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Minimizing total annualized cost per tonne of feed processed of a semicontinuous distillation process utilizing data-driven model predictive control

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ABSTRACT

Semicontinuous distillation is a separation technique used to purify multicomponent mixtures with low to medium throughput. This research addresses the problem of designing a Data-driven Model Predictive Control (MPC) approach that enables minimizing the Total Annualized Cost (TAC) of the semicontinuous process per tonne of feed processed while maintaining the required product purity. In lieu of typically unavailable first principles models, the manuscript demonstrates the implementation of data-driven technique using data collected from an Aspen Plus Dynamics simulation as a test bed. A subspace model identification technique is adapted to develop a multi-model framework to capture the dynamic behavior of the process and then utilized within a Shrinking Horizon MPC (SHMPC) scheme, to achieve the required objective. The simulation results demonstrate a lowering of the TAC/tonne of feed by 11.4% compared to the traditional PI setup used in the previous studies.

1. Introduction

Despite its energy-intensive nature, distillation remains the most important unit operation for separation in the chemical process industry. A significant amount of the plant's operating and capital cost is attributed to the distillation process (Kiss, 2014). This is particularly evident in the separation of mixtures containing three or more components, where both capital and operating cost are very high. Much research has been done in the past to reduce the operating and capital cost of the multicomponent separation process. For instance, the dividing wall column is one of the process intensification techniques that has been explored in previous studies (Dejanović et al., 2011; Yildirim et al., 2011) to minimize capital cost for multi-component separation. Semicontinuous distillation is another process intensification technique in which one or more middle vessels are integrated with a single distillation column for the separation of a multi-component mixture (Phimister and Seider, 2000a,b). The semicontinuous process has multiple modes of operation, namely charging, processing, and discharging. The main motivation behind the semicontinuous distillation process (Adams and Seider, 2008; Wijesekera and Adams, 2015; Adams and Seider, 2005) is to reduce the capital cost required for purifying n-component mixtures ($n \geq 3$) compared to a conventional continuous process for small to medium production rates. Semicontinuous distillation has been adopted for various simulated separation processes like ternary non-azeotropic distillation, azeotropic distillation, extractive distillation, pressure swing distillation, and distillation with chemical reaction (Adams and Pascall, 2012; Adams and Seider, 2009, 2006; Monroy-Loperena and Alvarez-Ramirez, 2004; Phimister and Seider, 2000c).

Semicontinuous processes are complex, dynamic, and have a cyclic behavior with three modes of operation. The design, tuning, and configuration of the control structure heavily impact the performance and TAC/tonne of feed processed of the semicontinuous distillation system. Variables that contribute to the operating cost portion of the TAC/tonne of feed processed include the service cost provided by chilled water to the condenser and the service cost provided by steam to the reboiler.

The initial studies with semicontinuous distillation columns focused on using the traditional PI controller setup in various configurations. Phimister and Seider (2000a,b) studied the performance of three widely proposed binary distillation control configurations on a semicontinuous process. The three configurations were LV configuration, (L/D)(V/B) configuration and DB configuration. The variables L, V, D and B represent reflux rate, boilup rate, distillate flowrate and bottom flowrate respectively and they are manipulated to control the product purities

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in these configurations. Even though it is usually inoperable for a traditional continuous binary distillation column, the DB configuration easily outperformed the remaining configurations for a semicontinuous system. The reason for not implementing a DB configuration on the binary distillation column is the overflow of liquid drums due to the interactions present between level controllers. But in the presence of a full liquid side draw, the sump and reflux drum do not overflow in the semicontinuous system. In the proposed DB configuration, the distillate and bottom products are controlled by manipulating distillate and bottom flowrates, the reflux drum and reboiler sump level are controlled using feed flowrate to the column and reboiler heat duty respectively, and condenser pressure is controlled by manipulating condenser heat duty.

This DB controller configuration formed a base system for the controller configurations proposed in subsequent research works. First, Adams and Seider (2009, 2008, 2006) proposed ideal side draw recovery (ISR) arrangement to improve this DB configuration by introducing a feed-forward model-based control for the sidestream and effectively demonstrated this configuration for semicontinuous reactive extraction, reactive distillation, and production of ethyl lactate. Then Pascall and Adams (2013) studied various control systems design themselves in much more comparative detail, and found ways of improving it, but ultimately still relied on a largely PI control structure with simple model-based feed-forward control for the sidestream. Finally, Madabhushi and Adams (2018) proposed a modified ideal side draw recovery (MISR) arrangement to improve the sidestream control but still kept the same PI-based structure.

More advanced techniques such as model predictive control (MPC) have been utilized extensively in the literature (Martin et al., 2013; Porfírio and Odloak, 2011; Richalet, 1993; Huang and Riggs, 2002) for binary distillation columns. MPC (Eaton and Rawlings, 1992; Garcia et al., 1989) makes use of a dynamic model of process which optimizes the input to the system based on the objectives specified.

The classical MPC approach (Foss and Cong, 1999) proposed in the earlier studies made use of first principle models to build a dynamic model of the distillation process. Building a first principle model using MESH equations (Singh et al., 2013) is highly complex and may be difficult to develop and maintain in practice. As an alternative, a neural network model could be utilized as a data-driven modeling scheme; however the utility of Artificial Neural Network models to capture the process dynamics while avoiding the problem of overfitting continues to be an active research focus. Hence a linear modeling technique is considered in this work to avoid overfitting. One such linear data-driven technique is subspace identification (Qin, 2006) where a Linear Time Invariant (LTI) model is developed between the input and output of the process. Subspace Identification has been previously used to successfully model continuous (Kadali et al., 2003; Pour et al., 2010) and batch (Corbett and Mhaskar, 2016) processes. Previous research has demonstrated successful application of data-driven MPC for various industrial processes like rotomolding (Chandrasekar et al., 2022), polymerization (Corbett et al., 2014), distillation (Jalanko et al., 2021) and bioreactor (Sarna et al., 2022).

In an earlier effort, Meidanshahi et al. (2017) data-driven MPC was implemented on a semicontinuous distillation column and compared with an already established PI controller configuration based on the cost analysis. The MPC controller was operated only during the processing mode. For the remaining two modes (charging and discharging), the process was switched to operate under the PI controller configuration. The semicontinuous distillation process operation, by design, goes through different modes of operation. Recent results Ubene and Mhaskar (2023) proposed a multi-model framework using subspace identification for batch operations where an individual model is built for each mode of operation and connected using a PLS connector model. Such approaches have so far not been adapted for semicontinuous operation.

The present work proposes a multi-model-based MPC to enable uninterrupted implementation of MPC and thus improve closed-loop performance. The rest of the paper is structured as follows: Section 2 describes the semicontinuous process and the simulation environment to generate the data, and reviews the subspace identification. Section 3 presents the proposed framework to build a multi-model state-space model and shrinking horizon model predictive control (SHMPC) formulation. The results of the process performance under both MPC and traditional PI configurations are shown in Section 4. Finally, the conclusion of this work is presented in Section 5.

2. Preliminaries

In this section, first, the semicontinuous process description and its simulation environment are described and then an overview of existing subspace identification of batch process.

2.1. Process description

A typical semicontinuous distillation process is performed in three modes of operation, charging, processing, and discharging. During charging mode, the mixture to be separated is fed to the middle vessel. Once the content in the middle vessel reaches 90% of the middle vessel height, the feed stream control valve is turned off, and the processing mode starts. In the processing mode, the mixture from the middle vessel is fed to the distillation column at a higher flowrate. The high volatile component and low volatile component are collected as distillate and bottom products. The sidestream from the column is always recycled to the middle vessel. As time proceeds, the sidestream enriches the middle vessel with the intermediate volatile component (component B). Once the desired composition of component B is reached in the middle vessel, the process is switched to discharging mode by turning on the discharge valve situated at the bottom of the middle vessel. During the discharging mode, the content present in the middle vessel is drained out. This marks the end of the separation of a batch through a semicontinuous distillation column. The same process is repeated for the remaining batches of feed. In this way, the components present in the entire mixture are separated. By avoiding n − 2 distillation columns, the semicontinuous distillation column is used as an alternate way to purify n-components present in the mixture by reducing the capital costs compared to conventional distillation column setup for low to medium throughputs. In an effort to avoid startup and shut down of the column during the process, a certain amount of liquid is always maintained in the middle vessel (at some safe lower-limit that ensures the feed never stops to the column). The comparison of conventional and semicontinuous process setup for the separation of n-component mixture is shown in Fig. 1.

The semicontinuous separation of an equimolar mixture of hexane, heptane and octane (HHO) is considered as the case study for this work. The design data for the column and middle vessel are taken from Wijesekera and Adams's (2015) work on the separation of the quaternary mixtures and were adapted appropriately for this ternary mixture separation. The design is done so products are separated to their desired purities of 95 mol% of hexane, heptane, and octane respectively. The condenser pressure of the column was designed to be at 1.013 bar and a pressure drop of 0.0068 bar at all the following stages. In our nomenclature, stage 1 is the condenser and the last stage is the reboiler. The column diameter was designed to be 3 ft. with an active tray area of 80%. The total middle vessel molar holdup at the start of a cycle is considered to be 100 kmol. Some of the required design data of the system is presented in Table 1. More detailed information on the simulation of the hexane, heptane and octane system can be found in the previous publication (Madabhushi and Adams, 2020).

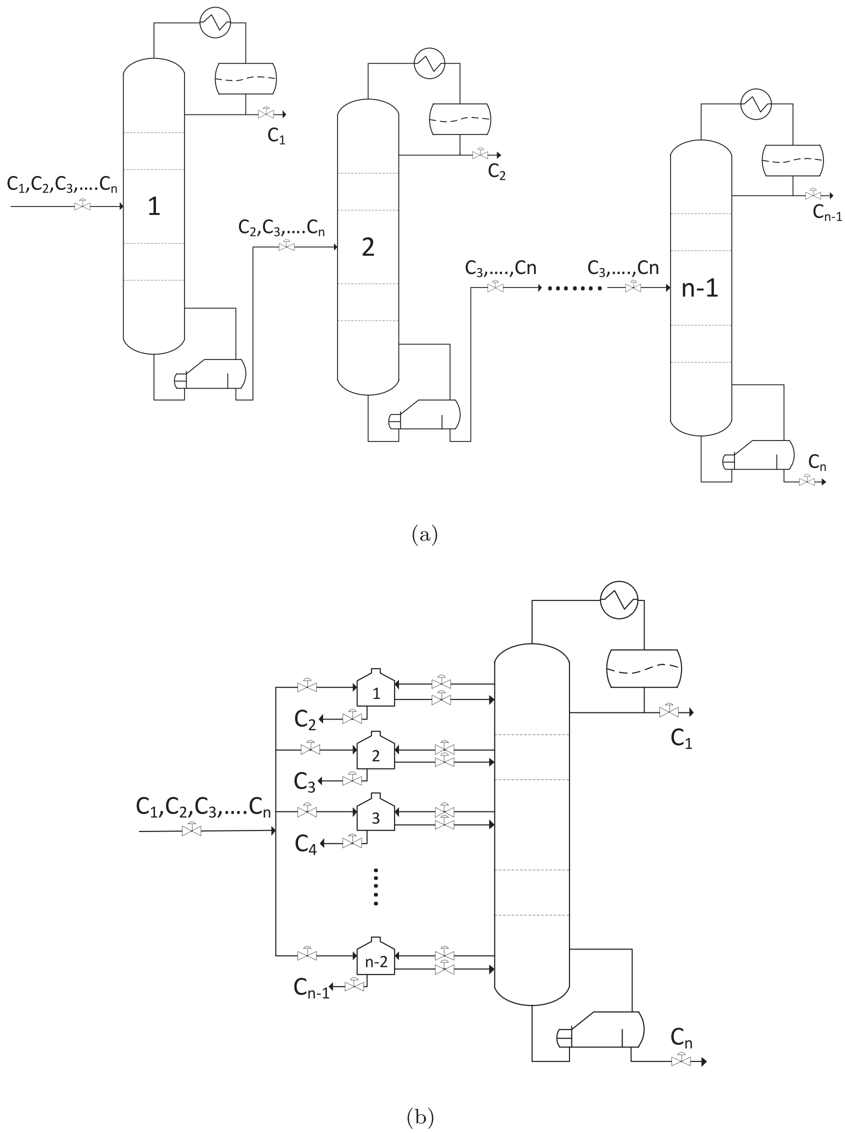


Fig. 1. (a) Conventional distillation column setup (b) semicontinuous distillation column setup for the purification of n-component mixtures.

Table 1
Key column design data for the separation of HHO mixture.

Design parameters	Value
Ternary mixture	Hexane, heptane and octane
Composition (mole frac.)	0.33, 0.34, 0.33
Number of stages (N_s)	40
Feed stage location (N_f)	25
Sidestream draw location (n_s)	14
Area of tray (m^2)	0.657
Area of reflux drum (m^2)	2.350
Area of reboiler sump (m^2)	2.746
Condenser (stage 1) pressure (bar)	1.013
Stage pressure drop (bar)	0.0068
Weir height (m)	0.0508
Weir length (m)	0.6644

Table 2
The manipulated and controlled variables of the process. CC = Composition controller, LC = Level controller, PC = Pressure controller, FC = Flow controller, Hliq. = Height of Liquid, comp. = component.

Controller	Manipulated variables	Controlled variables
Distillate CC	Distillate flowrate	Distillate composition
Bottom CC	Bottom flowrate	Bottom composition
Condenser PC	Condenser heatduty	Condenser Pressure
Drum LC	Feed flowrate to the column	Hliq. in Reflux drum
Sump LC	Reboiler heat duty	Hliq. in reboiler sump
Sidestream FC	Sidestream comp. flowrate	Sidestream flowrate

2.2. Simulation environment of the semicontinuous process

As described in Section 2.1, the semicontinuous process of hexane, heptane, and octane separation requires one middle vessel and a distillation column to separate the individual components in this mixture. Pascall and Adams (2013) proposed a control configuration where the purity of distillate and bottom products were controlled by their corresponding flowrates, the reflux drum and reboiler sump levels were controlled by the feed flow rate to the distillation column and reboiler heat duty respectively, the condenser pressure is controlled by condenser heat duty. Fig. 2 illustrates the current control structure in use. Table 2 displays the manipulated and controlled variables of all six PI controllers.

Recently, Madabhushi and Adams (2018) proposed a modified ideal side draw recovery (MISR) arrangement to improve the performance of the process under PI configuration. This study looked at the particular

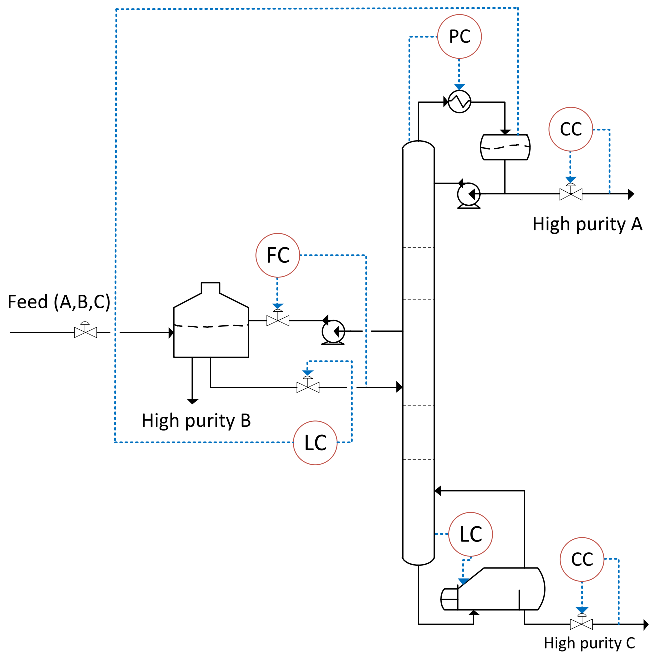


Fig. 2. PI controller configuration of a semicontinuous process. CC = Composition controller, LC = Level controller, PC = Pressure controller, FC = Flow controller.

structure of the model-based feed-forward control for sidestream control setpoint trajectory and found this arrangement performed better than the previously proposed control structure. In their configuration, the setpoint of the sidestream controller was given by Eq. (1) below:

$$S_{MISR}(t) = \frac{F_{MV,B}(t)}{x_{S,B}(t)} \tag{1}$$

where $S_{MISR}(t)$ is the setpoint of the sidestream controller. $F_{MV,B}(t)$ is the intermediate volatile component B flowrate in the feed to the distillation column, and $x_{S,B}(t)$ is the composition of intermediate volatile component in Sidestream flow. The modified ideal side draw recovery configuration is used in the current work to generate the process data.

A dynamic simulation of the semicontinuous process is utilized as the test bed. To simulate the process, a steady-state simulation of a semicontinuous process is first developed in Aspen Plus V12.1 and then converted to a pressure-driven dynamic simulation using Aspen Plus Dynamics V12.1. The inputs and outputs of the process are specified in Table 2. Like most dynamic simulators, Aspen Plus Dynamics requires the user to provide a consistent initial state (or enough information to solve for one), and then the solver can integrate the dynamic equations and advance the simulation dynamically. However, semicontinuous distillation systems are so complex that the only practical way to achieve any near-consistent initial state is to use a steady-state solution found with Aspen Plus. Once simulated, the semicontinuous distillation process functions takes a few cycles to reach a cyclical behavior with each cycle initially being somewhat different from the next in terms of the trajectories of the state variables, cycle times, and product qualities. In most cases however, these cycles tend to converge, with three to four cycles typically being sufficient. For analysis purposes, it is common to run ten cycles just to make sure that the system has converged. Hence, the first ten cycles are ignored and the data from the start of the 11th cycle is considered for this work. There have been other attempts in the literature to avoid this approach by solving for the cycles of semicontinuous distillation systems directly, but that method works with simplified models with a small number of equations (Madabhushi and Adams, 2020).

To generate data after cyclical behavior has been established, a pseudo-random binary signals (PRBS) is introduced to the setpoint trajectories of the Condenser Pressure and Reboiler sump level controllers. Since the motive behind this work was to demonstrate the key aspects of a multi-model framework and develop MPC architecture using a multi-model framework for semicontinuous distillation, the current simulation data does not consider the measurement noise. The integrated economics options available in Aspen V12.0 is used to compute the total capital cost associated with the semicontinuous distillation process. Equipment cost and Installation cost of the process are calculated based on book chapter 10 (Adams, 2018).

2.3. Subspace identification

In traditional subspace algorithm, a single model is developed to capture the dynamics of the process using obtained input–output data of the process. The traditional modeling approach is as follows: a dynamic state-space model is built between the Condenser Pressure setpoint ($CondSP$) and Bottom flow control valve opening percentage ($bval$) as the inputs and rate of distillate (ROD), rate of the bottoms product (ROB), condenser heat duty (CHD), reboiler heat duty (RHD), middle vessel composition of component heptane ($mvcomp$), distillate purity (x_d), and bottom purity (x_b) as the outputs. The inputs and outputs for the present process are shown in Eq. (2).

$$\begin{aligned} Input &= \begin{bmatrix} CondSP & bval \end{bmatrix} \\ Output &= \begin{bmatrix} ROD & ROB & CHD & RHD & mvcomp & x_d & x_b \end{bmatrix} \end{aligned} \tag{2}$$

To obtain a dynamic state-space model, a deterministic subspace identification technique is considered. The identification problem involves tuning the optimal number of states and obtaining the model matrices by fitting the state-space model to the input–output data that is obtained from Aspen Plus Dynamics simulations.

The identified model takes the following form:

$$x_{K+1} = Ax_K + Bu_K \tag{3a}$$

$$y_K = Cx_K + Du_K \tag{3b}$$

where $A \in R^{n\times n}$, $B \in R^{n\times m}$, $C \in R^{l\times n}$, $D \in R^{l\times m}$ are the associated system matrices and x_K denotes the state vector, n represents the number of states, m denotes the number of inputs, l denotes the number of outputs, u_K denotes the inputs of the model and y_K denotes the outputs of the model at the Kth time step.

There are various other subspace algorithms available in the literature which are designed to handle noise in the data, such as canonical variate analysis (CVA) (Larimore, 1990), the numerical algorithm for subspace state-space system identification (N4SID) (Van Overschee and De Moor, 1994), and the multivariable output error state-space algorithm (MOESP) (Shi and MacGregor, 2001). These techniques have not been explored in the current manuscript since the data used here is purely from simulations and is noise-free.

Remark 1. In the data generation phase, the PRBS is introduced in the reboiler level controller to overcome the simulator stability issue associated with the open-loop bottom composition configuration. Switching a controller configuration to an open-loop system causes material imbalance and leads to instability in the aspen simulation of the semicontinuous process.

2.3.1. Subspace quality model

Often there are key variables of interest in a process that are required to meet a desired specification by the end of the batch. These are commonly known as quality variables, and are commonly found in batch processes. One way to incorporate these quality variables is to relate them to the batch states at the end of the batch (Corbett and Mhaskar, 2016).

Although, the process under investigation is not a batch process, we do have few key variables like weight-averaged distillate and weight-averaged bottom purity, which act as quality variables in our case, and hence the above-mentioned technique can be used to model and control the quality variables. Specifically, they can be used to relate the states at the final time step of the sequence to the quality variables, using a Partial Least Squares (PLS) regression model represented as:

$$q = \beta x_{end} \tag{4}$$

where x_{end} is the state variable at the end of a batch, and q is the quality variable vector of the process at the end of a batch.

3. Proposed approach

In this section, the multi-model subspace identification and implementation of the multi-model structure in MPC formulation are described.

3.1. Multiple state-space model identification

As previously mentioned, the semicontinuous distillation process has three distinct modes of operation. In the conventional subspace algorithm approach (Moonen et al., 1989), a single model is fit on the entire input–output sequence to capture the dynamics of all three modes. However, in the present work, a novel multi-model identification algorithm has been proposed. This section describes the procedure for constructing separate models for the various modes without encountering discontinuities during mode switching.

One way of constructing data-driven multiple models, when the information about the mode switching criteria is given, is to split the data appropriately and apply the modeling algorithm (subspace identification in this case) on each of the data sets. However, doing so might not guarantee the continuity of the model states across the switch points. For example in the case of state-space models, there is no guarantee that the states of one mode are aligned with those of the next mode (due to the non-uniqueness of the state space representation) since the identification of each of the models is done independently on each of the data sets. Given this, there exist two alternatives tried in the literature; one, to find the appropriate similarity transformation matrix and ensure that all the models are in the same state-space domain (Verdult and Verhaegen, 2004), or to build a model connecting the two state spaces across the switch points (Ubene and Mhaskar, 2023) that can be used when moving from one mode to the other.

For the first case, obtaining the similarity transformation requires sufficient amount of data during the switch-over operation, and this cannot always be guaranteed in the plant. For the present case for instance, the switch occurs instantaneously. For the second case, although the overall modeling strategy gives better prediction accuracy than a single model, designing an MPC with such a modeling framework could get quite cumbersome and can get restrictive in terms of the kinds of MPC that can be designed. Hence, we present a modified subspace identification algorithm which can directly give multiple models without the issue of discontinuity in state-space, which in turn omits the requirement of additional connector models.

In the proposed approach, first, the deterministic subspace algorithm is applied on the input–output data. The way these algorithms work is first they generate the underlying state sequence for the entire time series, and then extract the model matrices A, B, C, D using regression on Eq. (3a) (Moonen et al., 1989). In the proposed approach, after the state sequences are generated, they are split and categorized based on the mode of operation. It must be noted that the entire data is labeled before hand, using information from other variables from the simulation. In the semicontinuous distillation process, the mode transition is based on the composition of IVC in the middle vessel and the height of liquid in the middle vessel. Using these two variables, state sequence and entire data are categorized based on their modes of operation. Subsequently, the model matrices are extracted from each of the mode using regression as mentioned above. While this might seem intuitive after the fact, applying the split after the formation of state sequence and not directly on the data and then forming the state sequences ensures that all the individual models lie on the same state-space domain, hence mitigating the discontinuity problem. The entire modeling strategy is shown in Fig. 3

Table 3
Comparison of normalized RMSE value using traditional and modified subspace algorithm.

Normalized RMSE	Traditional algorithm	Modified algorithm
Rate of distillate	0.16	0.15
Rate of bottoms	0.10	0.09
Condenser heat duty	0.19	0.17
Reboiler heat duty	0.19	0.17
Middle vessel composition	0.33	0.07
Distillate purity	0.30	0.20
Bottom purity	0.30	0.18

The database of the semicontinuous process is generated as explained in Section 2.2 of the semicontinuous process. As mentioned earlier, the data are generated under the closed-loop performance of a semicontinuous process with the PI controllers. In this work, a sequence of PRBS with various time periods is added to the nominal setpoint trajectory of the condenser pressure controller and reboiler level controller from the 11th to 30th cycle (the first 10 cycles represent the simulation settling; see Section 2.2 for a detailed reasoning). These two controllers manipulate the heat duties of the condenser and reboiler. The changes in the heat duty variables ensure we get a wide range of operational data. The data generated from cycles 11–30 are used as a training dataset to build the model.

The testing dataset is generated by changing the setpoint of the condenser pressure controller and reboiler level controllers to a value other than nominal setpoints (single step change) and letting it simulate for 10 additional cycles (cycles 31–40). The model is validated against the testing datasets to check the performance of the predicted model.

For operation of the semicontinuous column after the training is over, the initial state of the state-space model X_0 is unknown. To find the initial state estimate of the process, a Luenberger observer is used. The Luenbeger observer is of the following form:

$$\hat{y_k} = C\hat{x_k} + Du_k \tag{5a}$$

$$\hat{x_{k+1}} = A\hat{x_k} + Bu_k + L(y_k - \hat{y_k}) \tag{5b}$$

where L is the observer gain, $\hat{x_k}$ is the state estimate, u_k and y_k are the input and output of our process at time instance 'k' and $\hat{y_k}$ is the estimated output of the process using the state-space model at time instance 'k'. The observer is designed in such a way as to make sure $(A - LC)$ is within the unit circle and stable.

A state-space model of order 10 and Hankel rows 13 was found to sufficiently capture the dynamic of output variables associated with the process using the modified algorithm shown in Fig. 3. The comparison of the predictive behavior of the traditional subspace algorithm and the modified algorithm is shown in Figs. 4(a)–6. From Fig. 6 it is noticeable that the modified algorithm captures the dynamics of the middle vessel heptane composition better than the traditional algorithm. Predicting the accurate trend of the middle vessel heptane composition is very important as this is used in the MPC architecture to reduce the cycle time. The normalized RMSE value (Table 3) of all outputs except middle vessel composition is almost the same for both traditional and modified algorithms but the main difference is observed in the middle vessel composition prediction. The RMSE value of a variable is normalized to range of the respective variable.

Remark 2. During processing mode, the dynamic behavior of the process is determined by the distillation column and middle vessel

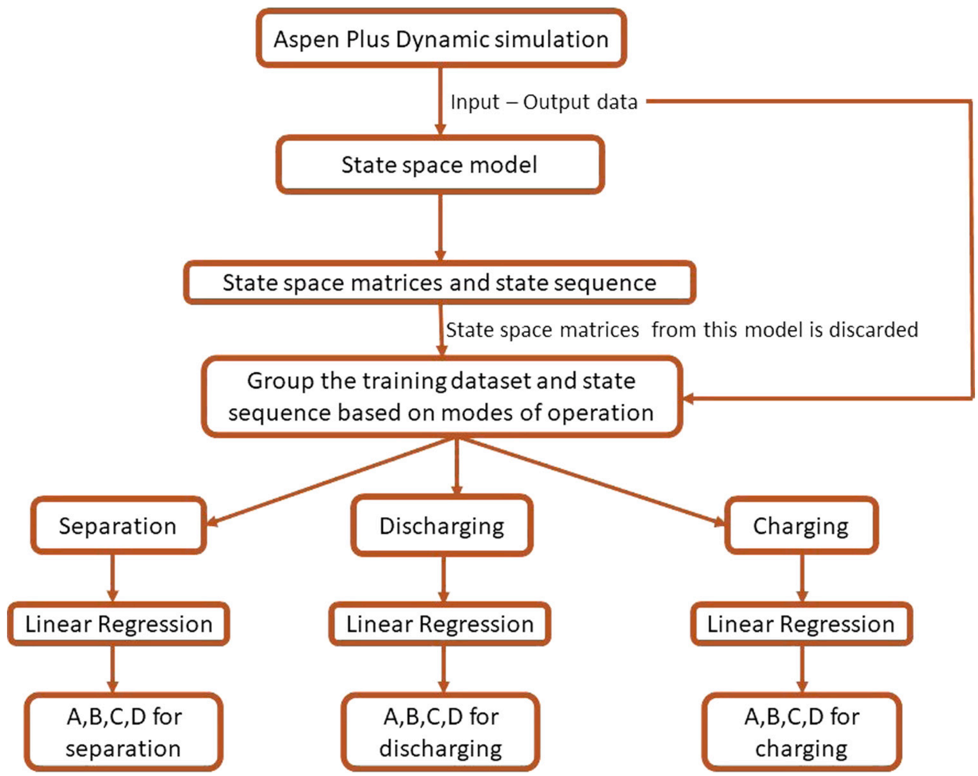


Fig. 3. Proposed algorithm for multiple state-space model.

whereas, in the charging and discharging mode, most of the dynamics of the process are associated with the middle vessel behavior. The processing mode contributes to 85% of the process cycle time (process data points). The traditional approach does not have enough information to differentiate between each mode of operation, hence the prediction ability of the traditional approach is limited (because of high processing mode data points compared to charging and discharging mode). One could attempt to put more 'weight' on the error associated with the middle vessel, but a single model approach would do that across all operation. On the other hand, in the case of multi-model approach, since the data of each mode of operation are segregated, the multi-model approach has enough information to differentiate the modes of operation and capture the dynamic of the process better than the traditional approach.

The next step is to predict the quality variables. In this work, average distillate and average bottom purity are considered quality variables. A point to be noted is during charging and discharging mode, no bottoms or distillate streams are drawn. Hence, only the average distillate and bottom purity of the processing mode are predicted. The average distillate and bottom purity of charging and discharging modes are not predicted as no products are drawn during these two modes.

The average product purity is defined as the total amount of product collected throughout the processing mode divided by the respective product's total flowrate collected during the processing mode. The average distillate and bottom purity are shown in Eqs. (6a) and (6b) below:

$$avg.x_d = \frac{\int_{t=t_{start}}^{t=t_{end}} Dx_d \times dt}{\int_{t=t_{start}}^{t=t_{end}} D \times dt} \tag{6a}$$

$$avg.x_b = \frac{\int_{t=t_{start}}^{t=t_{end}} Bx_b \times dt}{\int_{t=t_{start}}^{t=t_{end}} B \times dt} \tag{6b}$$

where $avg.x_d$ and $avg.x_b$ represents the average distillate and average bottom purity of a particular batch respectively. ($\int_{t=t_{start}}^{t=t_{end}} Dx_d \times dt$) and ($\int_{t=t_{start}}^{t=t_{end}} Bx_b \times dt$) represents the total amount of distillate products and bottom products collected throughout the processing mode respectively. Similarly, ($\int_{t=t_{start}}^{t=t_{end}} D \times dt$) and ($\int_{t=t_{start}}^{t=t_{end}} B \times dt$) represents the total distillate and bottom flowrates collected during the processing mode. The limits of $t = t_{start}$ and $t = t_{end}$ represent the time at the start and end of the processing mode of a batch respectively and the quality variable is given as:

$$q = \begin{bmatrix} Total\ Dx_d & Total\ Bx_b & Total\ D & Total\ B \end{bmatrix} \tag{7}$$

Figs. 7(a)–7(b) show the subspace modeling technique can capture the trends of quality variables. In the MPC design, product specifications for these variables are included as hard constraints.

In summary, simulations show that the dynamics of the semicontinuous process are well captured by the proposed multi-model approach, setting the stage for a model predictive control implementation.

3.2. MPC configurations on semicontinuous distillation process

In the proposed configuration, the MPC directly manipulates the bottom valve opening percentage and setpoint of the condenser pressure controller to optimize the semicontinuous system performance. Here, MPC indirectly manipulates the condenser heat duty by acting as a cascade controller to the condenser pressure controller. This configuration is shown in Fig. 8.

3.2.1. Shrinking horizon model predictive control formulation

The next part of this work in controlling semicontinuous process is to integrate the developed data-driven (multiple state-space technique explained in Section 3.1) model within a shrinking horizon MPC to demonstrate a reduction in the TAC per tonne of feed processed, computed as:

$$\begin{aligned} &\text{TAC} = \text{Annual Operating Cost} + \frac{\text{Total Capital Cost}}{\text{Payback Period}} \\ &\text{Total Capital Cost(USD)} = \text{Equipment Cost} + \text{Installation Cost} \\ &\text{Payback Period} = 3 \text{ Years} \end{aligned} \tag{8}$$

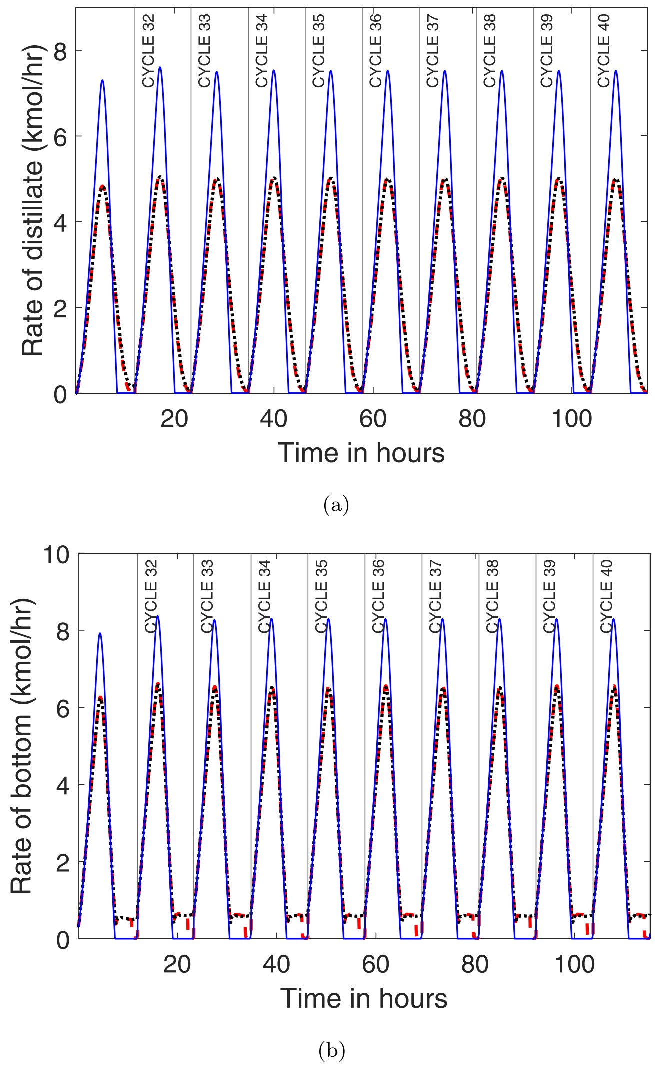


Fig. 4. The output behavior of (a) rate of Distillate (b) rate of bottom predicted by multimodeling framework and traditional subspace algorithm. Blue solid line represents process data, black dotted line represents the traditional algorithm approach, red dashed line represents multimodeling framework.

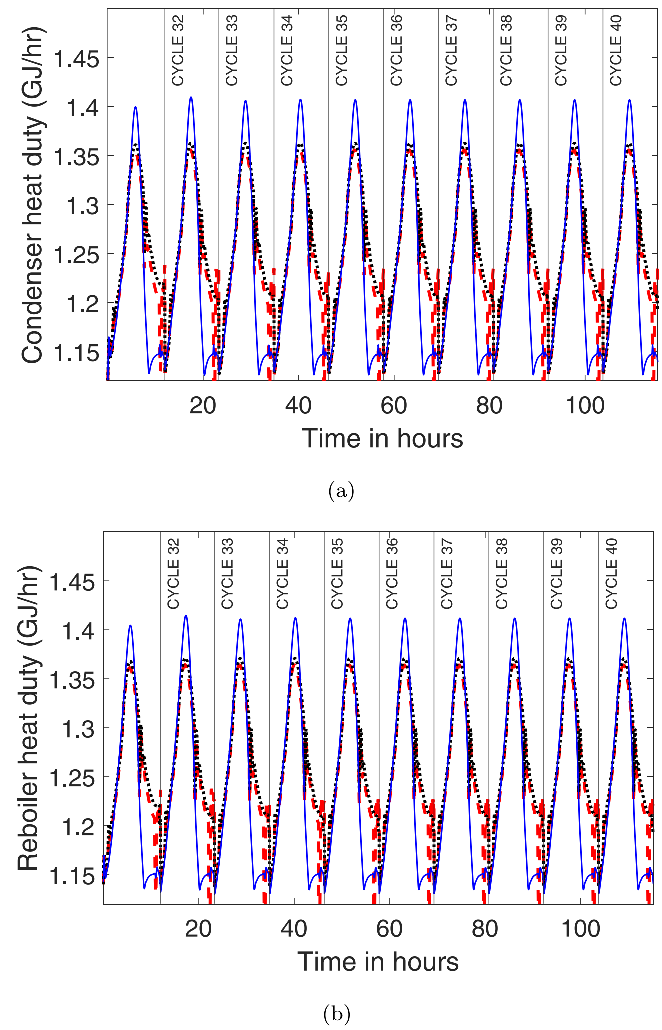


Fig. 5. The output behavior of (a) condenser heat duty (b) reboiler heat duty predicted by multimodeling framework and traditional subspace algorithm. Blue solid line represents process data, black dotted line represents the traditional algorithm approach, red dashed line represents multimodeling framework.

$$
\begin{aligned}
&\text{Total Operating Cost(USD)} = Q_{condenser} + Q_{reboiler} \\
&Q_{condenser}\text{(USD)} = \text{Amount of condenser cooling heat} \times \text{Cost of service} \\
&Q_{reboiler}\text{(USD)} = \text{Amount of reboiler heat} \times \text{Cost of service provided}
\end{aligned} \tag{9}
$$

where $Q_{condenser}$ and $Q_{reboiler}$ represent the cost of cooling service provided to the condenser by chilled water and the cost of heating service provided to the reboiler by steam respectively. Since the capital cost does not change between MPC and PI configurations, this work emphasizes reducing the total operating cost of the process. The processing mode constitutes 85% of the process cycle time.

In the Shrinking Horizon MPC, the prediction horizon (P) of the processing mode is chosen as the average length of the processing mode under the PI configuration plus 50-time instances as a buffer, in recognition of the fact that cycle time may be (and is) different under the MPC. During discharging and charging mode, the liquid is fed/discharged at a constant flow rate to the middle vessel. Therefore, for discharging and charging modes, the cycle length remains the same in both MPC and PI configurations. The prediction horizon (P) of the discharging mode and charging mode is the length of the respective mode under PI configuration plus 5-time instances. The control horizon (N) for all three modes is chosen to be 5-time instances.

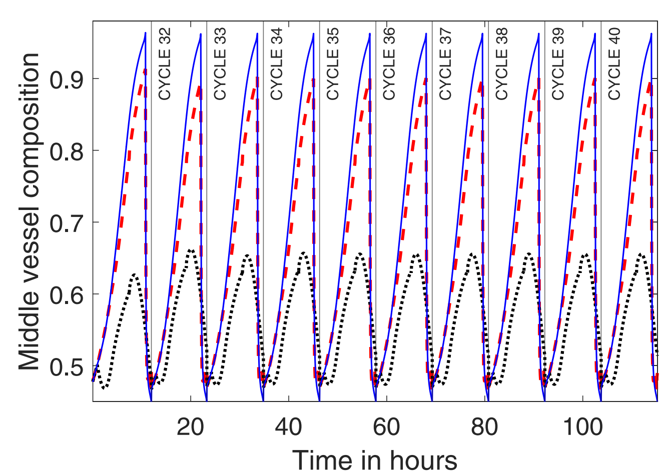
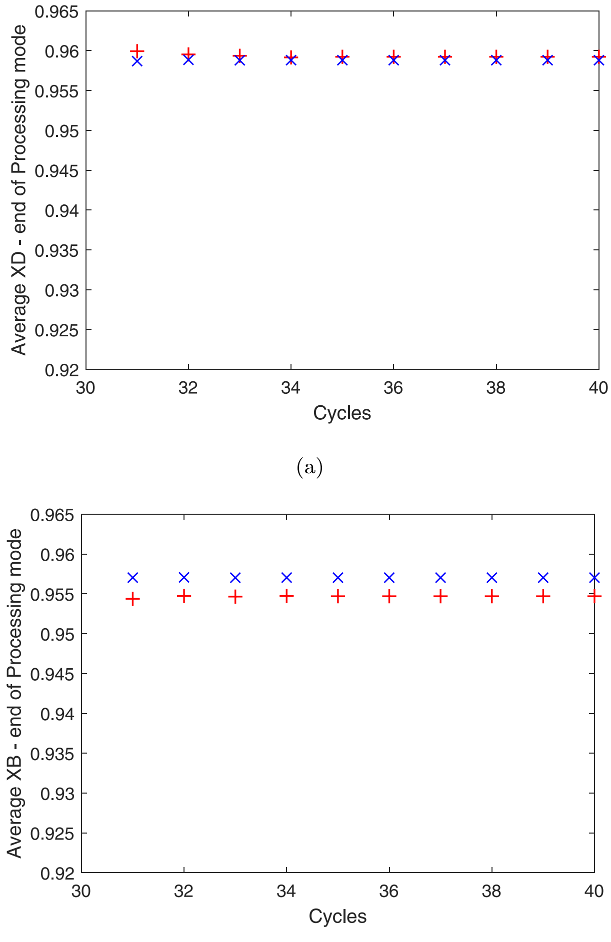


Fig. 6. Predicted comparison of middle vessel heptane composition by traditional algorithm (black dotted line) and multi-model framework (red dashed line) with process data (blue solid line).



(a)

(b)

Fig. 7. The quality model prediction of (a) average distillate purity (b) average bottom purity by subspace quality model framework (red + marker). Blue *x* marker represents process data.

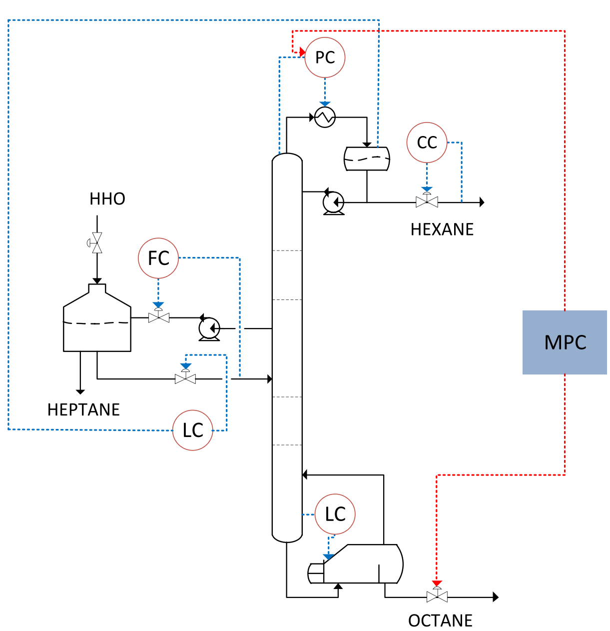


Fig. 8. MPC configuration proposed in this work.

In the semicontinuous process, electricity is primarily used for pumping fluids and producing chilled water through a cooling tower. The formulation mentioned in Eq. (8) already accounts for the electricity consumed in the production of chilled water. Moreover, the cost of electricity used for pumping fluids is negligible in comparison to the overall operating cost. These two considerations collectively lead to the exclusion of the electricity cost of the semicontinuous process in the total operating cost formulation for this work.

When formulating the SHMPC for the processing mode of a semicontinuous system, it is essential to consider that the control system must fulfill the following characteristics:

1. The average distillate and bottom purities at the end of the processing mode need to be greater than the desired specifications which are 0.95 in this work.
2. The manipulated inputs (condenser pressure setpoint and bottom valve opening) from the MPC controller should be within the operating range.
3. The Aspen Plus Dynamics simulation fails when there is a drastic change in the magnitude of successive inputs. Hence a hard constraint is implemented on change in the magnitude of successive inputs (this is in line with requiring control equipment such as valves to be not moved around too much too quickly).
4. Minimize the operating cost per tonne of feed processed. The operating cost calculation is explained in Eq. (9). A point to be noted is the amount of tonne of feed processed is indirectly proportional to the time taken by the process to complete a cycle. Hence, the operating cost of the process and the cycle time of the process are minimized separately in an effort to reduce the total operating cost per tonne of feed processed. The cycle time minimization is achieved by minimizing the sum of squared errors between middle vessel heptane composition and heptane desired purity which is 0.95. This forces the process to attain the processing mode switch to happen faster than the PI configuration

The first three characteristics are implemented as hard constraints in MPC formulation of processing mode. Characteristic 4 is included as soft constraints in the objective function of MPC formulation. The characteristic of MPC formulation of charging and discharging mode is shown below,

1. Minimize the sum of squared errors between process products (distillate and bottom) purity and their desired purity which is 0.95.

To implement the proposed control scheme on the Aspen Plus Dynamics simulation, MATLAB is connected to Aspen Plus Dynamics using VBA connecting software. VBA acts as a communication tool in this work. VBA accesses the MPC function file in MATLAB to generate the current input action and store it on the Excel sheet. Then the current input which is stored in Excel is passed to Aspen Plus Dynamics simulation to generate the output of the process. The control action is calculated and implemented at every 0.03 h time instance through MATLAB — Aspen interface using VBA [Fig. 9]. At a sampling instance, the optimal input trajectory is computed by solving the optimization problem described in Eqs. (10) and (11).

The cost of chilled water and cost of steam is chosen as 4.2 USD/GJ services and 4.5 USD/GJ services according to Ref. Deng et al. (2023). The condenser cooling heat and reboiler heat are predicted by the modified subspace algorithm. The average distillate and average bottom purity are predicted by the quality variable model.

As explained in the previous section, during the implementation of MPC, initial state estimates are required ($\hat{X}_0$). To estimate the initial state, a Luenberger observer (Eq. (5b)) is utilized. As the process measurements become available, the observer is updated until the output predictions converge to the measured outputs. So, the process is

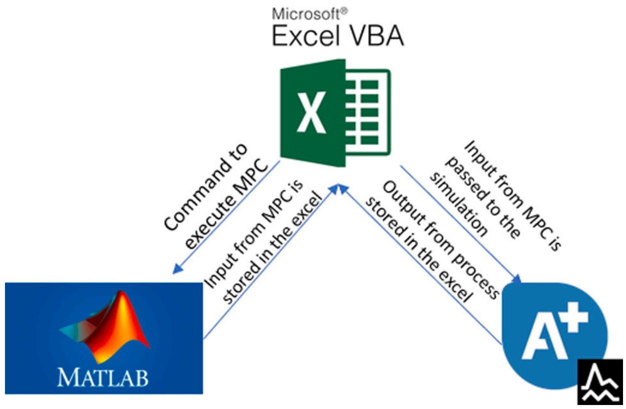


Fig. 9. VBA-MATLAB-Aspen communication.

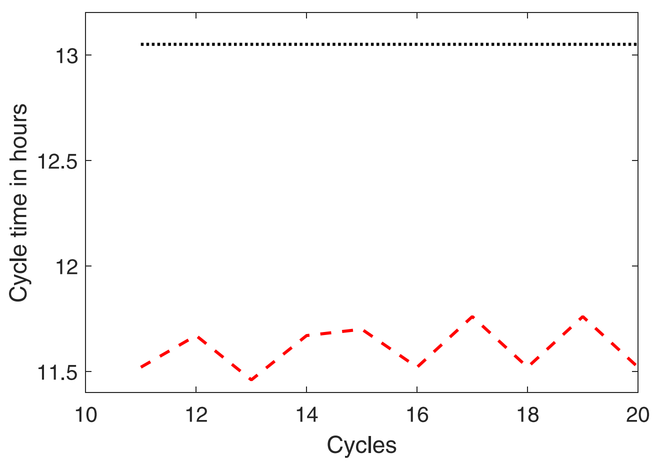


Fig. 10. Comparison of time taken by MPC (red slashed line) and PI (black dotted line) configurations for cycle 11–20.

first operated under PI controllers for the first ten cycles and the MPC controller is switched on at the start of the 11th cycle.

The MPC formulation of the processing mode is as follows:

$$\min_{U} \sum_{i=0}^{P-1} ((mvcomp - 0.95)^T Q(mvcomp - 0.95) + \mathrm{TOC})_i$$

Subject to:

$$\begin{aligned} &\hat{x_{k+1}} = A\hat{x_k} + Bu_k \\ &\hat{y_k} = C\hat{x_k} + Du_k \\ &u_{\min} \le u_k \le u_{\max}, \quad \forall\, 0 \le k \le N-1 \\ &\Delta u_{\min} \le \Delta u_k \le \Delta u_{\max}, \quad \forall\, 1 \le k \le N-1 \\ &\Delta u_k = u_k - u_{k-1} \\ &u_k = u_{N-1}, \quad \forall\, N \le k \le P-1 \\ &avg.x_d \ge 0.95 \\ &avg.x_b \ge 0.95 \end{aligned} \tag{10}$$

where A, B, C, and D represent the state-space matrices of the processing mode determined by the proposed multi-model framework, $\hat{x_k}$ and $\hat{y_k}$ represent the estimated state estimates and predicted output at time instance 'k' using the multi-model framework, $mvcomp$ is the middle vessel composition of heptane, TOC is the operating cost per hour which is calculated according to the Eq. (9), $avg.x_d$ and $avg.x_b$ are the average of distillate and bottom purity at end of the processing mode.

The MPC formulation during charging and discharging modes are as follows,

$$\min_{U} \sum_{i=0}^{P-1} ((x_d - 0.95)^T (x_d - 0.95) + (x_b - 0.95)^T (x_b - 0.95))_i$$

Subject to:

$$\begin{aligned} &\hat{x}_{k+1} = A\hat{x_k} + Bu_k \\ &\hat{y_k} = C\hat{x_k} + Du_k \\ &u_{\min} \le u_k \le u_{\max}, \quad \forall\, 0 \le k \le N-1 \\ &\Delta u_{\min} \le \Delta u_k \le \Delta u_{\max}, \quad \forall\, 1 \le k \le N-1 \\ &\Delta u_k = u_k - u_{k-1} \\ &u_k = u_{N-1}, \quad \forall\, N \le k \le P-1 \end{aligned} \tag{11}$$

where, A, B, C, and D represent the state-space matrices of the charging/discharging mode determined by the proposed multi-model framework, x_d and x_b are the purities of distillate and bottom products, N and P are the control and prediction horizon of the MPC formulation, $u = [u[0], u[1], u[2] \dots u[N-1]]^T$ are the set of decision variables consisting of condenser pressure setpoint and bottom valve opening percentage inputs at each sampling time instance over the control horizon. u_{min} and u_{max} are the lower and upper bounds of the operating range of our inputs. The values of u_{min} and u_{max} in the processing mode MPC formulation are $[0.95, 0]^T$ and $[1.1, 100]^T$. The values of Δu_{min} and Δu_{max} in the processing mode MPC formulation are $[-0.1, -22]^T$ and $[0.1, 22]^T$. The minimum and maximum values of condenser pressure setpoints are chosen to be within the operating range of the Aspen Plus Dynamics simulation. The Aspen Plus Dynamics simulation crashes out of this range. The value of tuning parameters Q is 15.5. The reason for choosing the tuning parameter Q value of 15.5 is explained in Section 4.1. Due to the structure of semicontinuous process, the constraint of average heptane product purity greater than or equal to 0.95 in MPC formulation is eliminated. The switch from processing to discharging mode occurs once the heptane composition in the middle vessel hits 0.95 from below (so it is rising). Hence the process makes sure that the average purity of the heptane product collected is always greater than or equal to 0.95.

In charging and discharging mode, the distillate and bottom flow rates are zero. Hence, instead of optimizing the TOC during these two modes, we let the process build up the bottom and distillate purity to 0.95. This in turn assists to reduce the processing mode time (as mentioned earlier time taken to complete charging and discharging mode cannot be lowered because of the constant liquid added/removed to the middle vessel during MPC and PI configurations). During charging and discharging mode, the values of u_{min} and u_{max} are $[0.95, 0]^T$ and $[1.1, 0]^T$ and the values of Δu_{min} and Δu_{max} are $[-0.1, 0]^T$ and $[0.1, 0]^T$.

The above-mentioned formulation is solved in MATLAB using the non-linear programming solver `fmincon`. The Luenberger observer within the MPC architecture helps to determine the state estimate at the next time instance using the current input–output data obtained from the process. The Luenberger observer is shown in Eq. (5b).

Remark 3. This particular work did not consider the effect of flooding in the MPC formulation because the flooding is assumed to be taken care of by the remaining PI controllers. In Meidanshahi et al. (2017), the flooding is avoided by implementing a constraint on the vapor velocity at the top and bottom trays of the column during the processing mode MPC configuration. However, the current work focuses on optimizing the performance of the semicontinuous process using variables which are easy to measure in real-time. Future work will consider utilizing inferential variables to monitor and control tower flooding.

Table 4
MPC performance for various tuning parameter value.

MPC versions	Value of Q	TAC per tonne of feed processed (USD)
Version1	180	65.8
Version2	85	65.5
Version3	35	65.4
Version4	28.3	65.3
Version5	28	65.3
Version6	20	64.8
Version7	17.5	64.7
Version8	15.5	64.1
Version9	14	64.1
Version10	12.7	64.1

Table 5
Split up of the Total Annualized cost per tonne of feed processed.

Name	Traditional PI	Proposed MPC
Tuning Parameters for MPC (Q)	–	15.5
Average Condenser cooling heat (GJ/h)	1.224	1.223
Average Reboiler heat (GJ/h)	1.227	1.232
Runtime per year (h)	8000	8000
Cost of chilled water per year (USD/yr)	41 100	41 100
Cost of steam per year (USD/yr)	44 200	44 400
Total Operating Cost per year (USD/yr)	85 300	85 500
Total Capital Cost/Payback period (USD/yr)	337 000	337 000
Average cycle time (h)	13.1	11.6 (11.45% lower)
Amount of feed processed (tonne) in a cycle	9.55	9.55
Amount of feed processed (tonne) in a year	5830	6590
TAC (USD) per metric tonne of feed processed	72.4	64.1 (11.46% lower)

Remark 4. Initially, the same MPC architecture was developed with single subspace model instead of multi-model framework. Due to the poor prediction of middle vessel composition variable by traditional subspace algorithm, the MPC — single subspace model architecture could not push middle vessel composition variable to 0.95 because of which the switch between processing and discharging mode did not happen, necessitating the design of the multi-mode MPC.

4. Simulation results

The proposed modeling and control strategy is demonstrated by implementing on the semicontinuous process in the Aspen Plus Dynamics simulation.

4.1. SHMPC formulation results

Recall that the first ten cycles of the process are discarded to wait for the cycle stabilization, and the trajectories are considered from the eleventh cycle. The performance of MPC and PI controller setups on semicontinuous process are compared where the process is operated for 8000 h/year. This is denoted as Case-1 where the price of utilities is used according to what is mentioned in the reference book (Deng et al., 2023).

The best value of Q is chosen based on the MPC controller's performance of reducing the TAC/tonne of feed processed best, resulting in a value of Q of 15.5. The simulation of MPC performance on various Q values is shown in Table 4.

From Table 4, it is noticeable the performance of MPC on the semicontinuous process saturates around versions 8, 9 and 10. Version 8 is chosen as the best MPC setup for this case. Next, the performance of PI on the semicontinuous process is compared with best-case MPC performance on the semicontinuous process. The capital cost of the process is 1,010,000 USD. The total operating cost is calculated according to Eq. (8). The entire split up of TAC/tonne of feed processed calculation for PI and MPC controller configuration is shown in Table 5.

Table 6
Average product purity of PI and MPC configuration.

Name	Average dis. purity	Average bot. purity
Setpoint	0.95	0.95
PI setup	0.958	0.957
MPC setup	0.959	0.953

Table 5 shows the improvement of semicontinuous system performance in reducing TAC/tonne of feed processed under MPC configuration over the PI controller configuration. The MPC reduces TAC per tonne of feed processed by 11.46%. This is mainly attributed to the condenser pressure setpoint (one of the manipulated variables) value chosen by MPC. The MPC configuration also reduces the cycle time by 11.45%. The cycle time comparison of PI and MPC controller configurations for cycles 11–20 are shown in Fig. 10.

Remark 5. An interesting observation drawn from Fig. 10 is the absence of a repetitive cycle under MPC. This is due to the discretization of the mode switch events in the VBA — Aspen Plus Dynamic setup. Normally, these events happen dynamically in Aspen Plus Dynamic simulation with the help of the task function. However, while using a VBA setup to pass input to process in the Aspen Plus Dynamic simulation, the task function in the Aspen Plus Dynamic gets deactivated. Hence the switch condition of the semicontinuous process has to be discretized to include mode switch. This results in the absence of cyclic behavior of the semicontinuous process under MPC configuration, and is essentially an artifact of the simulation environment.

The average distillate and bottom purity of case-1 for both configurations are also shown in Fig. 11. In both configurations, the average product purities are well above the desired specifications (see Table 6).

The comparison of the dynamic behavior (case-1) of manipulated inputs between MPC and PI configurations for cycles 19 and 20 is shown in Fig. 12. The distillate and bottom purity of case-1 for all three modes of operation are shown in Fig. 13. There is a clear difference in the behavior of the process under MPC and PI configuration which is indicated in Figs. 14(a)–14(d). Taking a closer look at the MPC setup (refer to Fig. 14(c)), it is evident that the peak value of the bottom flowrate is achieved at the beginning of the cycle. In contrast, the PI setup (refer to Fig. 14(d)) requires some time to reach this point, as it needs to build up the bottom purity and draw out more liquid.

To illustrate the ability of the controller to handle variability in market conditions, another case (case-2) is considered where the prices of utilities are increased. In this case, the cost of the cooling service provided by chilled water and the heating service provided by steam is increased to 6.7 and 8.4 USD per GJ service respectively. In order to achieve the optimal performance of case-2 under MPC configuration, the MPC was fine-tuned. The tuning parameter (Q) of MPC formulation for case-2 was found to be 28 and the MPC setup was simulated for 20 cycles. With the new formulation, the same VBA-Aspen-MATLAB setup is used to communicate and control the process using the proposed data-driven model predictive control approach. For this particular case (case-2), the TAC per tonne of feed processed for PI and MPC configuration is found to be 83.2 USD/t and 73.7 USD/t respectively. Even in the

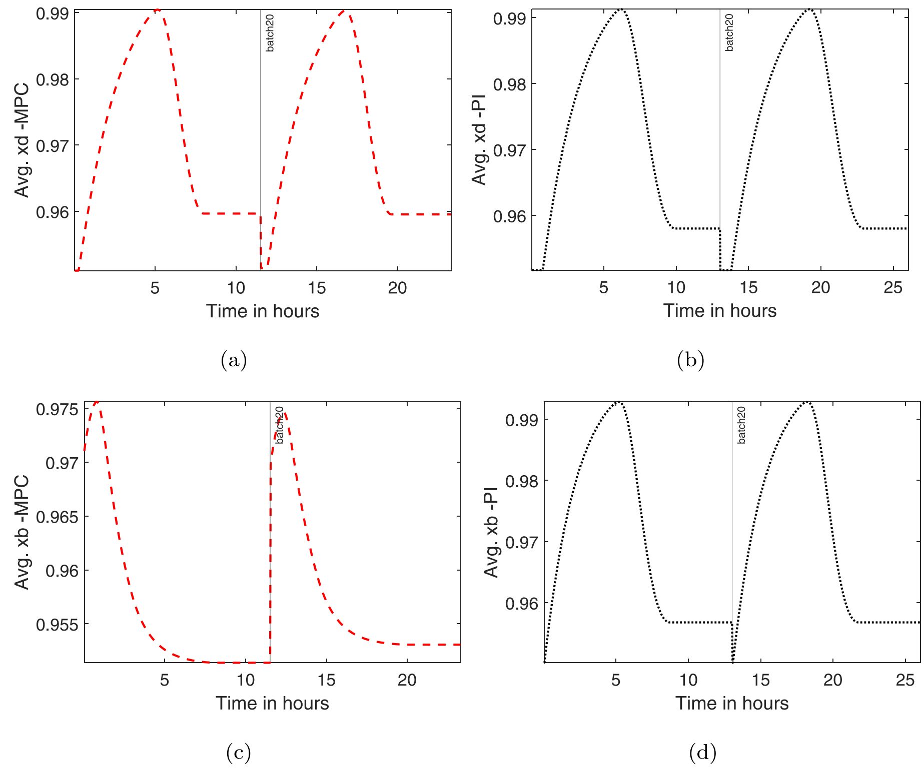


Fig. 11. Average distillate (avg. xd) purity of process (case-1) by (a) MPC configuration (b) PI configuration for cycle 19–20. Average bottom (avg. xb) purity of process (case-1) by (c) MPC configuration (d) PI configuration for cycle 19–20.

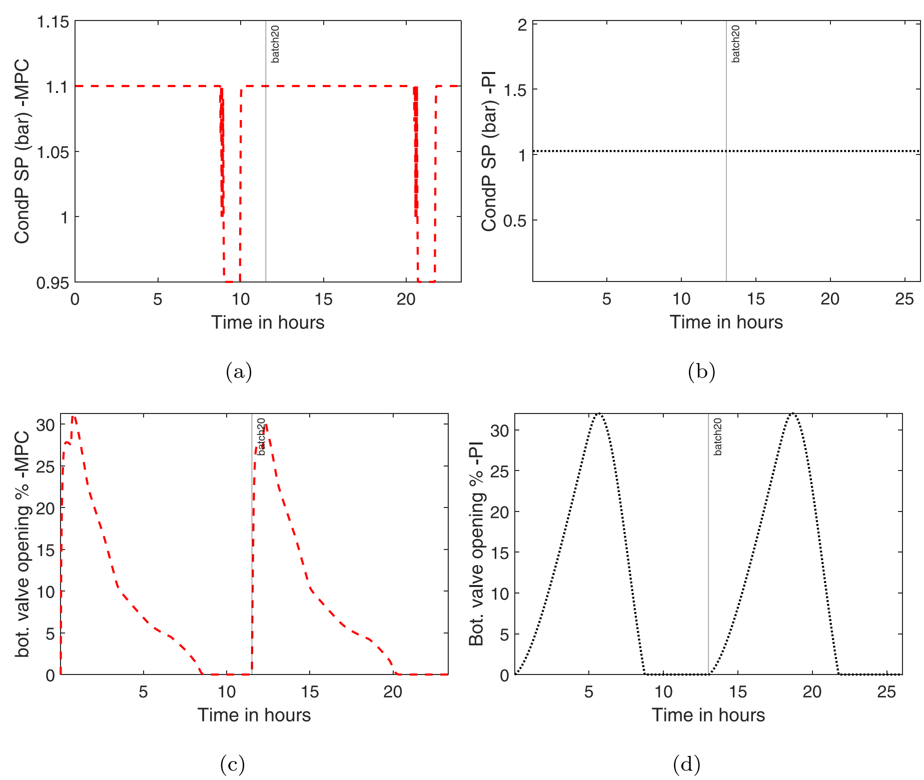


Fig. 12. The condenser pressure setpoint (CondP SP) behavior (Case-1) of (a) MPC configuration (b) PI configuration for cycle 19–20. Bottom (Bot.) valve opening percentage behavior (Case-1) of (c) MPC configuration (d) PI configuration for cycle 19–20.

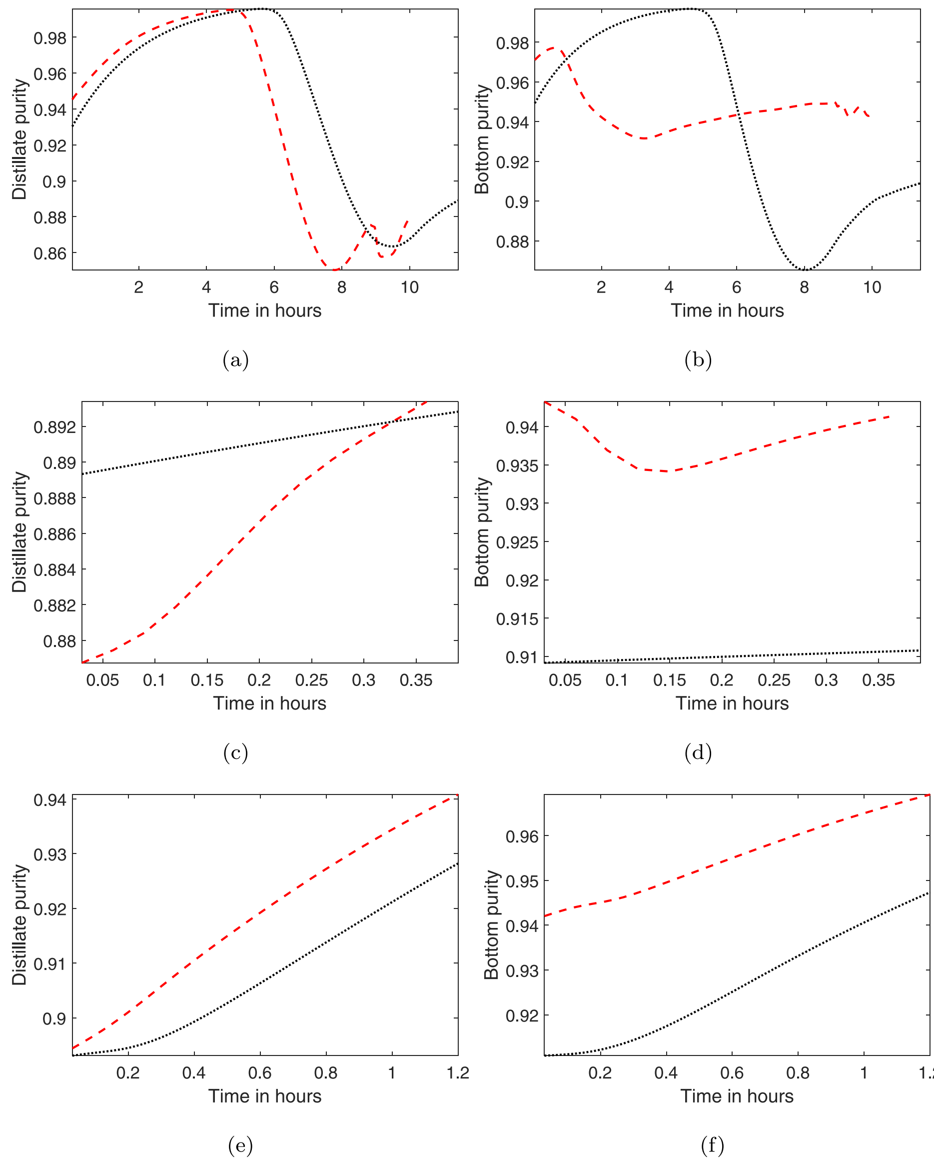


Fig. 13. Comparison of distillate purity behavior by MPC configuration (red slashed line) and PI configuration (black dotted line) for (a) processing (c) discharging (e) charging for cycle 19–20. Comparison of bottom purity behavior by MPC configuration (red slashed line) and PI configuration (black dotted line) for (b) processing (d) discharging (f) charging for cycle 19–20.

case-2 MPC outperforms PI configuration and reduces the TAC/tonne of feed processed by 11.42%

An interesting point to note is MPC found that a condenser pressure setpoint of 1.1 bar optimizes the process to perform better than the traditional PI configuration. A condenser pressure setpoint of 1.1 bar is the maximum operational range. Note that raising the condenser pressure setpoint to 1.1 bar in the standard PI configuration would not even be sought after if not for MPC. For both cases (case-1 and 2), TAC per tonne of feed processed for PI configuration with the condenser pressure setpoint of 1.1 bar is found to be 64.7 USD/t and 74.3 USD/t. The cost value is slightly higher than the most effective MPC setup for both case-1 (64.1 USD/t) and case-2 (73.7 USD/t). These values show the proposed MPC configuration performs better than the PI configuration with the condenser pressure setpoint of 1.1 bar too.

5. Conclusion

In this work, the problem of improving the economic performance of semicontinuous process using a data-driven, multiple model based model predictive control design is addressed. To achieve this, first, a multi-model subspace algorithm was designed. The dynamic behavior of the semicontinuous process was captured by the proposed subspace algorithm better than the traditional subspace algorithm. The semicontinuous process was controlled under MPC configuration to reduce TAC/tonne of feed processed by manipulating the condenser pressure controller setpoint and bottom valve opening percentage. For this particular case study, it was found that the MPC can lower the TAC per tonne of feed processed and cycle time by 11.4% compared to the traditional PI setup of the semicontinuous process. Finally, the ability of the MPC configuration to respond to market changes was illustrated by considering a change in the service utility cost of cooling water

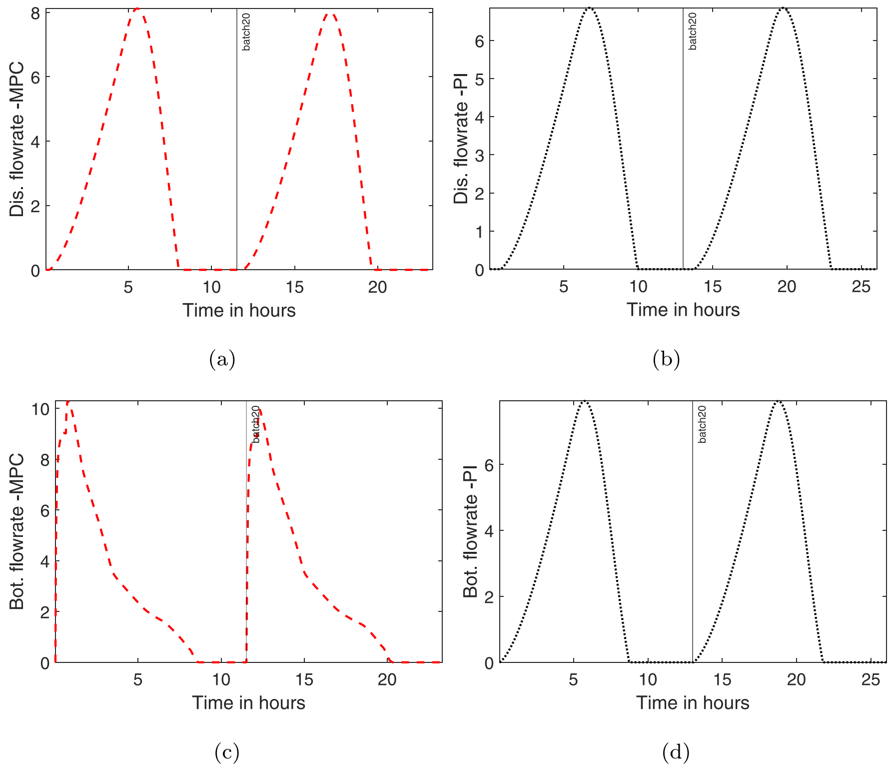


Fig. 14. The distillate (Dis.) and bottom (Bot.) flowrate behavior of ((a), (c)) - MPC configuration ((b), (d)) PI configuration for cycle 19–20.

and heating steam. It was found that MPC performs better than the traditional PI setup in responding to market changes.

CRediT authorship contribution statement

Sakthi Prasanth Aenugula: Methodology. **Aswin Chandrasekar:** Writing – review & editing, Methodology. **Prashant Mhaskar:** Writing – review & editing, Supervision, Methodology, Funding acquisition, Conceptualization. **Thomas A. Adams II:** Writing – review & editing, Supervision, Methodology, Funding acquisition.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Sakthi Prasanth Aenugula reports financial support was provided by Ontario Ministry of Colleges and Universities. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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