

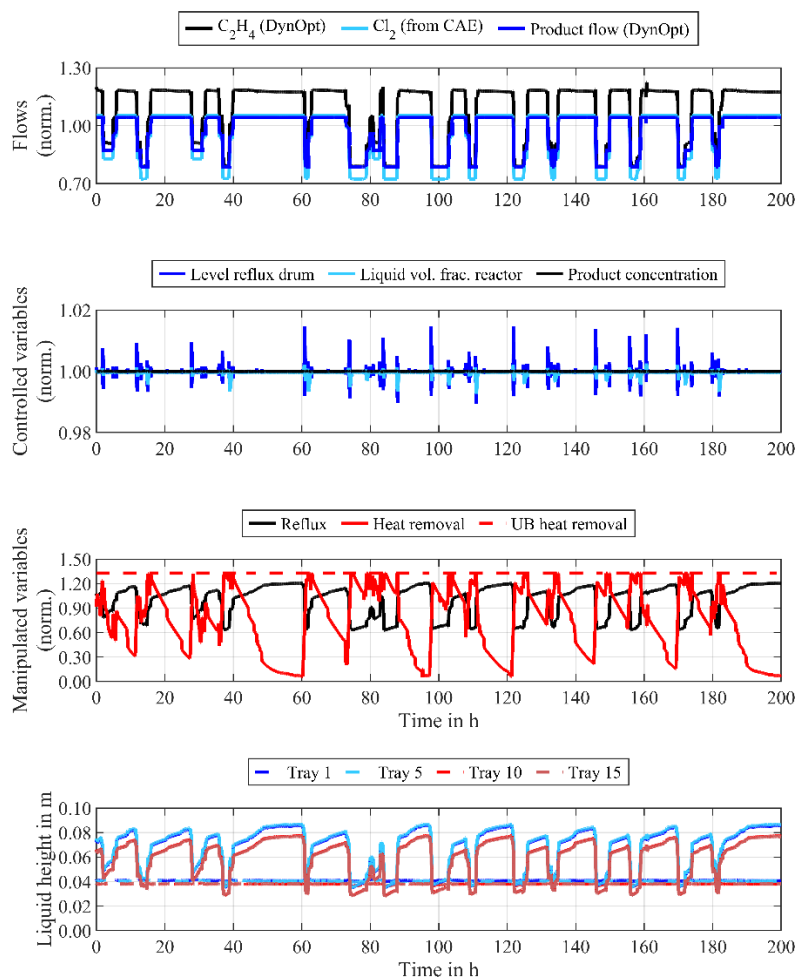


Fig. 5 Dynamic profiles of flows (top), controlled variables (top middle), manipulated variables (top bottom), and liquid heights (bottom) for case study 2. In the bottom figure, the dashed lines represent the height of the clear liquid whereas the continuous lines represent the height above the weir (the same color is used for variables that belong to the same tray). The first three figures are normalized as the results represent an actual industrial process.

Fig. 5 shows the results obtained for case study 2. Note that relevant variables have been normalized as the simulation is based on industrial data. The top subfigure visualizes how the chlorine feed changes over time because of the dynamic operation of the chloralkali electrolysis. Consequently, the optimizer adapts the ethene feed to the chlorine

feed. In addition, the product flow must match the ingoing streams. The second subfigure illustrates that the level in the reflux drum, the liquid volume fraction in the reactor, and the product concentration remain at their desired setpoints. The third subfigure shows the manipulated variables, i.e., the degrees of freedom in the optimization problem. During load increases, the heat removed by the heat exchanger at the bottom first increases due to an increased heat flow due to the reaction. When the heat flow reaches its upper bound, the heat removal decreases and the reflux increases. A more thorough discussion and the implications of these results for demand response can be found elsewhere [16].

The last subfigure illustrates the different liquid levels on different trays: the height of the clear liquid (dashed lines) and the height above the weir, which appears in the Francis weir formula. The model predicts that the liquid holdup on the tray (represented by the height of the clear liquid) hardly changes during operation. However, the height above the weir fluctuates, which indicates a varying weir load in the column over time. Such variations cannot be observed in models that apply the often-used assumption of constant holdup on a tray.

Conclusion and outlook

This contribution presented the application of a dynamic, pressure-driven model for distillation columns with trays that can be used for startup, shutdown, or dynamic operation of continuous and batch distillation columns. To demonstrate its applicability, the model was formulated for two case studies – the startup of a continuous distillation column to separate benzene and toluene, and a dynamically operated separator for 1,2-dichloroethane. Case study 1 showed that the model is able to qualitatively predict reasonable temperature and composition profiles during startup. Furthermore, case study 2 demonstrated that the model is also robust enough for dynamic optimization. In the future, we will study the dynamics of the included phenomena, such as weeping, for various tray types in our lab facilities to improve its overall accuracy and to make it applicable to safety-related events. In addition, the model will be extended to include phenomena at high gas load, such as flooding. This had not been included so far because it is challenging to describe the movement of the liquid on a flooded tray.

Acknowledgements

The authors gratefully acknowledge the financial support of the German Federal Ministry of Economic Affairs and Energy for the project ChemEFlex (project number 0350013A).

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