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Finding better limit cycles of semicontinuous distillation. Part 1: Back-stepping design Methodology

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Abstract

Semicontinuous ternary zeotropic distillation is a periodic process that is carried out in a single distillation column and a tightly integrated external middle vessel. In the state-of-the-art design procedure of this process, a continuous distillation process that separates the top and bottoms products to the desired purity is used to generate an arbitrary initial state for simulating the dynamics of the semicontinuous distillation process. Although this method is useful in estimating the limit cycle, it was later found that the operation of the process in this limit cycle was economically sub-optimal. In this study, a new algorithmic design procedure, called the back-stepping design methodology, is proposed to find better limit cycles for zeotropic ternary semicontinuous distillation using the aspenONE Engineering suite. The proposed methodology was applied to two different case studies using feed mixtures with different chemical components. A comparison with the current design procedure for the two case studies indicates that the new method outperforms the state-of-the-art by finding limit cycles that were 4% to 16% lower in separating cost, which was the chosen measure of cycle performance.

Introduction

The concept of semicontinuous distillation is intended for multicomponent separations, which are carried out in the intermediate production range. This intensified process has desirable features like higher flexibility, and lower capital investment than equivalent continuous distillation processes[1]. Indeed, the basis for process intensification was on its traditional viewpoint[2] rather than the newly developed concept of dynamic intensification by Yan et al.[3], who focused on operational regime changes. In their work, dynamic intensification in process plants was illustrated by using the properties of output multiplicity to devise a new periodic operating mode for binary distillation.

Industries undergoing a production scale-up from the batch mode, and separations in distributed biofuel production plants are ideal cases to implement the semicontinuous distillation process[4,5]. A semicontinuous configuration was illustrated to be beneficial in terms of cost and energy utilization in heterogeneous azeotropic distillation by Tabari and Ahmad[6] using dehydration of acetic acid as a case study. In this article, however, the focus is on the semicontinuous distillation of zeotropic ternary mixtures, which requires two pieces of equipment for separations of ternary mixtures: a distillation column and a process vessel called the middle vessel, and a control system which drives the process[4] (Figure 2). The batches of feed to be distilled are fed periodically to the middle vessel, which in turn continually feeds the distillation column. Simultaneously, a side stream from the distillation column is continually recycled to the middle vessel. The low and high volatile components in the ternary mixture are continually removed from the top and bottom of the distillation column, while the intermediate boiling component is periodically discharged from the middle vessel. This process is, therefore, different from cyclic distillation, which is a cyclic operating mode for the operation of distillation columns. The cyclic operation comprises of a vapor flow period when liquid is stagnant and a liquid flow period when vapor flow is stopped to improve energy use, increased throughput and separation performance[7].

Semicontinuous distillation is an example of an autonomous hybrid limit-cycle oscillator[8], which was defined mathematically by Khan et al. State-dependent discrete input actions, such as the periodic feed charges and product discharges, are responsible for changes in the system dynamics at discrete instants in continuous time, making it a hybrid system. Unlike continuous distillation, this process operates in a limit cycle (Γ), which is the periodic solution of the equations describing the semicontinuous distillation process. The design of the process involves finding the time-invariant parameter vector, $\mathbf{p}$, to operate the process in a desirable limit cycle. Typically, the metric that is used to evaluate the performance of a design is the separating cost, defined as the total annualized cost-per-production rate of a product.

In order to estimate the limit cycle of a semicontinuous distillation system for a particular value of $\mathbf{p}$, all previous studies[1,5,9–14] had relied on the 'brute force method[15]'. In this method, a dynamical system is numerically integrated to estimate the steady state (in this case, a limit cycle) by starting from an arbitrary initial state, provided this initial state is within the basin of attraction[15]. Although it is a reliable method, it suffers from limitations, such as linear convergence[16], and difficulty in steady-state identification. Despite these limitations, in this study, the brute force approach was chosen because it offers a practical way to approach a cycle (startup), and it features a simple computational method.

All previous studies[5,10–12,17,18] that used the brute force method determined the arbitrary initial state by designing a continuous distillation process (referred to as continuous middle vessel-column system in this study) which comprises of a distillation column with a side draw (Figure 1 - Top left). The continuous distillation process is designed to meet the top and bottoms product purities that is desired in the semicontinuous distillation process. However, the side draw does not satisfy the necessary purity requirements of the intermediate product.

The state of this process (represented by E) only roughly approximates the semicontinuous system's true state in a semicontinuous cycle (Figure 1 - Top right, and Figure 1 - Bottom). This approach was an effective way of obtaining a consistent initial condition that satisfied the dynamic model equations of the semicontinuous distillation system. From this state, the brute force method is applied to estimate the limit cycle, Γ (Figure 1 - Bottom). Furthermore, the continuous distillation process was used to estimate equipment sizes such as column diameter, side stream pump capacity, and valve sizes to be used in semicontinuous distillation. A stochastic optimizer was typically used to find a better semicontinuous distillation design by using the separating cost as the objective function and the controller tuning parameters as design decision variables.

The above described design methodology was known as the sequential design methodology and was first used by Pascall and Adams [5]. Later, Meidanshahi and Adams [11] included integer design decision variables in the optimization formulation along with the controller tuning parameters to find cost-effective designs.

Subsequently, Madabhushi and Adams [13] demonstrated the importance of the side stream flowrate function on process economics. The study directly leads to the hypothesis that the upper bound of the side stream flowrate (S^u), which is related to the side stream pump and valve design, is an important parameter in the search for finding cost-effective designs. The hypothesis was tested in the study by Madabhushi et al. [14], where the combined effect of changing S^u and the point E (in particular, the state of the distillation column) was demonstrated to have an impact on the cycle time (period T). This effect was also briefly demonstrated by Pascall and Adams [5]. Note here that varying S^u and the point E indirectly corresponds to changing the semicontinuous distillation system's time-invariant parameters and therefore affects the limit cycle wherein the system operates. Although these studies have shown that higher side stream recycle rates to the middle vessel could be advantageous,

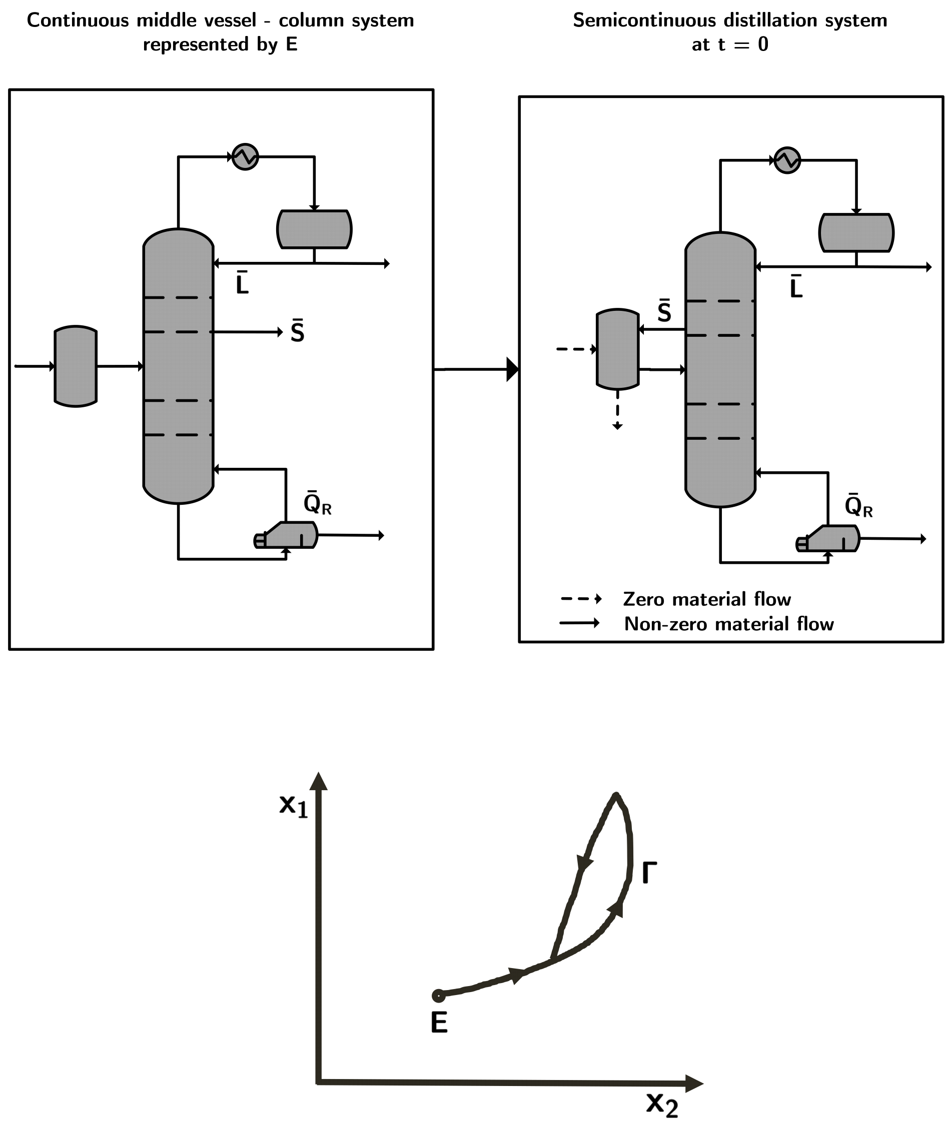

Figure 1: Top left: A schematic of the hypothetical continuous middle vessel-column system used for equipment design and to determine an arbitrary initial state for the semicontinuous system. Top right: A schematic of the semicontinuous distillation system at $t = 0$ on which the brute force method is applied. Bottom: An illustration of the evolution of the system trajectory in state space when applying the sequential design methodology.

care should be taken to ensure that the design is hydraulically feasible throughout the operation in the limit cycle to guarantee efficient separation.

The sequential design methodology does not prescribe a procedure to change the arbitrary initial state (E) once it is determined. However, varying this state is possible by changing the side stream flowrate ($\bar{S}$), the reflux rate ($\bar{L}$), and the reboiler duty ($\bar{Q}_R$), i.e., altering the design of the continuous middle vessel-column system. Variables are affixed with an overbar to indicate that they correspond to the point, E. Therefore, this paper builds upon the results reported by Madabhushi et al.[14] and presents a new algorithmic design procedure for semicontinuous distillation design, referred to as the 'Backtracking design methodology'. The application of this design procedure for semicontinuous distillation design in the aspenONE simulation environment is demonstrated using two different case studies. Most semicontinuous distillation studies have used Aspen Plus and Aspen Plus Dynamics software to simulate the semicontinuous distillation process, primarily due to the availability of rigorous process and physical property models. The scope of the new procedure is limited to finding the point E and S^u, which can lead to better feasible Γ in terms of cost than the state-of-the-art methodology. The next two sections focus on the detailed process description and a brief mathematical description of the process.

Detailed process description

The semicontinuous distillation system is comprised of three sub-systems (Figure2): the middle vessel, the distillation column, and the control system. The middle vessel sub-system has four material streams – two inlet streams and two outlet streams. However, the number of streams in use at any given time (i.e., non-zero flowrates) will always be less than the total number of available material streams. At the beginning of the cycle, the middle vessel contains the feed to be separated at a pre-specified upper limit in liquid height (h_v^u).

The liquid mixture in the middle vessel is separated into its constituents in the distillation column by drawing the most volatile component (A) from the distillate, the least volatile component (C) from the bottoms, and gradually concentrating the middle vessel with an intermediate volatility component (B) by recycling the side stream. Once product B has reached the desired level of purity in the middle vessel ($x_{B,v}^{desired}$), the contents of the middle vessel are discharged. Liquid is drawn from the middle vessel through the discharge stream ($F_d(t)$) while it continues to feed the distillation column. Once the height of liquid in the middle vessel ($h_v(t)$) reaches a pre-specified lower limit (h_v^l), the liquid discharge is stopped and fresh feed is charged ($F_c(t)$) to the middle vessel. The mixture to be separated is fed to the middle vessel while also still being fed into the distillation column. When the liquid height, $h_v(t)$, reaches a pre-specified upper limit (h_v^u) it signifies the end of the cycle. These switches in the operation are based on the state of the middle vessel sub-system. These states of the middle vessel can be classified into three modes of system operation, which are: separating mode, discharging mode, and charging mode[4].

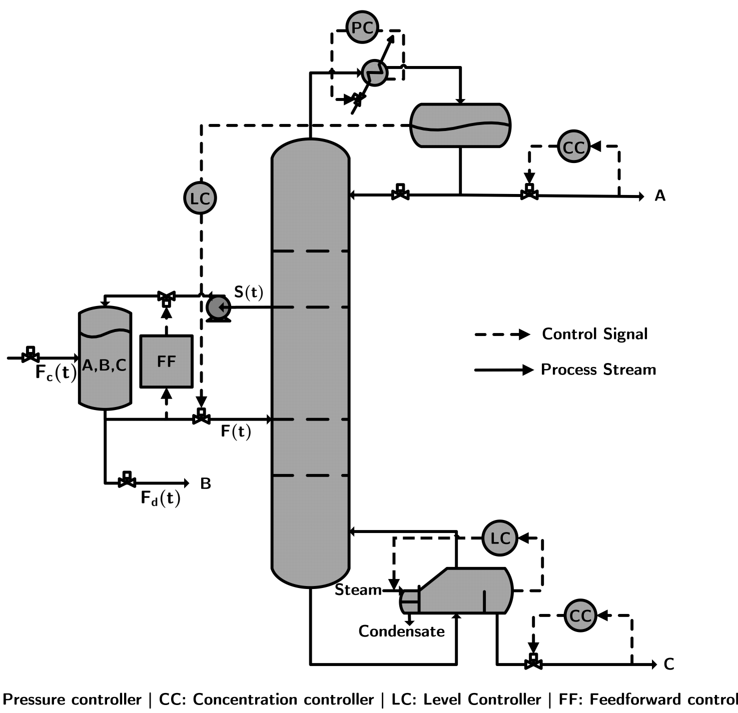

Figure 2: A schematic of the semicontinuous distillation system.

During all the three modes, the concentration of feed components changes continuously with time. Since the process is not self-regulating, a control sub-system is used to maintain the control outputs at the desired values. The most frequently used control sub-system in semicontinuous distillation studies was designed by Pascall and Adams[5]. In a subsequent study, Madabhushi and Adams[13] demonstrated that modifying the control configuration – specifically the side stream flow rate control – produced significant economic benefits. Madabhushi and Adams[13] controlled the side stream flow rate using the Modified - ideal side draw recovery feedback control implemented using a PI controller. The setpoint of the controller is varied according to Equation 1,

$$S_{MISR}(t) \coloneqq \frac{F(t)x_{B,v}(t)}{x_{B,S}(t)} \tag{1}$$

where $x_{B,v}(t)$ is the mole fraction of B in the middle vessel, and $x_{B,S}(t)$ is the mole fraction of B in the side stream.

Mathematical description

The mathematical model of the semicontinuous distillation process falls under the category of hybrid (discrete/continuous) limit-cycle oscillators, which allow for the presence of both discrete and continuous state trajectories that are closed, isolated, and time-periodic[8]. The continuous-time dynamics of this process varies in different 'discrete states' as a result of the changes to the mass and energy balance equations of the middle vessel sub-system. Changes to these equations are because of instantaneous events like the feed charges and product discharges, which alter the number of input streams to, and output streams from the middle vessel. A discrete state is the active mode of the process[19], which are: separating mode (mode 1), discharging mode (mode 2), and charging mode (mode 3). The mode trajectory (order of the modes visited by the system's discrete state) in a semicontinuous distillation cycle is as follows: $\{1, 2, 3, 1\}$. The mode-specific material balance, fugacity relations, summation equations, enthalpy balance, and hydraulic flow equations are represented compactly as:

$$\mathbf{f}^{(k)}(\dot{\mathbf{z}}^{(k)}, \mathbf{z}^{(k)}, \mathbf{y}^{(k)}, \mathbf{u}^{(k)}, \mathbf{p}) = \mathbf{0}, \ k = 1, 2, 3 \tag{2}$$

where $\mathbf{z}$ represents the differential states, $\mathbf{y}$ represents the algebraic states, $\mathbf{u}$ represents the vector of the control variables, $\mathbf{p}$ represents the vector of time-invariant parameters such as equipment design variables and the tuning parameters of the controllers in the modified Pascall-Adams multi-loop control configuration. The index that designates the discrete state is represented by k. As an example, the middle vessel sub-system's component mass balance in the three modes would be,

$$\text{mode 1}: \left\{ \frac{\mathrm{d}M_\alpha^{(1)}(t)}{\mathrm{d}t} = S^{(1)}(t)x_{\alpha,S}^{(1)}(t) - F^{(1)}(t)x_{\alpha,v}^{(1)}(t), \quad \alpha = A, B, C \right. \tag{3}$$

$$\text{mode 2}: \left\{ \frac{\mathrm{d}M_\alpha^{(2)}(t)}{\mathrm{d}t} = S^{(2)}(t)x_{\alpha,S}^{(2)}(t) - F^{(2)}(t)x_{\alpha,v}^{(2)}(t) - F_d^{(2)}(t)x_{\alpha,v}^{(2)}(t), \quad \alpha = A, B, C \right. \tag{4}$$

$$\text{mode 3}: \left\{ \frac{\mathrm{d}M_\alpha^{(3)}(t)}{\mathrm{d}t} = F_c^{(3)}(t)x_\alpha^{(3)}(t) + S^{(3)}(t)x_{\alpha,S}^{(3)}(t) - F^{(3)}(t)x_{\alpha,v}^{(3)}(t), \quad \alpha = A, B, C \right. \tag{5}$$

where, α designates the components A, B, and C, respectively, and $M_\alpha(t)$ is the liquid molar holdup of the component, α, in the middle vessel.

The transition from one mode to another (discrete dynamics) is based on a transition condition ($L_j^{(k)}$), where j is the next mode in the sequence[20]. Ternary semicontinuous distillation has three simple transition conditions, which are:

$$L_2^{(1)} : x_{B,v}^{(1)} \geq x_{B,v}^{desired} \tag{6}$$

$$L_3^{(2)} : h_v^{(2)} \leq h_v^{l} \tag{7}$$

$$L_1^{(3)} : h_v^{(3)} \geq h_v^{u} \tag{8}$$

with the superscripts l, and u representing the pre-defined lower and upper limits, respectively. Since these are state dependent transitions, the event time is implicitly defined by these conditions. Specifically, these transitions are triggered by discrete control signals computed based on the system's state. Thus, the closed-loop hybrid system is an autonomous-switch hybrid limit-cycle oscillator[21]. Given that commercial process-simulation software can simulate such systems, the aspenONE Engineering suite was used in this study because of its rigorous phenomenological and control models available in the process model library, which makes it easier to model the semicontinuous distillation sub-systems. The discrete dynamics were modeled using the "Tasks" functionality in Aspen Plus Dynamics V10[22]. In this study, the focus is on designing the system using the aspenONE Engineering suite by varying the side stream pump and valve capacities (via $\bar{S}$), the controller tuning parameters, and the reflux rate ($\bar{L}$), which are time-invariant parameters in the semicontinuous distillation model.

Design - Optimization problem formulation

The point E, which refers to the steady-state solution of the continuous middle vessel-column system in the sequential design methodology does not represent any of the three modes of semicontinuous distillation. This state is used as the arbitrary initial state (E) for applying the brute force method on the semicontinuous distillation model. In the sequential design methodology, identifying a specific separation to be carried out in the continuous middle vessel-column system, for example, separating the top and bottoms products to the desired purity, locks the value of the reflux rate (a time-invariant parameter) in the semicontinuous distillation model to $\bar{L}$. Additionally, the side stream flowrate ($\bar{S}$), a degree of freedom of the continuous middle vessel-column system, is used to determine the capacities of the semicontinuous distillation system's side stream pump and valve, which are also fixed parameters in the semicontinuous distillation model. Therefore, to change the limit cycle in which the semicontinuous distillation process operates, the continuous middle vessel-column design should be altered by varying its degrees of freedom ($\bar{S}$, $\bar{L}$, and $\bar{Q}_R$). Although $\bar{Q}_R$ is not a time-invariant parameter of the semicontinuous distillation system, it is included here because its choice could affect the selection of the modified Pascall-Adams controller tuning parameters.

A set (Θ) can be defined to contain all possible continuous middle vessel-column steady-states that can be generated by varying the values of $\bar{S},\ \bar{L},\ \bar{Q}_R$.

$$\Theta = \{(\bar{\mathbf{z}},\ \bar{\mathbf{y}}) : \mathbf{f}^{(E)}(\mathbf{z},\ \mathbf{y},\ \bar{S},\ \bar{L},\ \bar{Q}_R) = \mathbf{0}\} \tag{9}$$

where $\mathbf{f}^{(E)}$ is a system of nonlinear algebraic equations that describes the continuous middle vessel-column system. The optimization problem ($\mathbf{P}$) to be solved to find the best semi-continuous distillation design in the space of the design variables considered, which includes selecting E from Θ is shown below,

$$
\begin{aligned}
\underset{\bar{S},\,\bar{L},\,\bar{Q}_R,\,\mathbf{p}'}{\text{minimize}} \quad & SC^{(\Gamma)} \\
\text{subject to} \quad & \mathbf{f}^{(k)}(\dot{\mathbf{z}}^{(k)}, \mathbf{z}^{(k)}, \mathbf{y}^{(k)}, \mathbf{u}^{(k)}, \mathbf{p}) = \mathbf{0},\ k = 1, 2, 3 \\
& \text{mode 1 (Separating Mode)} : \begin{cases} L_1^{(3)} : h_v^{(3)} \geq h_v^u \\ F_c(t) = 0 \\ F_d(t) = 0 \end{cases} \\
& \text{mode 2 (Discharging mode)} : \begin{cases} L_2^{(1)} : x_{B,v}^{(1)} \geq x_{B,v}^{desired} \\ F_c(t) = 0 \\ F_d(t) = F_d \end{cases} \\
& \text{mode 3 (Charging mode)} : \begin{cases} L_3^{(2)} : h_v^{(2)} \leq h_v^l \\ F_c(t) = F_c \\ F_d(t) = 0 \end{cases} \\
& \text{Hydraulic constraints}^{\ (\Gamma)} \\
& \text{Quality constraints}^{\ (\Gamma)} \\
& \text{Variable bounds} \\
& \mathbf{f}^{(E)}(\mathbf{z},\ \mathbf{y},\ \bar{S},\ \bar{L},\ \bar{Q}_R) = \mathbf{0}
\end{aligned}
$$

where, $\mathbf{p}'$ represents the controller tuning parameters and is a subset of $\mathbf{p}$. In this study, Aspen Plus V10 was used to design the continuous middle vessel-column system. The arbitrary initial state (E) that was generated in Aspen Plus V10[23] by solving the nonlinear system, $\mathbf{f}^{(E)}$, was used to start the numerical integration of the differential-algebraic equations (DAEs) describing the semicontinuous distillation process, which was carried out in Aspen Plus Dynamics V10.[22] The objective function was evaluated only after converging to the limit cycle (Γ) because it is a metric that is defined for the limit cycle and not elsewhere. Similarly, the hydraulic constraints (flooding, weeping, and weir loading), which are inequality-path constraints with an implicit dependence on state variables, should be satisfied during column operation in the limit cycle. The quality constraints are mass-average purities of the top and bottoms products (end-point constraints), which have to be satisfied at the end of Γ. In practice, however, different blending/mixing tanks are used (column downstream) to collect and blend the top and bottoms products separately over the time period of the cycle so as to ensure on-spec product quality.

Simulation of the embedded system in P

Simulating the embedded hybrid system in the optimization problem, $\mathbf{P}$, using the aspenONE Engineering suite is a two-step process as briefly described above. An initial condition for the dynamic simulation of semicontinuous distillation process was obtained by first solving the continuous middle vessel-column equations in the Aspen Plus steady-state simulation software[23]. All equipment sizes, including the side stream pump and valve, were determined at this stage using the steady-state flowrates. The simulation was then exported to the Aspen Plus Dynamics software to simulate the dynamic behavior. Once the equipment sizes were fixed, solving $\mathbf{f}^{(E)}$ within the Aspen Plus Dynamics V10[22] environment to generate a new E with a different side stream pump and valve size proved to be challenging because of numerical convergence issues. Therefore to overcome this practical issue, the idea of using a control system to move from one steady state to another for a fixed side stream pump and valve size was implemented in Aspen Plus Dynamics V10. Nevertheless, the new design methodology also includes a procedure to change the side stream pump and valve capacities (thus affecting S^u) and is discussed in the subsequent section.

Modifications were made to the continuous middle vessel-column model in Aspen Plus V10 to implement the idea mentioned above, and thus, the semicontinuous distillation model in Aspen Plus Dynamics V10. The continuous middle vessel-column model was modified in

Aspen Plus V10 to include two side streams: S_1, recycled to the middle vessel with zero liquid flowrate, and S_2, wherein there was liquid flow, but was not recycled to the middle vessel. A new control system, called the continuous control configuration, was added to this modified continuous middle vessel-column superstructure in Aspen Plus Dynamics V10 to transition from one steady state to another. This control system was in addition to the modified Pascall-Adams control configuration used in semicontinuous distillation. The continuous control configuration includes two flowrate controllers: one for feed flow, and one for column side stream flow (S_2). It further includes two level controllers, which maintain the reflux drum and sump levels by varying the distillate and bottoms flowrates, respectively. The modified continuous middle vessel-column state was moved from one E to another by introducing a step change in the setpoint of the S_2 flowrate controller, the reflux rate ($\bar{L}$), and the reboiler duty $\bar{Q}_R$, while maintaining the feed flow rate. This process results in the addition of a new mode called continuous mode or mode 0. This mode precedes modes, 1, 2, and 3 in the hybrid system description of the semicontinuous process. Figure 3 illustrates the superstructure that was used to enable the mode transition from the continuous regime to the semicontinuous operating regime.

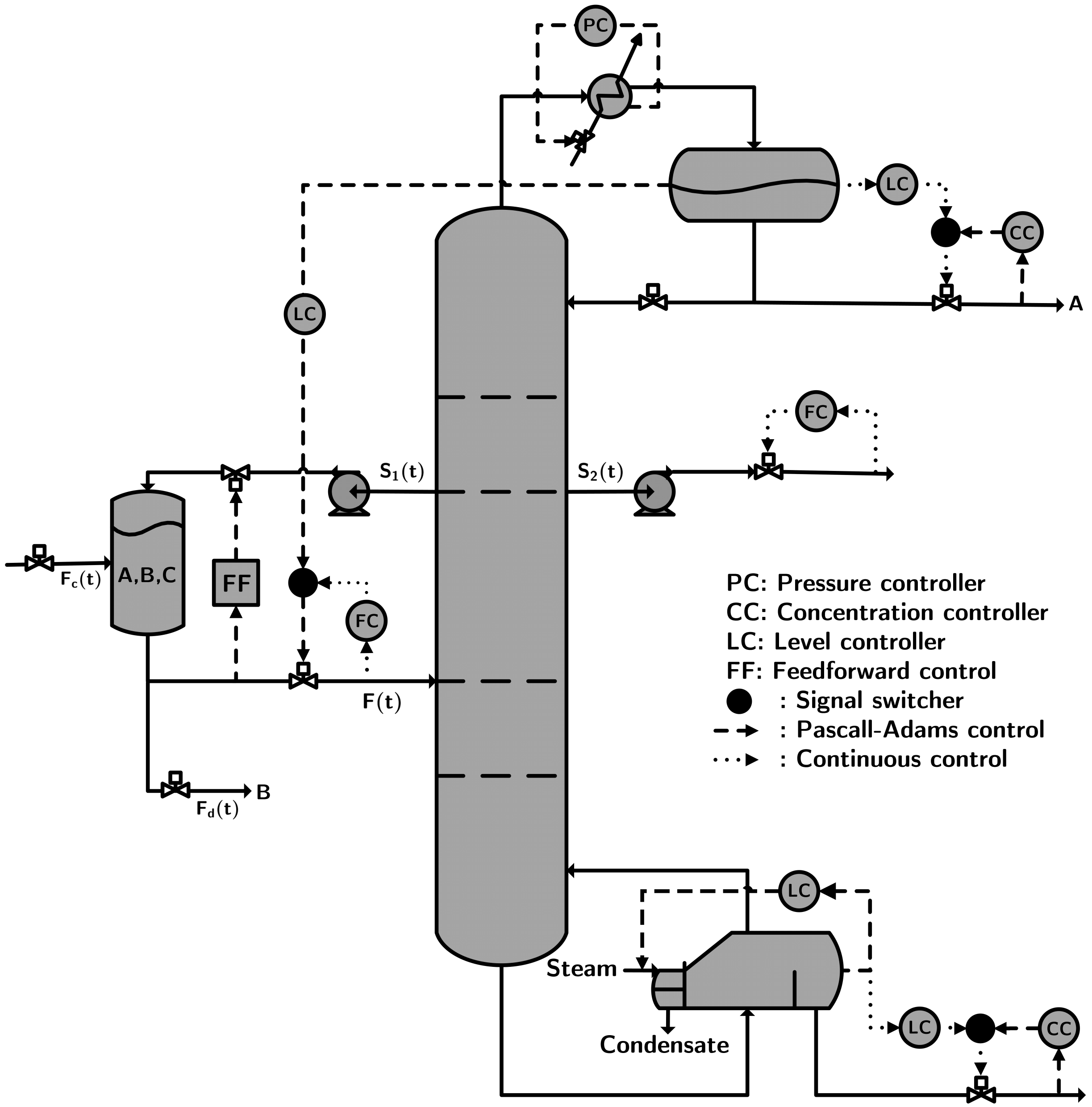

Figure 3: A schematic of the modified continuous middle vessel-column superstructure.

The recycle stream to the middle vessel (S_1) is operational only during semicontinuous operation (modes 1, 2, and 3), and the column side stream (S_2) is operational in the continuous mode (mode 0) only. Once a new steady state in mode 0 is reached, the semicontinuous operation begins; this transition is modeled as a time event. At this mode transition, the control system is changed from the continuous to the modified Pascall-Adams control configuration by using a switching block, and flow is introduced in S_1 while shutting down S_2.

The mode trajectory in the beginning is $\{0,1,2,3,1\}$, and once the semicontinuous operation begins, the mode trajectory is $\{1,2,3,1\}$. Since discrete control signals were used to switch from continuous operation to semicontinuous operation at a specific time, the hybrid model no longer has pure autonomous switches; rather, it has a combination of both controlled and autonomous switches. The events that govern the mode transitions, which are modeled using the 'Tasks' functionality[22], are shown below,

$$L_1^{(0)} : t^{(0)} = t \tag{10}$$

$$L_2^{(1)} : x_{B,v}^{(1)} \geq x_{B,v}^{desired} \tag{11}$$

$$L_3^{(2)} : h_v^{(2)} \leq h_v^{l} \tag{12}$$

$$L_1^{(3)} : h_v^{(3)} \geq h_v^{u} \tag{13}$$

Since waiting for the limit cycle is not a practical option, any cycle after the initial transient phase can be chosen to represent the limit cycle for evaluating the SC and enforcing the constraints. The cycle number is the index that is used to identify this cycle, and Γ is replaced by this representative limit cycle i.e.,

$$SC^{(\Gamma')} = \begin{cases} \dfrac{\frac{\text{Total Direct Cost}}{\text{Payback Period}} + \text{Annual Operating Cost}}{\text{Annual amount of Product Processed}} & \text{Cycle Number} = \Gamma' \\ 0 & \text{otherwise} \end{cases} \tag{14}$$

Side stream flowrate – Pump and valve design

In the optimization problem formulation $\mathbf{P}$, all bounds on the decision variables can be chosen independently except for the upper bound on the variable $\bar{S}_2$ (or $\bar{S}_1$), which is a function of the side stream pump and valve design in the aspenONE Engineering suite. The design of the side stream pump and the valve happens during the process of exporting the simulation from Aspen Plus to Aspen Plus Dynamics based on steady-state flowrates. Specifically, the design procedure uses the value of $\bar{S}_2$, which is a degree of freedom in the design of the continuous middle vessel-column system. The exported simulation in Aspen Plus Dynamics V10 has fixed equipment design variables, which are difficult to change.

Madabhushi et al.[14] demonstrated that a high $\frac{\bar{S}_2}{\bar{F}}$ ratio is preferable for good cycle performance in terms of cycle time, which indicates that pump and valve designs with maximum possible operational flexibility – the range of flowrates that can be accommodated by equipment of a known capacity – are necessary. Additionally, after extensively studying several simulation cases, it was observed that cycles generated from an arbitrary initial state that violates the flooding constraint, or close to the flooding constraint are infeasible hydraulically. Hydraulically infeasible means that the hydraulic path constraints are not satisfied at some/all points in the limit cycle. This infeasibility was a result of drawing more than acceptable liquid content from the column during the cycle. Obviously, the operational flexibility of the side stream pump and valve should be selected such that the semicontinuous operation is feasible. However, to vary the operational flexibility by changing the values of the equipment design variables (specifically, the pump), a different steady state has to be re-simulated in Aspen Plus and then exported again to Aspen Plus Dynamics to avoid any model inconsistencies. Therefore, the new design procedure includes iteratively back-stepping from $\frac{\bar{S}_2}{\bar{F}} \approx 1$ in order to design a side stream pump and valve with enough operational flexibility to maintain hydraulic constraint feasibility. Three to four iterations were required to find a suitable $\frac{\bar{S}_2}{\bar{F}}$ ratio based on the different case studies carried out. Note that although the side stream pump and valve design was fixed even before solving the optimization problem, $\mathbf{P}$, $\bar{S}_2$ was still used as a decision variable as it may affect the choice of the modified Pascall-Adams controller tuning parameters and the reflux rate.

Proposed algorithmic design procedure - Back-stepping Design Methodology

Based on the information provided in the above three sections, the following new algorithmic design procedure is proposed to find a better limit cycle (in terms of SC) of the semicontinuous distillation process than the state-of-the-art. This design procedure consists of the steps listed below (Figure 4).

- **Step 1**: Select a value of $\frac{\bar{S}_2}{\bar{F}} \approx 1$. The value of $\bar{S}_1$ is fixed at zero.
- **Step 2**: Solve $\mathbf{f}^{(E)}(\mathbf{z},\ \mathbf{y},\ \bar{L},\ \bar{Q}_R;\ \bar{S}_1,\ \bar{S}_2) = \mathbf{0}$ by varying $\bar{L}$ and $\bar{Q}_R$ such that the flooding, weeping, and weir loading constraints are satisfied. If a solution is found, jump to Step 4; if no solution is found, continue on to Step 3.
- **Step 3**: Lower the ratio of $\frac{\bar{S}_2}{\bar{F}}$ by a factor of m $(0 < m < 1)$ and return to Step 2. Repeat Step 3 until a solution is found and then jump to Step 4.
- **Step 4**: Export the simulation from Step 2 to Aspen Plus Dynamics and add the controllers required for continuous state transition and semicontinuous operation with the help of the signal-selector block. Add tasks to switch between different modes. Additionally, the distillate and bottoms flow-valve sizes are adjusted to allow for greater operational flexibility.
- **Step 5**: Run simulations at Latin hypercube points by varying the decision variable values and collect information about the type of steady-state and hydraulic inequality path constraint feasibility at these points.
- **Step 6**: Check if the hydraulic path constraints are satisfied for at least some sampling points in the domain of interest to ensure cycle feasibility. If there is no feasible point, repeat Steps 3 to 5.

- **Step 7**: Use the sequential direct approach (see “Optimization problem solution" section below) to solve the optimization problem **P** in the domain of interest. If optimizer finds a solution near/along the edge of the, then relax the domain and repeat Step 7.

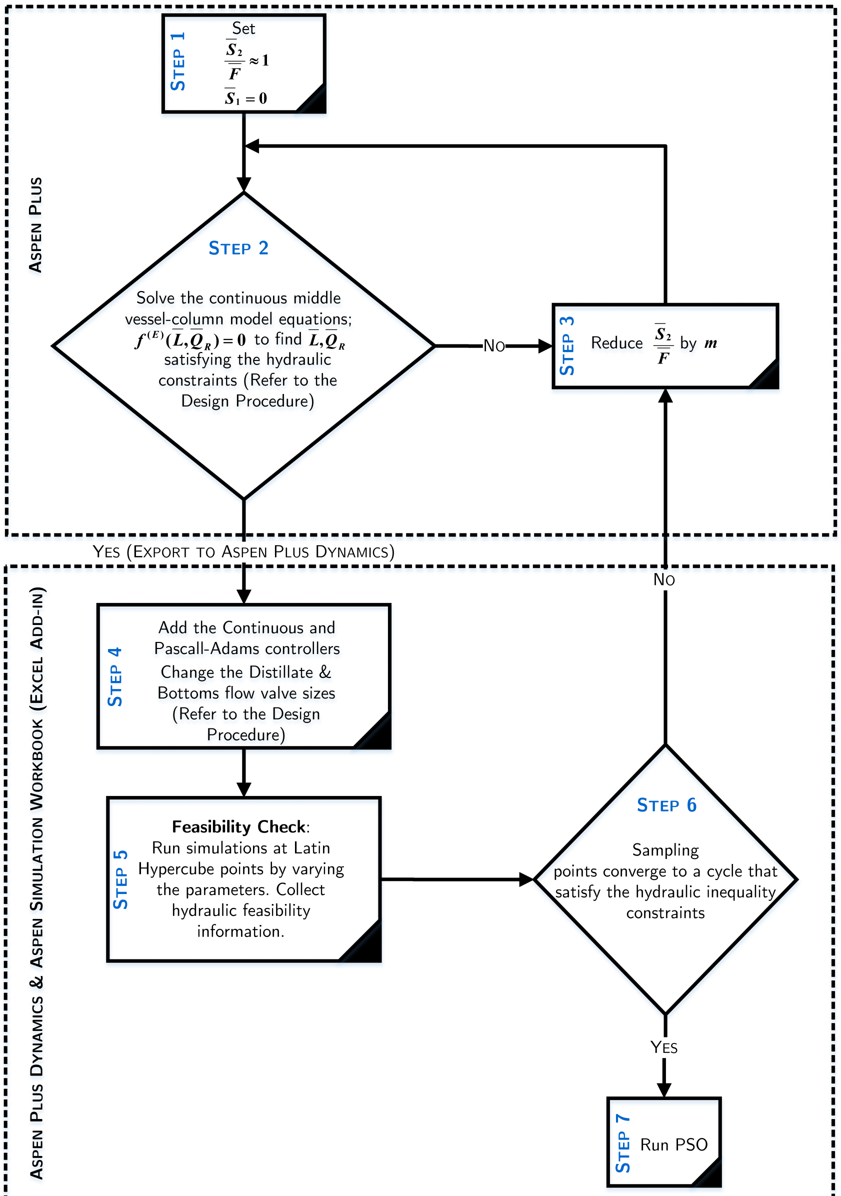

Figure 4: Flowchart illustrating the back-stepping design methodology.

Optimization problem solution

In the past, researchers have made several attempts to solve optimization problems with embedded models of processes with periodic forcing using the variational approach[24,25]. The most recent review of dynamic optimization of forced-periodic systems was by Guardabassi et al.[26]. Most of these studies were entirely theoretical based on mathematical analyses of simple systems having not more than three differential states. But, rigorous models of semicontinuous distillation have more than 50 differential states, and thus direct methods of dynamic optimization are more appropriate.

The optimization problem **P** falls under the category of multi-stage dynamic optimization because of the hybrid limit-cycle oscillator's fixed mode sequence. The sequential direct method is a reliable, practical method for solving multi-stage dynamic optimization problems like **P**, as a nonlinear program (NLP)[19]. In this method, the problem is divided into two subproblems: (1) the initial value subproblem (IVP), and (2) the nonlinear program (NLP) master problem. A gradient-based method or a derivative-free method can be used to solve the master NLP problem depending on the case. A gradient-based method could be used to solve parametric autonomous hybrid system optimization problems when the sequence of events in the parametric domain of interest is unchanged, and when the sensitivities do not jump at the event time because in these cases the Master NLP is smooth[27].

On the contrary, if the sequence of events varies from region to region in the parametric space, a derivative-free algorithm is the preferred choice, as this behavior suggests that the Master NLP may be nonsmooth[20]. In this study, the solution of the sensitivity equations of the embedded hybrid system in **P** can vary a lot because the system can have very different limiting behavior for arbitrarily close initial conditions as a result of the sequence of events changing in the parametric space. Furthermore, gradient-based local solvers embedded within Aspen Plus Dynamics were found to be ineffective[13] for the current case. Because of these two reasons, the derivative-free alternative (a stochastic NLP solver) was used in this study.

The particle swarm optimization (PSO) algorithm has repeatedly yielded good results in semicontinuous distillation studies[5,11]. In this stochastic search method, many particles are spread across the search space in a Latin hypercube grid. Each particle has personal objective and constraint function values. The particles' movement to new points in the decision variable space for subsequent iterations is computed based on their social interactions. Termination of the algorithm happens when all of the particles gather in some arbitrarily small neighborhood, or after reaching the maximum number of iterations[28].

In this method, the embedded hybrid dynamic model is treated as a black box. A predefined stopping criterion should be satisfied for terminating the dynamic simulation. In this study, the stopping criterion is ten complete cycles with the transition condition from mode 3 to mode 1 as the endpoint. PSO is time-consuming because a large number of dynamic simulations of the system have to be run for many values of the decision variables, which are the particle positions in the decision variable space. Furthermore, these simulations must be run iteratively, further increasing the computational time. Also, solution optimality, including local optimality, cannot be guaranteed due to the heuristic termination criteria. Therefore, PSO is intended only to produce a solution that is an improvement on the best-known solutions.

In this study, all constraints were handled using the penalty method wherein the objective function is penalized appropriately for violating any constraints[29]. The end-point and inequality path constraints were handled within the master NLP using a penalty function ($max\{\}$ function), where the function value is zero if the constraint is not violated and large if it is violated. In the case of inequality path constraints, the maximum constraint violation along the path was used as a measure to quantify the amount of constraint violation. The constraint violation was measured as a linear function of the distance from the boundary of the constraint. Also, the penalty parameter associated with the penalty function was a constant value during the PSO iterations and was chosen based on the scale of the objective function value.

Case studies

The proposed design algorithm was applied to two different case studies involving increasingly difficult separations of two different zeotropic mixtures. The first case study (Case 1) is the semicontinuous separation of a near equimolar mixture comprised of three alkanes: hexane, heptane, and octane (HHO). The continuous middle vessel-column design data for this case study were taken from the Wijesekera and Adams [17] seminal study on the separation of quaternary mixtures and were adapted appropriately for ternary mixture separation. The products were separated to minimum purities of 95 mol%, 96 mol%, and 95 mol% of hexane, heptane, and octane, respectively. The selected column pressure was 1.013 bar with a stage pressure drop of 0.0068 bar. The column was designed to have a diameter of 3 ft with an active tray area of 80%. The second case study (Case 2) is the semicontinuous separation of a near equimolar mixture of benzene, toluene, and o-xylene (BTX). All three products were separated to 99 mol% purity. The data to design the continuous middle vessel-column for this case study were directly taken from Madabhushi and Adams [13] without any modifications. A summary of some of the required design data is presented in Table 1.

The middle vessel was designed to hold 100 kmol of feed in Case 1 [17], and 200 kmol of feed in Case 2 [13]. Since property methods were validated before they were used in the respective studies, they were directly used here without any validation. The present analysis also considered the variations in total direct costs (does not include the cost of controllers)

Table 1: Continuous middle vessel-column design data for the two case studies. Murphee stage efficiency = 75%. Stage 1 is the condenser, and the last stage is the reboiler. $\bar{F}$ is the feed flowrate to the middle vessel and thus the column. P is the top stage pressure, ΔP is the stage pressure drop.

Case	Feed Mixture	Upstream feed mole fraction			Stages	Stage Location		P (atm)	ΔP (atm)	$\bar{F}$ (kmol/hr)
		x_A	x_B	x_C		F	S			
1	HHO	0.33	0.33	0.34	40	25	14	1	0.0068	39.66
2	BTX	0.33	0.33	0.34	40	25	14	0.37	0.0068	100

because of changes to equipment capacities as a result of continuous middle vessel-column design changes when iterating between, either Step 3 to Step 2 or Step 6 to Step 2. The capital costs were estimated using the Aspen Capital Cost Estimator V10 program[30]. As with all prior semicontinuous distillation studies, the operating cost only factored in the duties of the reboiler and the condenser. The utility prices used in these case studies were taken from Madabhushi and Adams[13]. The dynamic simulation in Aspen Plus Dynamics V10 is pressure-driven.

The implementation of the PSO algorithm for semicontinuous design optimization was done in Microsoft Excel VBA. The direct sequential method of dynamic optimization was carried out by linking Microsoft Excel to Aspen Plus Dynamics V10 using the Aspen Simulation Workbook V10-Excel add-in. The PSO parameters used in this study were taken from Adams and Seider[29]. The hydraulic feasibility constraints of operation during the PSO iterations was selected as follows:

- the flooding approach had to be less than 0.8,
- weir loading had to be greater than the minimum of 4.47 m^3/h-m (default value in Aspen Plus V10[23]),
- the vapor velocity should be greater than the weeping velocity.

Note that these constraints are path constraints. Since there were no noticeable changes after the 3rd or 4th cycle usually, the 10th cycle was chosen to be the representative cycle (Γ') to calculate the SC for the two case studies.

Case 1 - results

Three iterations of Steps 3 to 5 of the back-stepping design methodology were required to find a desirable continuous middle vessel-column design. The values of the design degrees of freedom of this continuous system, $\bar{S}_2$, $\bar{L}$, and $\bar{Q}_R$ were identified to be 20.43 kmol/h, 54.56 kmol/h, and 1.67 GJ/h, respectively. The capacities of the side stream pump and the valve were determined using the above-obtained value of $\bar{S}_2$.

The decision variable value that yielded the best SC during the hypercube sampling in Step 5 was used to initialize a particle in the PSO routine. The best-known point resulting from the sequential design methodology was not used to initialize any PSO particle in the back-stepping design methodology. The optimizer returned an improved decision variable vector after 20 iterations with 30 particles (600 simulation runs). The resultant limit cycle from the proposed design procedure has a cycle time that is approximately 9.28% lower, and an SC of almost 4.25% lower compared to the best-known design obtained by using the sequential design methodology. The SC includes the total direct cost changes due to variations in equipment size as a result of using the back-stepping design methodology. The mass-averaged product purity at the end of the reference cycle, and the hydraulic constraints during the reference cycle ($\Gamma' = 10$) were met. Good control of the top and bottoms products purities with the help of the distillate and bottoms concentration PI controllers (Figure 5) helped in meeting the mass-averaged product purities by the end of a cycle.

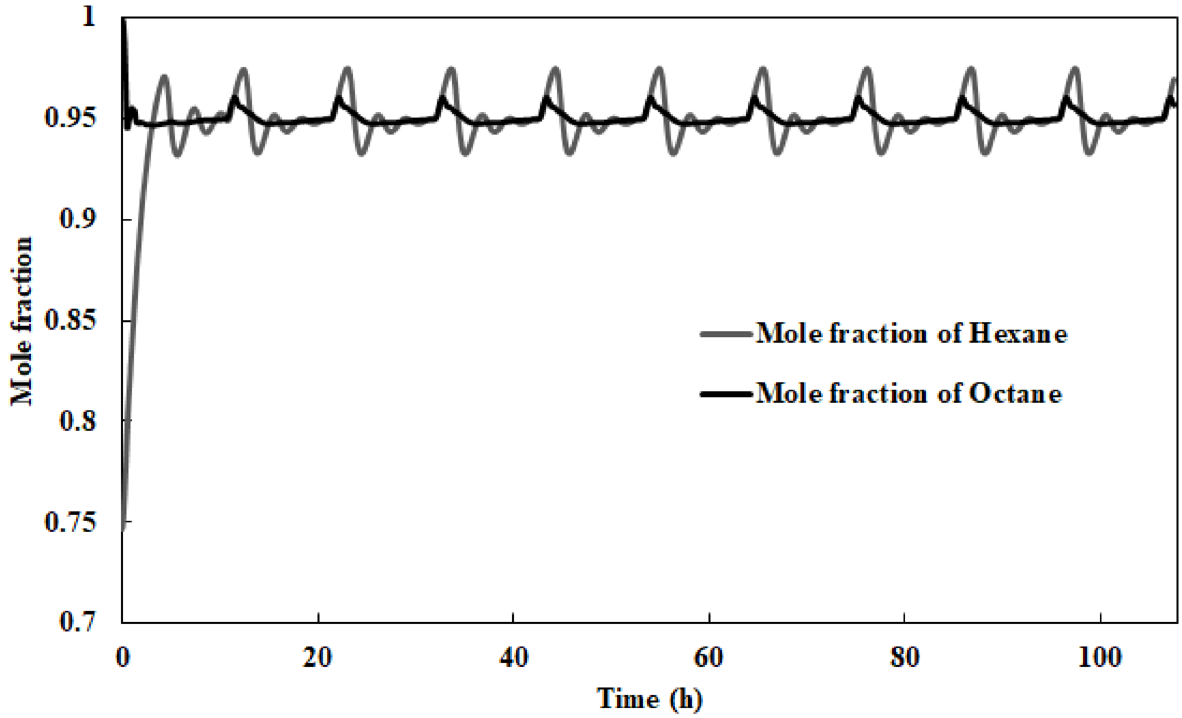

Figure 5: Mole fraction trajectory of the top and bottoms products in Case 1. The last cycle is the representative cycle ($\Gamma' = 10$). The desired values of mole fraction of the top and bottoms products are 0.95, and 0.95, respectively.

Figure 6 demonstrates the hydraulic feasibility of operating in this reference cycle. Note that the weir loading constraint becomes active on some of the column stages. Active weir loading constraint indicates withdrawal of a large quantity of liquid from the column.

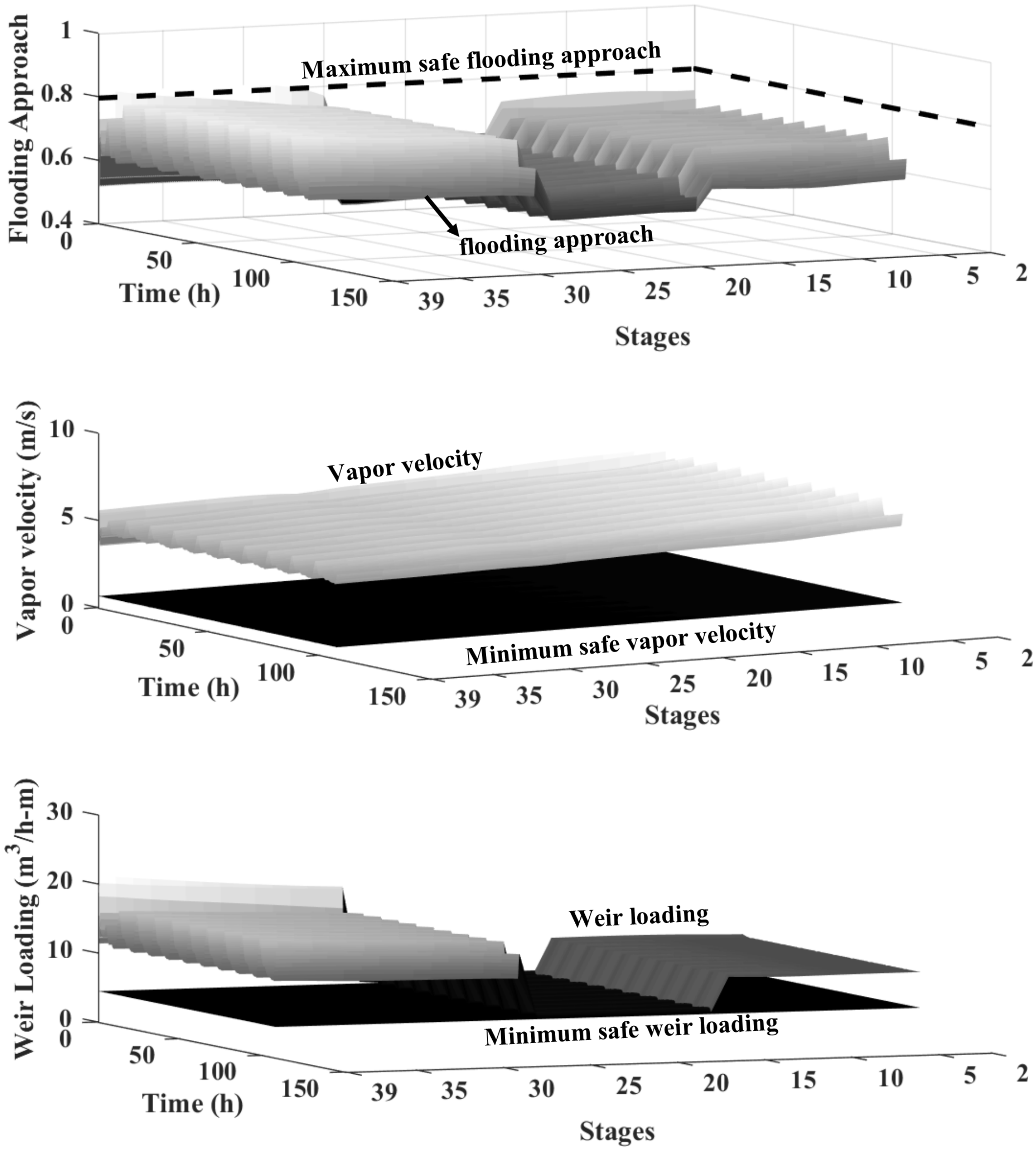

Figure 6: Plot illustrating the hydraulic feasibility of the representative cycle ($\Gamma' = 10$) found using the back-stepping design procedure for Case 1.

The reason why the design obtained using the new methodology has a lower cycle time than the previously best-known design is because the former design has a larger side stream pump and valve capacity than the latter. Thus, the side stream controller in the new design can take control actions where the recycle rate to the middle vessel is larger than the maximum possible recycle rate in the old design. The rate at which the middle vessel vessel becomes pure in the intermediate boiling component is dependent on the recycle rate, thus affecting the cycle time and in turn the separating cost.

In Figure 7 the approach to a limit cycle from the arbitrary initial state is illustrated. The initial points are attracted to different limit cycles since the designs (time-invariant parameters) obtained by following the design procedures are different.

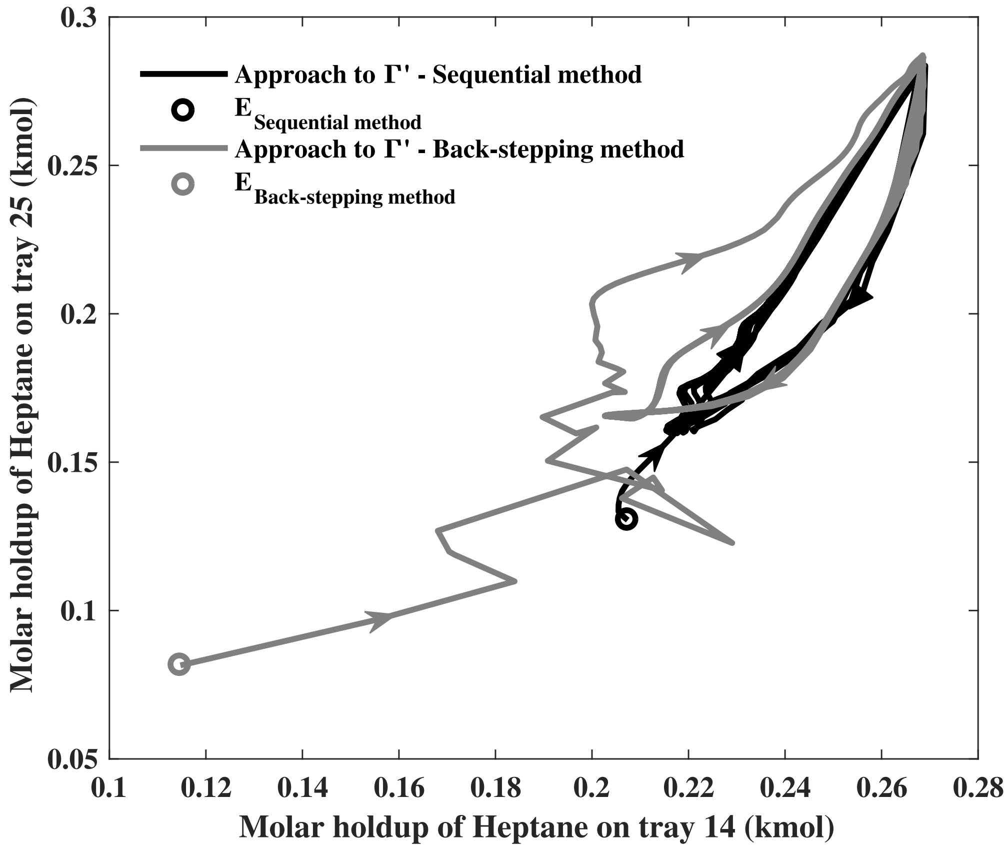

Figure 7: Phase plot illustrating different limit cycles found using the two design procedures in Case 1.

Case 2 - results

Application of the back-stepping design methodology to Case 2 resulted in a continuous middle vessel-column design that was desirable after two iterations of Steps 2 and 3. Upon close observation of this continuous middle vessel-column design, the weir loading constraint was found to be violated, although the dynamic simulation of the semicontinuous distillation resulted in hydraulically feasible cycles. In other words, the best known feasible semicontinuous design was found using an infeasible initial state. The continuous middle vessel-column design degrees of freedom variable values were as follows: $\bar{S}_2 = 75$ kmol/h, $\bar{L} = 102.04$ kmol/h, and $\bar{Q}_R = 3.69$ GJ/h. As in Case 1, an analysis of the information obtained from the 100 latin hypercube points sampled in Step 5 revealed that the selected decision variable values from the domain of interest only converged to limit cycles.

Initialization of a particle before running PSO with the best-known decision variable values from Step-5 as in Case-1, and the total number of simulation runs for PSO was set the same as in Case-1. The resultant design from the new methodology operates in a limit cycle that has 26% lower cycle time, and a 16% lower SC than the best-known design obtained using the sequential design methodology. As opposed to Case 1, the previously best-known design had significantly lower side stream recycle rate and was not close to any of the hydraulic feasibility constraints. This distance from the constraints gave the back-stepping design algorithm enough wiggle room to find better designs by increasing the side stream recycle rate. The SC improvement again includes the total direct cost changes as in Case-1. The mass-averaged product purity at the end of the reference cycle ($\Gamma' = 10$) was satisfied and the hydraulic constraints were met throughout the cycle. The top and bottoms product purities were well-controlled in the reference cycle by the distillate and bottoms PI controllers (Figure 8), thus meeting the mass-average product purities by the end of the cycle.

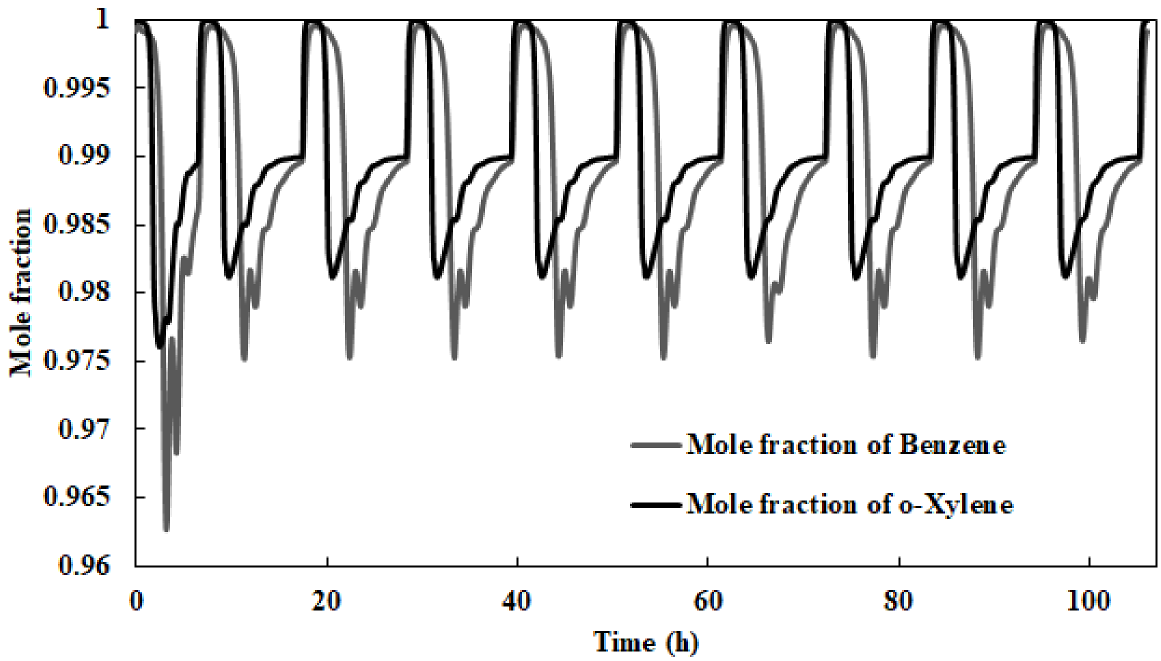

Figure 8: Mole fraction trajectory of the top and bottoms products in Case 2. The last cycle is the representative cycle ($\Gamma' = 10$). The desired values of mole fraction of the top and bottoms products are 0.99, and 0.99, respectively.

The hydraulic feasibility plot (Figure 9), again as in Case 1, illustrates that a substantial quantity of liquid was withdrawn through the side stream and thus, the weir loading constraint becomes active on some stages. The flooding and weeping constraints were however satisfied.

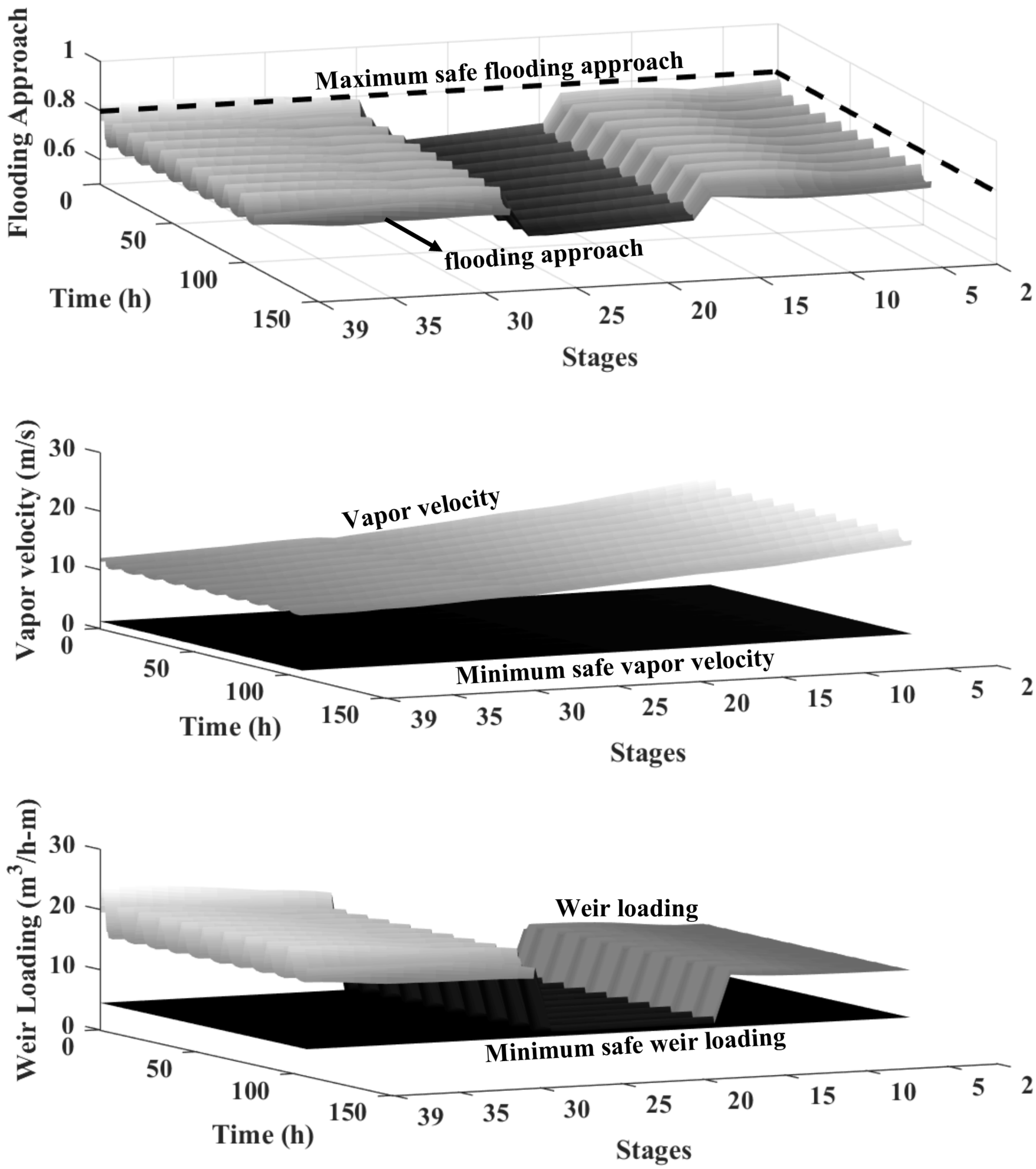

Figure 9: Plot illustrating the hydraulic feasibility of the representative cycle ($\Gamma' = 10$) found using the back-stepping design procedure for Case 2.

Figure 10 shows the approach to a limit cycle from an arbitrary initial state. From the plot, it can be observed that there is a large variation in the liquid molar holdup of toluene in the distillation column in the cycle from the new design compared to the cycle from the previous state-of-the-art methodology. This deviation was observed because a larger capacity side stream pump and valve design was specified through the new methodology, and thus withdrawal of more liquid content from the side stream stage is possible whenever required by the side stream controller.

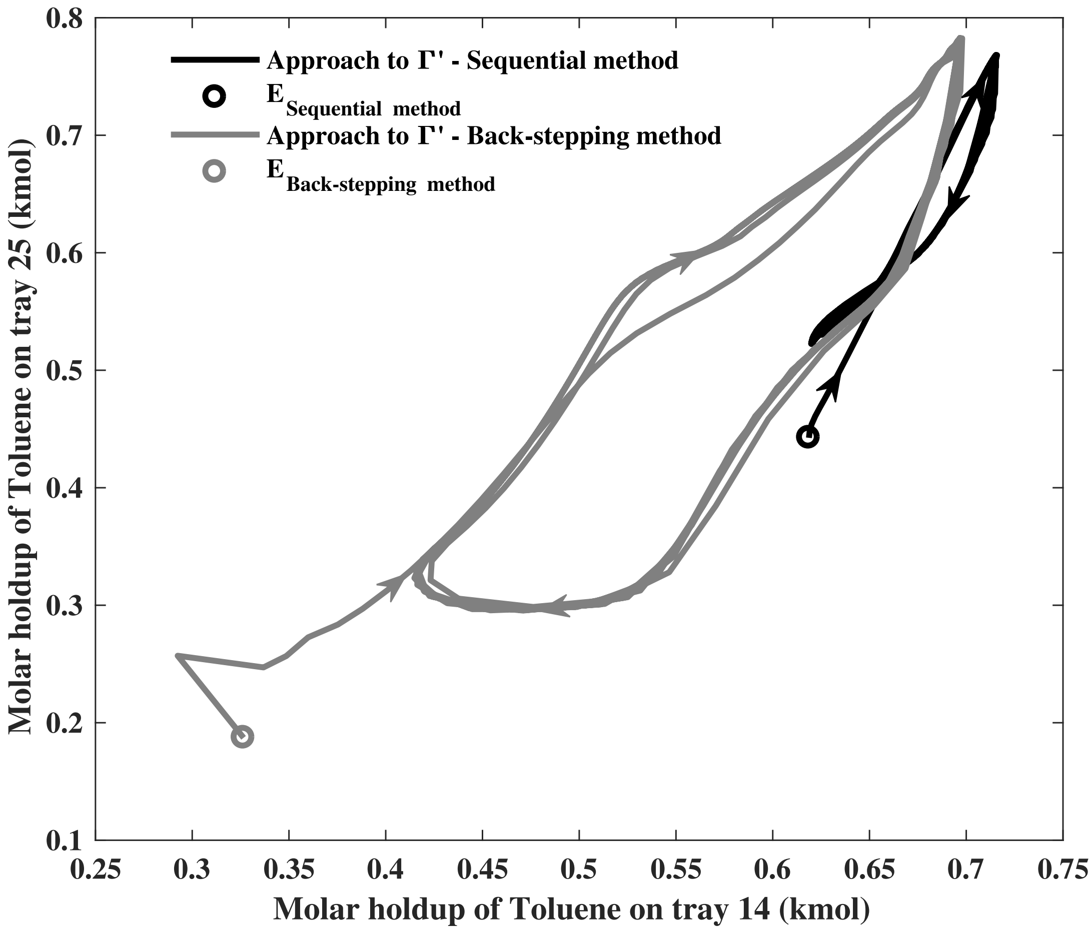

Figure 10: Phase plot illustrating different limit cycles found using the two design procedures in Case 2.

A summary of the results, which includes the values of SC, and decision variables $\bar{L}$ and $\bar{S}$, of the two case studies are presented in Table 2.

Table 2: Results of the case studies.

	System	
	HHO (Case-1)	BTX (Case-2)
	Best-known using sequential method	
$\bar{L}$ (kmol)	42.72	116.7
$\bar{S}$ (kmol)	15.86	39.0
SC (\$/kmol)	8.18	7.16
Wall-clock simulation time (min)	1.68	1.38
	New best-known using back-stepping method	
$\bar{L}$ (kmol)	45.53	132.44
$\bar{S}$ (kmol)	22.08	69.54
SC (\$/kmol)	7.83	6.02
% decrease in SC	4.28%	16%
Wall-clock simulation time (min)	2.06	1.8

Conclusions

This paper detailed a new semicontinuous distillation design procedure, known as the back-stepping design methodology. This new procedure is capable of yielding excellent results in relation to its ability to find more cost-effective designs for zeotropic ternary semicontinuous distillation. Indeed, the application of this algorithmic design procedure on the two case studies confirms that the limit cycles found were 4% to 16% lower than the limit cycles found using the status quo design methodology. Although this method is intended to find a limit cycle for known column and middle vessel sizes, it can also be extended to include integer variables. Furthermore, despite being computationally intensive, this procedure is an easy to implement approach of finding a limit cycle in the absence of prior system knowledge. Further research is required to assess the applicability of this method to other distillation processes like pressure swing distillation, azeotropic distillation, etc., which can be operated semicontinuously[4]. In part-2 of the paper, the back-stepping design procedure is extended to restrict the domain of search during optimization to a parametric space where the semi-continuous distillation dynamics asymptotically converge to a limit cycle.

All simulation files are available on LAPSE: `http://psecommunity.org/LAPSE:2019.0423`

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Nomenclature

Abbreviations

DAEs Differential Algebraic Equations

IVPs Initial value problems

NLP Nonlinear program

PSO Particle swarm optimization

SC Separating Cost

Greek Letters

α designates components, $\alpha = A, B, C$

Γ limit cycle (periodic steady-state)

Γ' representative limit cycle

Θ set containing all possible continuous middle vessel-column steady-states

Other Symbols

$\bar{F}$ feed flowrate to the column at $t = 0$

$\bar{L}$ reflux rate at E - a time-invariant parameter in semicontinuous distillation

$\bar{Q}_R$ reboiler duty at $t = 0$

$\bar{S}$ side stream flowrate at $t = 0$

A most volatile component

B intermediate volatility component

C least volatile component

P Optimization problem

$\mathbf{f}^{(E)}$ system of nonlinear algebraic equations that describes the continuous middle vessel-column system

$\mathbf{f}^{(k)}$ a system of differential-algebraic equations describing the semicontinuous distillation dynamics in mode k

$\mathbf{p}'$ controller tuning parameter vector and is a subset of $\mathbf{p}$

$\mathbf{p}$ time-invariant parameter vector

$\mathbf{u}$ represents the vector of control variables

$\mathbf{y}$ represents algebraic states

$\mathbf{z}$ represents differential states

E continuous middle vessel-column state (or) initial state of the semicontinuous distillation system

$F_c(t)$ liquid flowrate of the middle vessel charging stream

$F_d(t)$ liquid flowrate of the middle vessel discharge stream

$h_v(t)$ height of liquid in the middle vessel

h_v^l lower bound of height of liquid in the middle vessel

h_v^u upper bound of liquid height in the middle vessel

j index that describes the next mode in the sequence

k index designating the discrete state, $k = 1,2,3$

$L_j^{(k)}$ transition condition for transition from one mode to another

$M_\alpha(t)$ liquid molar holdup of the component α in the middle vessel

S_1 side stream recycled to the middle vessel in the modified continuous middle vessel-column system

S_2 side stream not recycled to the middle vessel in the modified continuous middle vessel-column system

T cycle time

t time

$x_{B,S}(t)$ molefraction of B in the side stream

$x_{B,v}(t)$ molefraction of B in the middle vessel

$x_{B,v}^{desired}$ desired purity of intermediate volatility component in the middle vessel

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