ADVANCES IN DESIGN, OPTIMIZATION AND CONTROL OF SEMICONTINUOUS DISTIL-LATION PROCESSES

ADVANCES IN DESIGN, OPTIMIZATION AND CONTROL OF SEMICONTINUOUS DISTILLATION PROCESSES

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Abstract

Semicontinuous distillation is a process intensification technique for purification of ternary mixtures to desired specifications. Where conventional continuous process requires two distillation columns for ternary separation, a semicontinuous process utilizes only one distillation column and integrates it with a simple storage tank (called middle vessel) to perform the same task. Therefore, with a lower total direct cost, a semicontinuous system has a lower total annualized cost (TAC) for low to intermediate production rates compared to the continuous configuration. However, the operating cost of the semicontinuous system is higher than the continuous counterpart.

The objective of this thesis is to improve the economics of semicontinuous distillation by reducing the operating cost and the TAC of the process. This study investigates potential enhancements of the process by modifying the design, optimizing the design parameters and implementing more efficient control strategies on the process.

In this work, a novel intensification technique for purification of ternary mixtures is proposed. The process can purify three components to desired purities in a single distillation column without the necessity of a middle vessel and is called semicontinuous without middle vessel (SwoMV). The proposed configuration reduces the side stream recycling and consequently lowers the operational and the direct costs of a semicontinuous process.

Subsequently, the integration of design and control of semicontinuous processes is studied. A methodology is presented to simultaneously obtain locally-optimal structural and operational parameters of the system to minimize the TAC of the process. A mixed integer dynamic optimization (MIDO) problem is formulated and the outer approximation (OA) and the particle swarm optimization (PSO) methods are used to solve the problem.

Finally, for the first time, the implementation of model predictive control (MPC) on the semicontinuous process is studied. The subspace identification method is adopted to identify a linear state-space model. Subsequently, a shrinking horizon MPC is implemented on the system to reduce the operating cost of the process while maintaining the desired product purities by the end of the cycle.

Research contributions and highlights

- A novel semicontinuous without middle vessel (SwoMV) configuration is proposed in this work.
- By changing the operational policy of the semicontinuous system, the SwoMV configuration can reduce the operating cost and the TAC of the process up to 45% and 43%, respectively.
- The proposed SwoMV configuration can facilitate the retrofit of available distillation columns for purification of ternary mixtures.
- A methodology is presented to simultaneously design the operational and the structural parameters of the semicontinuous process using a mixed integer dynamic optimization (MIDO).
- Integration of design and control of semicontinuous process has resulted up to 33% and 35% reduction in the operating cost and the TAC of the process.
- A deterministic outer approximation (OA) and a heuristic particle swarm optimization (PSO) methods are compared in solving the resulting MIDO problem.
- For the first time, the process is simulated in the equation oriented gPROMS software and a detailed design procedure is presented.
- The advantages and the disadvantages of simulating the semicontinuous process in Aspen Plus Dynamics and gPROMS software packages are discussed.
- The implementation of advanced model predictive control (MPC) on the semicontinuous process is studied, for the first time.
- The subspace model identification technique is used to identify a linear state-space model for a highly nonlinear distillation process, for the first time.
- The MPC implementation has resulted in about 11% reduction in the operational cost of the semicontinuous process and has increased the production rate by about 10%.

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Dream, work, achieve! The last four years was a life-changing experience for me. I am very grateful for the opportunity that I was given. It was an amazing journey and its accomplishment was not possible without the help and the support of people that I had the honour to meet and to work with.

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Thank you all!

Table of contents

Nomenclature

B	Benzene
C_v	Valve coefficient ($\frac{cm^{1.5} gr^{0.5}}{atm^{0.5}\ s}$)
CT^T	Conditional trays on top
CT^M	Conditional trays in the middle
CT^B	Conditional trays on bottom
d_H	Tray hole diameter (m)
D	Middle vessel diameter
ET^T	Eliminated trays on top
ET^M	Eliminated trays in the middle
ET^B	Eliminated trays on bottom
F	Flow rate (kg/s)
f_{min}	Minimum gas load ($Pa^{0.5}$)
g	Acceleration due to gravity (m/s^2)
H	Middle vessel height (m)
k	Gain
$\boldsymbol{M}$	Penalty matrix on quality variables
N	Number of stages
$\boldsymbol{P}$	Penalty matrix on input moves
$\boldsymbol{q}$	Quality variable
$\mathrm{Q_{condenser}}$	Condenser heat duty (kJ/s)
$\mathrm{Q_{reboiler}}$	Reboiler heat duty (kJ/s)
t_f	Final time (s)
T	Toluene
$\boldsymbol{u}$	Input variables
u_{min}	Minimum vapour velocity (m/s)
V	Valve
$\mathrm{v_1}$	Cost of condenser heat duty ($/kJ)
$\mathrm{v_2}$	Cost of reboiler heat duty ($/kJ)

w_1	PSO parameter
w_2	PSO parameter
y_1	Binary variable
y_2	Binary variable
X	*o*-xylene
$\boldsymbol{x}$	State variables
$\tilde{\boldsymbol{x}}$	Subspace states
x_B^{dis}	Purity of benzene in the distillate stream (mass %)
x_X^{bot}	Purity of *o*-xylene in the bottom stream (mass %)
$\boldsymbol{y}$	Output variables

Greek Letters

ρ_L	Liquid density (kg/m^3)
ρ_V	Gas density (kg/m^3)
φ	Relative free area
τ	Reset time

Abbreviations

BTX	Benzene, Toluene, *o*-Xylene
CSC	Conventional semicontinuous
DAE	Differential algebraic equation
ISE	Integral squared error
MPC	Model predictive control
MVCC	Middle vessel continuous distillation column
MV	Middle vessel
NRTL	Non-random two-liquid
PI	Proportional integral
PID	Proportional integral derivative
PML	Process model library
PRBS	Pseudo-random binary sequence
SQMPC	Subspace quality model predictive control

SwoMV	Semicontinuous without middle vessel
TAC	Total annualized cost ($/yr)
VLE	Vapour liquid equilibrium

Chapter 1

Introduction

1.1 What is a semicontinuous process?

Conventionally for purification of ternary mixtures via distillation, two columns are required. In a direct sequence separation, the light boiling point component is removed from the mixture in the distillate stream of the first column. The remaining mixture is fed to the second column where the intermediate and heavy boiling point components are removed in the distillate and bottom streams of the second distillation column, respectively (Figure 1) [1].

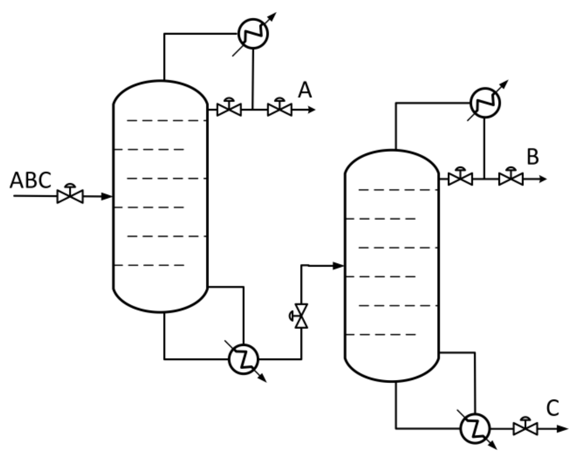

Figure 1- Conventional continuous system for purification of an arbitrary ternary mixture of ABC.

However, distillation columns are expensive pieces of equipment and their operational costs constitute the major fraction of a chemical plant's operating cost [2]. Therefore, process intensification techniques have been developed in this area aiming to reduce the total annualized cost (TAC) of distillation processes [3]. One successful process intensification technique in this field is the semicontinuous distillation process which was proposed by Phimister and Seider in 2000 [4].

In a semicontinuous process one expensive distillation column is omitted from the process and is replaced with a much cheaper storage tank which is called a middle vessel (Figure 2). The semicontinuous process purifies the ternary mixture in a dynamic, cyclic manner. Initially the middle vessel is charged with fresh feed. The middle vessel's charging and discharging valves are then closed and the middle vessel feeds the column. The light and the heavy boiling point components are continuously removed from the system in the distillate and bottom streams of the column, respectively. The purities of these streams are kept at or close to the desired specifications for the products by utilizing composition controllers such that the integral square error (ISE) of the purities from their setpoints are minimized during the cycle.

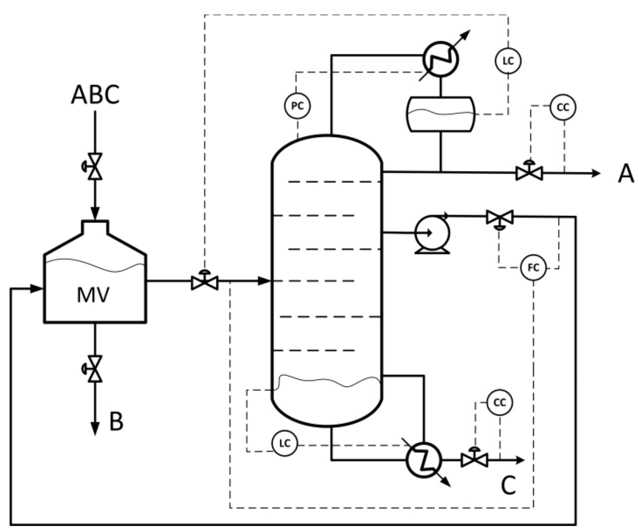

Figure 2- Semicontinuous process for purification of an arbitrary ternary mixture of ABC.

As the system depletes from the light and heavy boiling point components, the concentration of the intermediate component in the middle vessel reaches the desired specification for this product. Subsequently, the middle vessel's discharge valve is opened and the product is collected. Then the discharge valve is closed and the charging valve is opened and the middle vessel is recharged with fresh feed and a new cycle begins. The middle vessel never gets emptied completely. Therefore, it keeps feeding the column during the discharging mode. Therefore, the column does not go through any shut-downs or start-ups.

Although all material streams entering and exiting the column are always flowing, the flow rates themselves vary throughout the cycle. Also, the middle vessel is periodically being charged and discharged. Therefore, the process is somehow in between the classification of batch and continuous processes and for that reason it is called the semicontinuous process.

The process is control-driven and the control structure determines the operational policy of the system. In all previous studies on the process, only multi-PI control loops have been employed. Pascall and Adams have investigated eight different PI control configurations for the process and have evaluated the performance of each control configuration in terms of disturbance rejection, operating cost and maintaining the product purities [5]. The control structure shown in Figure 2 was found to be the best structure that satisfies all criteria.

In this control structure, the purities of the distillate and bottom streams are controlled by manipulating their respective flow rates. The reflux drum and sump levels are controlled by the feed flow rate to the column and the reboiler heat duty, respectively. The column pressure is controlled by the condenser heat duty and finally the ideal side draw control is used to determine the flow rate of the side stream. The ideal side draw control is based on mass balance and manipulates the side stream flow rate to be equal to the flow rate of the intermediate component in the feed stream [6].

1.2 Applications of semicontinuous process

By eliminating one distillation column, semicontinuous separation can significantly reduce the total direct cost of a process. On the other hand, the operating cost of the process becomes higher than the corresponding conventional continuous system. However, the reduction in the total direct cost is significant enough to compensate for the increase in the operating cost of the process at lower production rates and shorter payback periods. Thus, the TAC of the semicontinuous process is lower than the conventional continuous system for low to intermediate production rates. As the production rate of the process increases, a column with a larger diameter is required for the separation. This adds to the capital costs of the process and consequently, diminishes the superiority of the semicontinuous system over the conventional continuous system. Therefore, there is a certain range of production where the semicontinuous process is more economical than the conventional continuous system.

Over the last 16 years, since the introduction of the process, different studies have explored the applicability of the semicontinuous system for purification of different mixtures [7]. A detailed literature review is provided in the introduction section of Chapter 2. All studies in the open literature to date have confirmed that the semicontinuous process is more economical than the conventional continuous system at low to intermediate production rates. It has also been shown that where flexible separation in terms of purities is required, semicontinuous separation is a suitable choice [8]. Therefore, this separation technique can be used effectively for the production of bio-fuels and pharmaceuticals where the production rates are usually lower [9]. Several studies have shown that constructing multiple distributed, smaller bio-refineries instead of one large, centralized plant can reduce the transportation costs of biomass, which can reap significant benefits [10]. As such, it is probable that semicontinuous processes would be more suitable for these smaller, distributed plants and possibly even shift the optimum sizes down even more.

1.3 Challenges and solutions

While promising, semicontinuous systems have limitations such as the scales at which they are economical and also having higher operating costs than the conventional continuous systems. This study tries to tackle these issues by enhancing the semicontinuous system from a number of different aspects:

1- Reducing the operating cost of the process by improving the operational policy of the system. The process is inherently wasteful by constantly recycling the purified side stream back to the un-purified middle vessel. In this work, a novel configuration is proposed that reduces the recycling in the semicontinuous process and consequently lowers the energy consumption.

2- Reducing the TAC of the process by optimizing the design and the operational parameters of the system such as number of stages, feed and side stream locations, middle vessel hold up and the tuning parameters of the PI controllers. Due to the complexities of the process, the optimization of the process was not studied well in the literature. Previous attempts to optimize the process were limited to a subset of design parameters [5, 11]. Thus, in this work an efficient optimization methodology is presented to design the structural and the operational parameters of the process simultaneously.

3- Reducing the operating cost and increasing the production rate of the process by implementing advanced control strategies. The control configuration of the semi-continuous separation is the fundamental driver of the process and enhancing it will improve the operation of the system.

The successful implementation of these methods will result in considerable cost savings, a wider applicability of the semicontinuous process for purifying mixtures and ultimately bringing down the costs of bio-fuels and pharmaceutical products which are set to gain the most benefit from using the semicontinuous separation.

1.4 Chapters and publication summaries

Chapter 2 contains the first peer-reviewed publication resulting from this thesis. In this chapter a detailed literature review on the semicontinuous process and its applications is presented. Followed by that, the procedure to design and simulate a semicontinuous process in Aspen Plus Dynamics is discussed. The rest of the chapter introduces a novel semicontinuous configuration.

The scope of this chapter is to reduce the operating cost of a semicontinuous process from the design aspect. It is noticed that one reason for higher operational cost of the semicontinuous process is the constant recycling of the side stream back to the middle vessel. Therefore, if this inefficiency can be lessened by minimizing the recycling of the side stream, higher efficiencies can be obtained.

The new proposed process intensification technique is called semicontinuous without middle vessel (SwoMV). The configuration is capable of performing the same separation as a semicontinuous system process in just one distillation column but without the integration to a middle vessel. The purification is achieved by changing the operational policy of the column in two different operational modes which are producing and non-producing modes.

The advantages of the proposed configuration are:

1- Elimination of the middle vessel and the consequently the charging–discharging modes of operation.
2- Lowering the TAC of the process compared to the semicontinuous system.
3- The SwoMV process can facilitate the retrofit of available distillation columns for purification of new products.

The full paper citation is as follows:

Meidanshahi, V., Adams II, T.A., 2015. A new process for ternary separations: Semicontinuous distillation without a middle vessel. Chemical engineering research and design. 93: 100–112.

Chapter 3 contains the second peer-reviewed publication resulting from this thesis. This chapter addresses the main challenge of the semicontinuous process, which was designing the operational and the structural parameters of the system such that the process has the lowest TAC. There are heuristic design procedures available in literature that provide guidelines to design a semicontinuous process [12-13]. These heuristic methods suggest a sequential design approach in which first the structural parameters of the system are determined and then the control structure and its tuning parameters are designed. Subsequently, in a trial-and-error procedure, the design parameters are changed to obtain a better design with a lower TAC. Therefore, the design procedure can be quite time consuming. On the other hand, selecting the tuning parameters of the PI controllers that have high interactions can be quite tedious.

In this work, for the first time a simultaneous approach is suggested for designing the semicontinuous system in which the structural and operational parameters of the system are determined simultaneously in a mixed integer dynamic optimization problem. The benefit of the proposed method is lowering the computational time required to design a semicontinuous process for an arbitrary mixture.

Another advantage of integration of design and control of a semicontinuous process is consideration of the interactions of structural and operational parameters of this dynamic process in the design stage.

The full paper citation is as follows:

Meidanshahi, V., Adams II, T.A., 2016. Integrated design and control of semicontinuous distillation systems utilizing mixed integer dynamic optimization. Computers and Chemical Engineering. 89, 172–183.

Chapter 4 contains the third full paper of this thesis. This chapter addresses the control challenges of the semicontinuous process. The semicontinuous distillation is highly nonlinear with high variable interactions. The process has operational constraints which should be satisfied to ensure safe and stable operation. Although PI control configurations are shown effective to control the process but advanced control strategies such as model predictive control (MPC) can potentially enhance the economics of the process by providing a better control.

In this work, implementation of the MPC on the semicontinuous process is studied for the first time. This chapter describes the identification method adopted to find a linear data-driven model for the MPC. Two MPC configurations for the semicontinuous process are studied. Finally, the economic benefits of the MPC are explored in two case studies in this chapter.

The full paper is submitted to the following journal:

Meidanshahi, V., Corbett, B., Adams II, T.A., Mhaskar, P., 2016. Subspace Model Identification and Model Predictive Control of Semicontinuous Distillation Process. Computers and Chemical Engineering (Submitted).

In Chapter 5 the final remarks, suggestions for future works and the conclusions are presented.

1.5 Author's contributions to papers

As the author of this thesis, I can confirm that I was the primary investigator, developer of any and all methods, presented in chapter 2 and 3. As for chapter 4, the identification and SQMPC Matlab codes of Corbett and Mhaskar were adopted for control studies. However, I was solely responsible for the implementation of the methods on the semicontinuous process and the obtained results.

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Chapter 2

A new process for ternary separations: Semicontinuous distillation without a middle vessel

The content of the following chapter is a **published reprint** of the following peer-reviewed publication:

Meidanshahi, V., Adams II, T.A., 2015. A new process for ternary separations: Semicontinuous distillation without a middle vessel. Chemical engineering research and design. 93, 100–112.

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A new process for ternary separations: Semicontinuous distillation without a middle vessel

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A B S T R A C T

In this work, a novel semicontinuous process for the separation of ternary mixtures is presented. The new semicontinuous without middle vessel (SwoMV) configuration is a process intensification technique that makes separation of three components to desired purities possible in a single distillation column without the necessity of the middle vessel as opposed to the conventional semicontinuous processes. The elimination of the middle vessel omits the charging and discharging modes of conventional semicontinuous processes, reduces the direct costs of plant and facilitates the retrofit of available distillation columns for purification of new products. Furthermore, SwoMV configuration improves the conventional semicontinuous system by reducing the energy consumption in most cases and expanding the range of system capacities at which it is economically optimal. The separation of benzene, toluene, and *o*-xylene is used as a case study to show the feasibility of the SwoMV configuration. An economic analysis is performed, and conventional continuous distillation, conventional semicontinuous, SwoMV and single side stream column configurations are compared by calculating the total annualized cost of these systems over a range of production rates. The results show the feasibility, applicability and profitability of the novel proposed configuration.

Keywords: Semicontinuous separation; BTX; Semicontinuous without middle vessel; Ternary separation; Economic evaluation

1. Introduction

Distillation is one of the most common unit operations for purification of mixtures into more valuable high-purity components. Since it is a mature and well-studied unit operation, most recent advances in distillation system design have come in the form of advanced process intensification strategies. The semicontinuous distillation configuration proposed by Phimister and Seider (2000a) was one such strategy. For the separation of ternary mixtures to any desired purities using conventional continuous distillation configurations, two distillation columns are required. However, the novelty of the proposed configuration by Phimister and Seider was to eliminate one of the distillation columns and replace it with a simple storage tank (called a middle vessel, MV) and purify all three components to their desired specifications using an unsteady-state approach.

In the semicontinuous distillation configuration, the middle vessel is charged with fresh feed. It continuously feeds the column and a side draw is collected is recycled back to the tank. As the light and heavy components are removed from the system in a continuous fashion in the distillate

Abbreviations: BTX, benzene, toluene, *o*-xylene; CSC, conventional semicontinuous; ISE, integral squared error; MV, middle vessel; NRTL, non-random two-liquid; SwoMV, semicontinuous without middle vessel; TAC, total annualized cost ($/yr); VLE, vapour liquid equilibrium.

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Nomenclature

B	benzene
C_v	valve coefficient ($cm^{1.5}$ $gr^{0.5}$/($atm^{0.5}$ s))
d_H	tray hole diameter (m)
f_{min}	minimum gas load ($Pa^{0.5}$)
g	acceleration due to gravity (m/s^2)
N	number of stages
T	toluene
u_{min}	minimum vapour velocity (m/s)
V	valve
X	o-xylene
Greek letters	
ρ_L	liquid density (kg/m^3)
ρ_V	gas density (kg/m^3)
φ	relative free area

and bottom streams, respectively, the intermediate-boiling component concentrates in the middle vessel. When its concentration reaches the desired specification, the middle vessel is discharged and the product is gathered. The middle vessel is then charged again with fresh feed for the next cycle.

Several studies have investigated the range of applicability of the semicontinuous separation for various systems. Phimister and Seider (2000b,c) have showed application of the semicontinuous configuration for extractive and pressure-swing distillation. To model the system, they used the simplifying assumption of pseudo-steady-state energy balances in their simulations, and integrated the resulting dynamic MESH equations in FORTRAN 90. In 2004, Monroy-Loperena and Alvarez-Ramirez studied a semicontinuous separation process and compared it to continuous and batch process alternatives. They modelled the system under the assumptions of negligible vapour holdup, theoretical trays, and constant operating pressure.

Adams and Seider (2006, 2008, 2009a) investigated the feasibility of integration of reaction and separation in a semi-continuous configuration where the reaction took place in the middle vessel. They concluded that when reactive distillation is infeasible the semicontinuous distillation with chemical reaction in a middle vessel process is an economical option for a wide range of production rates.

Adams and Seider in 2009b further developed the semicontinuous separation process by designing a packed distillation column which switches between reactive extraction and reactive distillation for separation of 1,3-propanediol from a dilute mixture with water obtained from an upstream biofermentation process.

In 2013, Pascall and Adams looked into the applicability of semicontinuous separations for biofuel production. They used Aspen Plus and Aspen Dynamics software for their studies. They concluded that by using semicontinuous technology, a remarkable reduction in the cost of producing bio-DME can be achieved for small-scale distributed networks.

In 2013, Niesbach et al. proposed the use of semicontinuous distillation for the separation of butyl acrylate from a mixture of several light and heavy boiling point impurities. When the bio-resource feedstock used to produce butyl acrylate is changed (such as switching between different types of wood), different impurities might be produced in the product. They concluded that by using the semicontinuous system, high purities of product can be achieved without changing the operating conditions of the column. Furthermore, they showed that this process is quite flexible with respect to variations in the impurities present in the feedstock.

To recap, the profitability of semicontinuous separation over conventional continuous and batch systems for low to intermediate production rates has been well-illustrated in the existing literature and it has been shown that where flexible separation in terms of purities is required, semicontinuous separation is a good choice. Therefore, this separation technique can effectively be used for the production of bio-fuels (such as biodiesel, where plant capacities are low (Wen et al., 2009)) and down-stream purifications are essential to achieve fuel-grade quality. Several studies have shown that constructing multiple, distributed, smaller bio-refineries instead of one large, centralized plant can reduce the transportation costs of biomass, which can reap significant benefits (Carolan et al., 2007). For example, Bowling et al. (2011) used a mathematical programming model to determine the optimal location and size of biorefineries. Using this systematic method they concluded that the smaller distributed configurations usually are better options over the large, centralized plants. Sultana and Kumar (2012) performed a similar study for Alberta and concluded that the distributed facilities were more preferable. Depending on the geographical distribution of biomass, both of these studies have showed that smaller distributed biofuel plants may be more economically favourable. As such, it is probable that semicontinuous processes would be more suitable for these smaller distributed plants, and possibly even shift the optimum sizes down even more.

However, while promising, semicontinuous separations have limitations such as the smaller scales at which they are economically optimal and generally higher operating costs than conventional continuous systems. This study tries to tackle these issues by proposing a novel configuration called semicontinuous without middle vessel (SwoMV). This configuration is a process intensification technique that makes the separation of three components to desired purities possible in a single distillation column without the necessity of the middle vessel as opposed to the “conventional” semicontinuous process used in all prior semicontinuous studies. The elimination of the middle vessel omits the charging and discharging modes of the conventional semicontinuous process, reduces the direct costs of the plant, and depending on the initial composition of the feed, reduces the operating costs, thereby increasing the economical range of production. Furthermore, the new process facilitates the retrofit of existing distillation columns for purification of new products or elimination of introduced impurities in the process without installing any new vessels or columns.

In the SwoMV configuration the side stream is recycled back, mixed with the fresh feed and re-fed to the column. The required product purities are achieved by adjusting the total feed flow rate to the column in two modes of operation. It is worth mentioning that a distillation column with several side streams (without recycling) is a popular configuration for fractional distillation. Fractional distillation is commonly used in petroleum refineries to separate a multicomponent feedstock into multiple fractions via each side stream of the column. Each fraction consists of a group of components with similar boiling points. To further purify each fraction to pure components, subsequent distillation columns are required. However, if the feed consists of only three components, any desired product purities may be obtained by using a single column with a side stream and no recycling. However, a column utilizing a side stream has been shown in prior work to only be economical compared to the conventional continuous system (two consecutive distillation columns) when the mole percent of the intermediate component in the feed is above 80% (Doukas and Luyben, 1978). For other feed compositions, the side stream column has been shown to be uneconomical since it requires generally higher operating costs and column diameters (therefore capital costs), leading to higher total annualized costs (Alatiqi and Luyben, 1985). An economic analysis is performed in this study to compare the SwoMV and the single side stream configuration.

To study the feasibility of the SwoMV configuration, the separation of benzene, toluene, and o-xylene (BTX) to high purities is chosen as a case study. BTX separation is an important part of petrochemical refineries in which BTX is produced in a naphtha reforming process and are then separated for sale or other use (Chauvel and Lefebvre, 1989). In conventional refineries, the products are separated to high-purity benzene, toluene, xylene and heavy components successively in three consecutive columns with binary distillation. The first two columns of the fractionation process in the naphtha reforming unit are replaced with one distillation column working in a semicontinuous mode in this study.

BTX separation is also a good choice for a case study in demonstrating the new SwoMV concept because of the relative volatilities (7.1, 2.2 and 1) and normal boiling points (80–144 °C) of the species are in easily manageable ranges. Furthermore, BTX separation may be necessary in biorefineries which produce transportation fuels via Fischer–Tropsch synthesis (Demirbas, 2009), and such refineries are likely to be optimal at lower production rates where semicontinuous systems are likely to be optimal. However, it is important to note that the proposed SwoMV system can be applicable to a wide variety of other chemical mixtures.

After designing the SwoMV configuration and its appropriate control structure, simulations are performed in Aspen Dynamics and economic analyses are performed to compare the profitability of conventional continuous, conventional semicontinuous, single side stream, and SwoMV, systems.

2. Process modelling

2.1. *Conventional continuous process*

Fig. 1 shows the optimum configuration of the conventional continuous system for the separation of an equimolar feed of BTX with high purities of 99 mol%, according to the work of Ling and Luyben (2009). The equimolar BTX mixture at 358 K and 0.5 bar is fed to the first column just above stage 14. The first column is modelled with 30 equilibrium stages and the reflux drum operates at vacuum pressure (0.37 bar) such that cooling water can be used as a cooling medium. Benzene is recovered in the distillate stream and the mixture of toluene and o-xylene recovered in the bottoms is fed to the second column on tray 14. This column has 28 stages and the reflux drum operates at 0.13 bar. A pressure drop of 0.0068 bar per tray and Murphree efficiency of 0.75 is used for both columns. Simulations are performed using Aspen Plus V8 with the RadFrac equilibrium-based model for distillation columns. The vapour–liquid equilibria (VLE) are modelled using the NRTL model with ideal gas

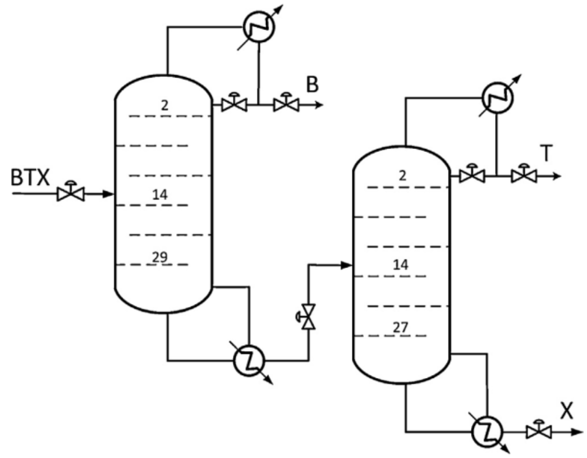

Fig. 1 – Schematic of the conventional continuous BTX separation system.

and Henry's law (Kiss and Rewagad, 2011). These specifications were chosen to be consistent with the aforementioned work.

In this study, the optimum configuration of the conventional continuous system for two other cases with different feed compositions is also determined. For both the toluene-rich feed composition case (10, 80 and 10 mol% of BTX, respectively) and toluene-lean feed composition case (45, 10 and 45 mol% of BTX), all design parameters are the same as the equimolar feed case, except that the feed enters at stages 15 and 17 in the first and second columns, respectively.

2.2. *Conventional semicontinuous process*

In the conventional semicontinuous (CSC) ternary distillation configuration, which is shown in Fig. 2, one distillation column is replaced with a middle vessel which is integrated tightly with the distillation column in the system. The process operates in a stable limit cycle consisting of three operational modes.

In mode 1, the middle vessel is charged with fresh feed. After the tank is charged valve V1 is closed and mode 2 begins.

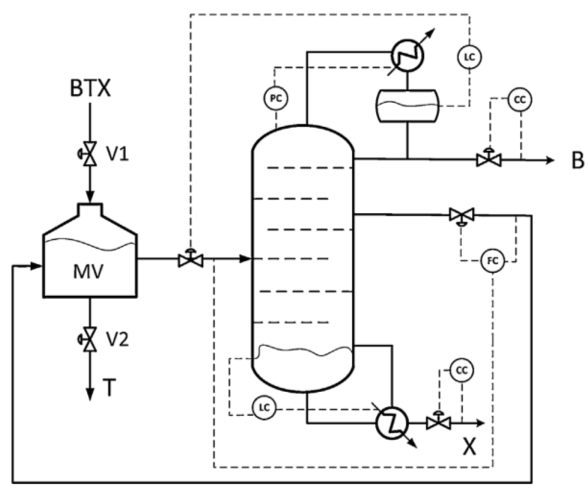

Fig. 2 – Schematic of the conventional semicontinuous configuration applied to a BTX system.

During this mode, the middle vessel feeds the column and the light and the heavy boiling point components (benzene and *o*-xylene, respectively) are withdrawn from the system at the desired purity of 99 mol% in the distillate and bottom streams, respectively. The side stream (rich in the intermediate component, toluene) is recycled back to the middle vessel. As the middle vessel is gradually depleted of benzene and *o*-xylene, the concentration of toluene increases in the vessel. When the desired concentration of toluene is achieved (99 mol% in this study) mode 3 starts by opening valve V2 and discharging the toluene product. Subsequently, valve V2 closes when the level of the middle vessel reaches a specified small value and the system cycles back to mode 1.

During all modes, the middle vessel continuously feeds the column, and the distillate and bottom products are withdrawn such that the column is always in operation without any shutdowns or start-ups. However, there are no steady-states during any part of the cycle since the composition and flow rate of the feed to the column changes over time.

Before dynamic simulations can commence, key design information must be determined, such as the number of stages, feed and side stream locations, column diameter, reflux drum size, and sump height. In addition, an initial state of the column is needed. To do this, an analogous flow sheet at steady-state is first simulated in Aspen Plus V8. Although the semicontinuous process is never at steady-state, the Aspen Plus model is a very good guess at a snapshot of the dynamic system at the beginning of mode 2. The column is modelled using the equilibrium-based RadFrac model in Aspen Plus, which is then exported to Aspen Dynamics, where additional modifications are necessary to complete the model. Our methodology is described next.

The pressure condition for the conventional semicontinuous column is considered to be the same as the first column in the conventional continuous configuration (reflux drum pressure of 0.37 bar). The number of column stages, as well as the feed and side draw locations, are determined as is explained later. Note that the side stream leaving the column is not connected to the middle vessel in the Aspen Plus model in order to enable convergence to a steady-state solution. Next, the design heuristics of Luyben (2006) is implemented to size the reflux drum and sump to allow for 5 min of liquid holdup when the vessel is 50% full, based on the total liquid entering or leaving these vessels. The middle vessel was sized such that it initially holds 100 kmol of fresh feed and the valves are sized to handle 3 bar pressure drop. These values are reasonable choices for a base case study based on a comparison with similar systems (Pascall and Adams, 2013).

At present, the distillation column model in Aspen Dynamics uses an equilibrium-based model and does not have a dynamic rate-based model available. Therefore, in order to incorporate the effect of sub-equilibrium behaviour (tray efficiencies of less than 100%) in the dynamic simulations, steady-state rate-based simulations were performed in Aspen Plus for a range of feed flow rates and compositions that might be encountered at different times during the semicontinuous cycle starting with an equimolar feed composition. The rigorous rate-based RadFrac model in Aspen Plus is then used to estimate tray efficiencies. As an example, the tray efficiencies calculated based on the rate-based model for the 50 stage design are shown in Fig. 3. The tray efficiencies are fairly constant throughout the cycle and depend very little on feed flow rate and composition. Therefore, a tray efficiency of 0.75 was

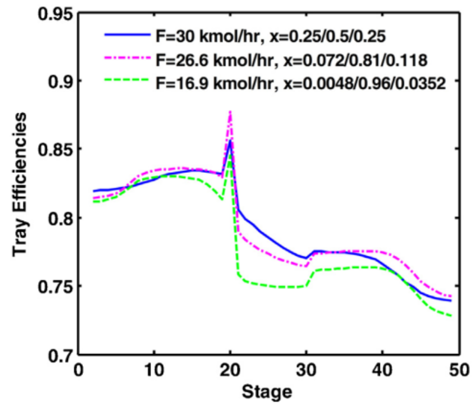

Fig. 3 – Calculation of tray efficiencies using rate-based simulations in Aspen Plus for different scenarios.

adopted for all stages of the column (a conservative estimate) for the equilibrium-based model.

Once all of this was completed, the simulation was exported to Aspen Dynamics as a pressure-driven simulation. After an initialization run is completed in Aspen Dynamics, a control system was added and the side stream was connected to the middle vessel. Because the system operates in a limit cycle, a well-designed control structure is needed to drive the cycle and achieve the desired performance. Pascall and Adams (2013) have looked into this issue and compared the performance of eight different control structures. Based on their work, the control structure shown in Fig. 2 was implemented for the simulation, which was identified to be the best in terms of controller performance, cycle stability, and robustness in the face of disturbances.

In this control structure, the reflux drum and sump levels are controlled by manipulating the feed flow rate to the column and the reboiler heat duty, respectively. The column pressure is controlled by manipulating the condenser heat duty. The purities of the distillate and bottom streams are controlled by manipulating the flow rate of these streams. The ideal side-draw recovery arrangement is implemented to control the side stream (Adams and Seider, 2008). A dead time of 3 min is assumed for composition analysers in the simulation. Proportional-integral (PI) control is used for composition and pressure loops while proportional-only (P) control is implemented for level and side stream flow. Controllers are tuned for each case of different initial feed compositions by hand such that the integral squared error (ISE) of benzene composition in the distillate and *o*-xylene in the bottoms are minimized. The event-driven task feature is used within Aspen Dynamics to handle the switching of the control system to different operational modes.

For the conventional semicontinuous process, the number of stages, column diameter, feed location, and side draw location are key design parameters which significantly affect the performance of the cycle and the total annualized cost (TAC). Furthermore, for each combination of those four key design parameters, there is some optimum set of control parameters (such as the controller gains and integral time constants) required to achieve a stable, functioning limit cycle with the minimum cost. There are many constraints which must be satisfied, such as ensuring that flooding and weeping never occur in the column at any point in the cycle (see Section 3.2).

Therefore, it can be quite challenging to find the parameters which yield the optimum design (the lowest TAC). The equation-based dynamic optimization tools provided with Aspen Dynamics are not suitable for semicontinuous systems because they do not work for systems with discrete events (such as mode switching) for which the exact times of their occurrences are not known a priori. Previous attempts to optimize semicontinuous systems in Aspen Dynamics using black-box techniques such as particle swarm optimization have been successful, but required very long run times due to both the length of time required to perform each dynamic simulation (about 4 min) and the high degree of dimensionality (Pascall and Adams, 2013). To make matters worse, this must be repeated for each individual production rate studied, since the column and corresponding control system must be re-designed to handle different flow rates, resulting in approximately 1 cpu-year of computation time required for formal optimization.

Consequently, we have adapted a shortcut procedure to achieve very good (but probably suboptimum) results in a much more reasonable amount of time. A series of steady-state simulations were performed in Aspen Plus to mimic the conditions of what the column would be at the beginning of mode 2. A range of number of stages was considered. For each number of stages considered, the feed tray location and side draw location was determined such that the operating cost of utilities are minimized and design specification of 99 mol% purities of the distillate and bottoms products are achieved by using the NQ curves tool in Aspen Plus. The NQ Curves tool optimizes the number of trays and feed locations in a RadFrac column using rigorous column simulation by plotting the heat load versus the number of stages. The NQ curves analysis performs an intelligent search, varying the number of stages in a column, optimizing the location of one feed stream at each step, and adjusting the locations of other feed and side-draw streams according to rules the user specifies. Subsequently, the column diameter necessary to prevent flooding was calculated using the results of the analysis, which is then used to compute the total direct costs of the column using the Aspen In-Plant Cost Estimator V8 software tool available from within Aspen Plus V8. The total direct costs include the equipment, piping, civil, instrumentation, electrical, paint, installation, and other details.

The operating costs were calculated considering only the utility costs of steam and cooling water. The cost of steam for the reboiler was estimated using the method of Towler and Sinnott (2012) which estimates the cost using the price of natural gas ($2.51/MMBtu (USEIA, 2012)) and the electricity price ($0.0491/kWh (IESO, 2012)). According to a similar methodology (Towler and Sinnott, 2012), the cooling water cost was estimated based on the electricity price ($0.0491/kWh (IESO, 2012)) and the water make-up and chemical treatment price ($0.02/1000 US gal (Towler and Sinnott, 2012)). Electricity is typically used to recirculate water and its cost is usually between 1 and 2 kWh/1000 US gal of circulating water (Towler and Sinnott, 2012). The electricity cost constitutes a significant portion of the cooling water cost and its variation has a significant effect of the price of cooling water. The resulting cost of steam at 147.75 °C is $0.5655 per GJ of heating load and the cost of cooling water at 24 °C is $0.3164 per GJ of cooling load. Therefore, the steam price is about 1.78 times the cooling water cost. For equimolar feed composition, the condenser and the reboiler heat duties are approximately in the same order therefore the cooling water cost represents approximately about 35% of the total operating cost.

Together, the energy costs and capital costs are combined to compute the TAC (assuming a 3-year plant lifetime and 8400 h per year of operation) according to Eq. (1) (Luyben, 2010).

$$\mathrm{TAC} = \frac{\text{Total Direct Cost}}{\text{Payback Period}} + \text{Annual Operating Cost} \tag{1}$$

When completed, a few cases with the lowest TAC are selected for further consideration. These analyses were based on the steady-state results which mimic the conditions of what the column would be at the beginning of mode 2, and not the entire cycle. Therefore, these candidate cases are then explored further in Aspen Dynamics considering the entire mode of operation.

For each of these candidate cases (i.e., columns with different numbers of stages with corresponding feed and side draw locations), dynamic simulations are performed over a range of production rates. The control system for each case was designed and tuned manually in order to complete the design objectives, minimize the energy costs, and ensure that flooding and weeping are prevented throughout the cycle. Some of the cases were found to not satisfy the purity constraints when considering the entire cycle and all ranges of production rates and were discarded. The TAC is then calculated for each remaining case. Subsequently, the case with the lowest TAC which satisfies the purity constraints of all three streams over the entire cycle was then selected as the best configuration.

This procedure is repeated for three cases of feed compositions and the results are listed in Table 1. This methodology reduces the number of simulations significantly to find a good configuration in a reasonable amount of time. Although the result is sub-optimal, it is still very good. In this case, 40 stages was always the most economic choice; anything larger had higher TAC and anything lower had purity constraint violations at some point during the cycle. However, a detailed dynamic optimization is required to find the optimum configuration which possibly could improve the performance of the system even more. This is outside the scope of this work.

2.3. *Semicontinuous without middle vessel (SwoMV)*

The new configuration proposed in this work aims to exploit the semicontinuous technique for ternary separation and modify it so that the middle vessel is eliminated from the system to further reduce the direct and operating costs of the process, and also to eliminate the charging and discharging modes of the conventional semicontinuous system. We call the new configuration semicontinuous without middle vessel (SwoMV).

The SwoMV configuration is shown in Fig. 4. The distillation column for the SwoMV design has the same structural and design parameters as the column in the conventional semicontinuous design. In this configuration, the bottoms and distillate streams are always collected (albeit at varying flow rates) in the same manner as in the conventional semicontinuous design. However, the fresh BTX feed from upstream is continuously fed to the system (though at variable rates), and the intermediate component (toluene) is now collected directly via the side draw, with a variable purity over the course of the cycle.

The system has two modes: the non-producing mode and the producing mode. Toluene is collected according to the

Table 1 – Column parameters of conventional semicontinuous system.

Feed of B/T/X (mol%)	Number of stages	Feed stage	Side draw stage
45/10/45	40	35	15
33/33/34	40	24	14
10/80/10	40	25	20

following policy. First, an upper and lower bound for purity of the intermediate component is defined, and should be chosen such that the average purity that is in between the bounds would be the desired purity. In this example, we have chosen an upper bound of 99.5 mol% and a lower bound of 98.5 mol% to achieve an approximate average purity of 99 mol%.

The side stream splits into two streams (see Fig. 4). The cycle starts with the non-producing mode during which the purity of the toluene in the side stream is below the upper bound. During this mode valve V1 is closed, valve V2 is fully open, and the side stream is recycled back (mixed with the fresh feed and fed to the column). During this mode, the purity of the side draw gradually increases. Once the purity of the side stream reaches the desired *upper* bound, the producing mode starts, valve V1 is fully opened, and toluene product is withdrawn. The rate at which toluene is collected is a degree of freedom and is discussed in Section 3.3. Note that because stream flow is simulated using a pressure-driven model, valve V2 must be partially closed in order to achieve the desired recycle ratio during the producing mode. The open fraction of V2 was pre-determined manually using off-line tests. The purity of the side draw now gradually decreases. As soon as the purity of this stream falls below the *lower* bound, V1 closes and V2 opens completely, and a new cycle begins. The opening and closing functions of valves V1 and V2 during producing and non-producing modes are determined by using Aspen Dynamics event-driven task.

The rest of the control structure is essentially the same as in the conventional semicontinuous system and the controllers are tuned in the same way. Note that the fresh BTX feed from upstream is now manipulated in order to manage the reflux drum level, instead of the feed to the column (after mixing with the side draw). As a result, the flow rates of all of the streams vary throughout each cycle.

2.4. *Side stream column*

For the purpose of economic comparison, a single distillation column with a side stream is also simulated (Fig. 5). The column is designed to have the same structural and design parameters as the column in the conventional semicontinuous and SwoMV designs. The distillate flow rate, the side draw rate and the reflux ratio of the column are adjusted such that the required purities of all three products are obtained.

3. Results and discussion

3.1. *Performance of the conventional semicontinuous process*

The performance of the conventional semicontinuous system is illustrated in this section for the example using a feed composition of 45, 10 and 45 mol% of BTX. As shown in Fig. 6a, the middle vessel is initially charged with fresh feed. The liquid level in the MV drops as it feeds the column, and the benzene and *o*-xylene are withdrawn from the system. After about 32 h, the desired purity of 99 mol% for toluene is attained in the middle vessel as shown in Fig. 6b, and the toluene product is discharged (seen in Fig. 6a as a sharp drop in the MV level). To avoid any shut-downs and start-ups, the MV does not discharge completely, which is why the initial concentration of toluene is higher than the fresh feed of 10 mol% in Fig. 6b. The middle vessel is subsequently charged with fresh feed at time 35 h and the second cycle starts.

As the cycle proceeds, the mole fraction of benzene and *o*-xylene in the middle vessel and the feed stream decreases as they are removed, thus making it more difficult to maintain the purity of the distillate and bottom stream. As a result, the control system gradually increases the reflux and boilup ratios as can be seen in Fig. 7. Simultaneously, the control system

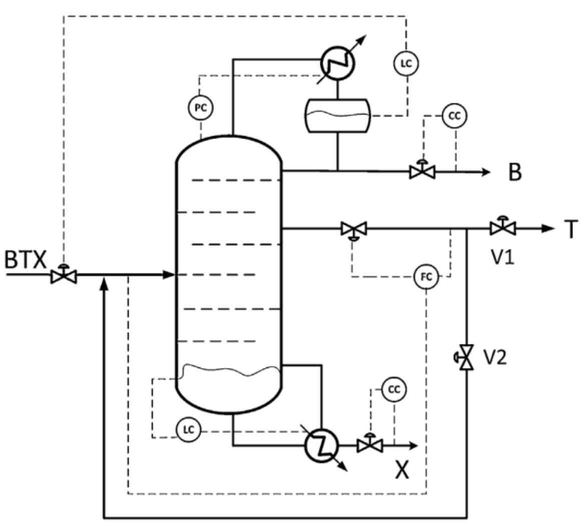

Fig. 4 – Schematic of the novel SwoMV system.

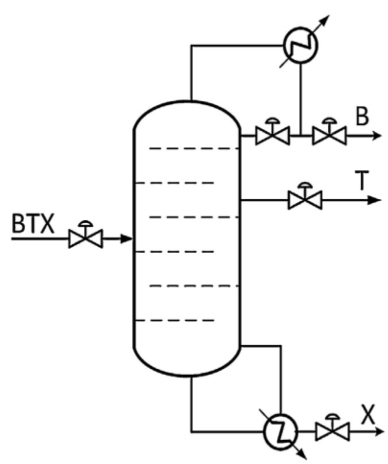

Fig. 5 – Schematic of the side stream column for BTX separation.

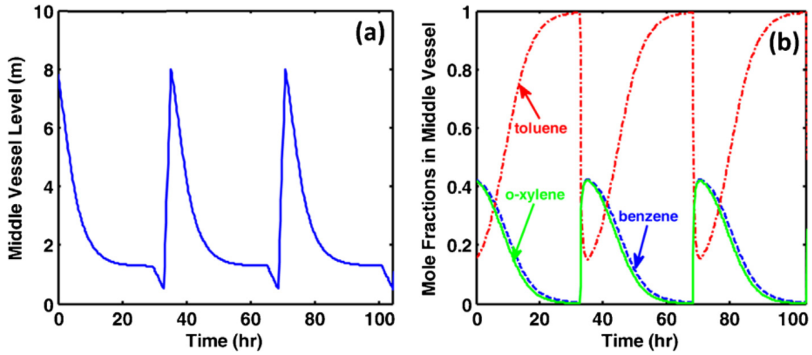

Fig. 6 – The (a) level and (b) mole fraction of the middle vessel during three conventional semicontinuous cycles for feed composition of 45, 10 and 45 mol% of BTX.

also decreases the feed flow rate to the column (see Fig. 8a) in order to maintain a constant reflux drum level. Ultimately, this serves to keep the internal liquid and vapour flow rates in the column balanced such that flooding and weeping do not occur. As the feed flow rate is reduced, the distillate and bottoms flow rates are reduced as well (Fig. 8b). Overall, the control system successfully maintains the desired 99 mol% purity of the distillate and bottom streams as shown in Fig. 8c.

3.2. *Performance of SwoMV process*

In order to illustrate the performance of SwoMV, the separation of a BTX mixture with 45, 10 and 45 mol% is studied. The column has the same design parameters as the conventional semicontinuous system (Table 1). The SwoMV cycle starts with the non-producing mode during which the side product valve (V1) is closed and all of the side stream flow is recycled back to the column, shown for example in Fig. 9a. During this mode, the recycle flow rate increases (Fig. 9b) and the flow rate of the fresh feed decreases since this stream is being manipulated to control the reflux drum level. On the other hand, the feed to the column (which is the combination of the fresh feed and the recycled side stream) increases at first due to increases in the recycled stream flow rate, but then eventually decreases as the fresh feed flow rate declines. The distillate

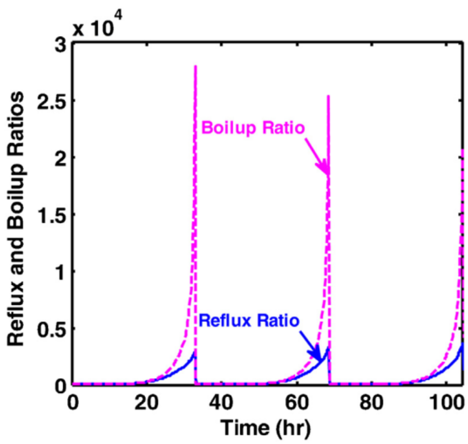

Fig. 7 – Reflux and boilup ratios during three conventional semicontinuous cycles for feed composition of 45, 10 and 45 mol% of BTX.

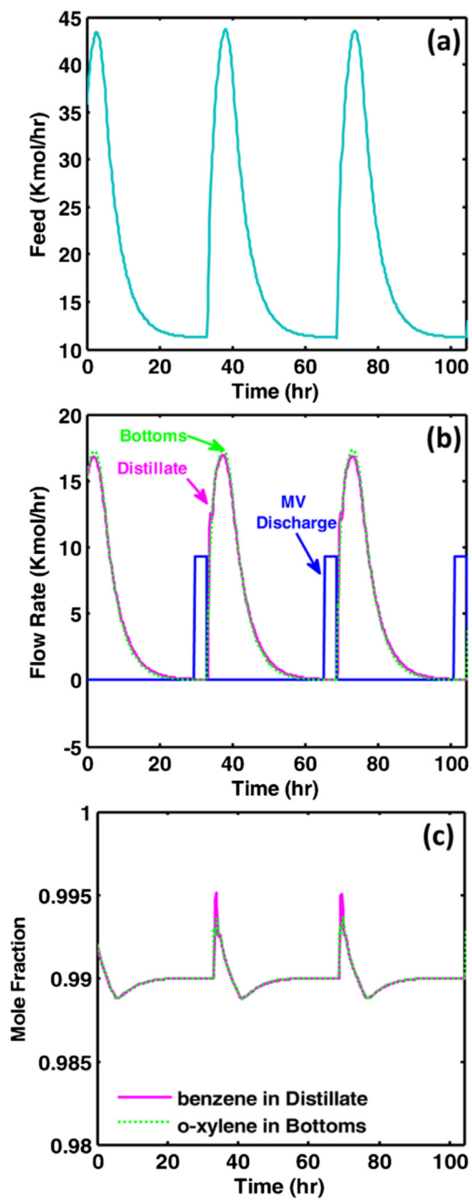

Fig. 8 – Flow rates of (a) feed, (b) product streams and (c) mole fractions during three conventional semicontinuous cycles for feed composition of 45, 10 and 45 mol% of BTX.

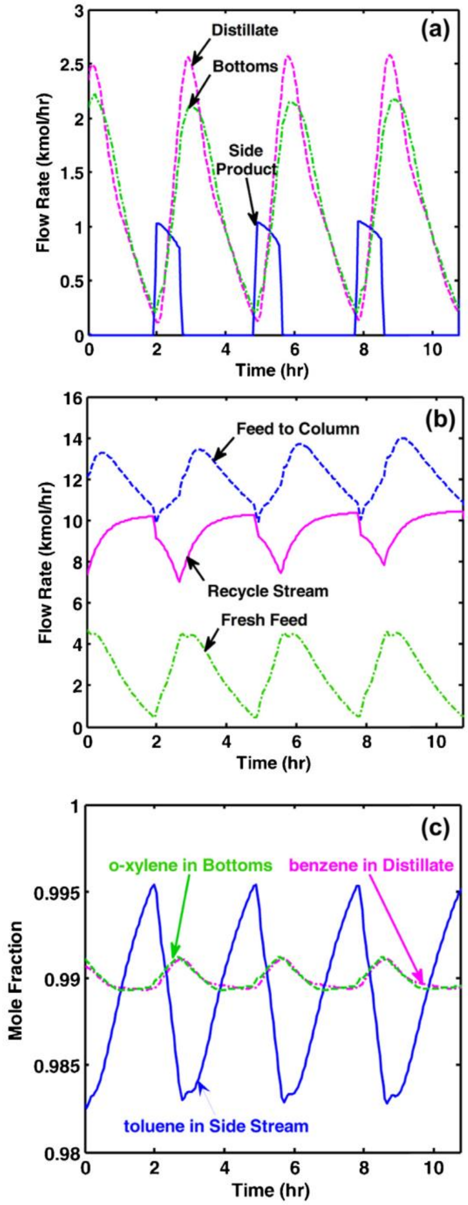

Fig. 9 – Cyclic behaviour of SwoMV for separation of BTX with feed composition of 45/10/45 mol%.

and bottom flows follow the same trend as the feed to the column (Fig. 9a) as a result of the control system acting to maintain purities as the fresh feed flow rate decreases and the amounts of light and heavy components in the system are reduced (Fig. 9c).

At about time 2 h, the concentration of the side stream reaches the upper defined value of 99.5 mol% percent as shown in Fig. 9c, valve V1 opens, and part of side stream is withdrawn as the product (Fig. 9a). During this producing mode, the flow rate of fresh feed, distillate, and bottoms increases, which results in a reduction of side stream purity. When the side-stream purity reaches the defined lower bound of 98.5 mol%, V1 closes and the system goes back to the non-producing mode and a new cycle begins.

During the SwoMV cycles, the purity of the distillate and bottom streams has a minor fluctuation around the desired

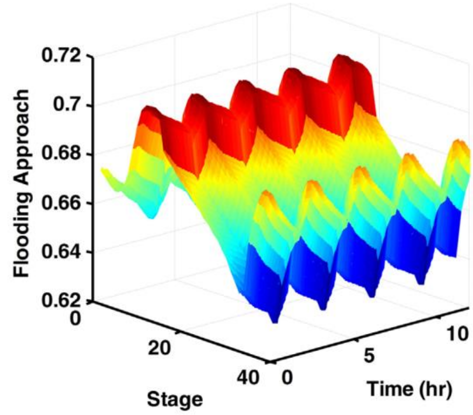

Fig. 10 – Flooding approach profile for SwoMV configuration for four cycles.

purity of 99 mol% (Fig. 9c) and the purity of the side product fluctuates between the lower and upper bounds. However, with proper controller tuning parameters, the 99 mol% time integral average purity for all three streams is achieved.

For both the conventional semicontinuous and the SwoMV system, weeping and flooding calculations are performed throughout each cycle to ensure that weeping and flooding do not occur at any point during the operation of the column. The Fair correlation is used to calculate the flooding approach (Fair et al., 1997) for this purpose. Typically, columns are designed such that the flooding approach is about 0.75–0.85 (meaning that the flow rates are about 75–85% of the flooding limit), providing enough "wiggle room" to ensure that the approach to the flooding limit never reaches 1.0 (Seider et al., 2008). For example, the flooding profile for each stage in the SwoMV example over the course of four cycles never goes above 0.8, as shown in Fig. 10, and therefore remains within safe operating limits.

To calculate the weeping velocities Eqs. (2) and (3) are used (Mersmann et al., 2011):

$$f_{\min} = \varphi\sqrt{0.37 d_H g \frac{(\rho_L - \rho_V)^{1.25}}{\rho_V{}^{0.25}}} \qquad (2)$$

$$u_{\min} = \frac{f_{\min}}{\sqrt{\rho_V}} \qquad (3)$$

where $F_{\min}$ is the minimum gas load, φ is the relative free area, d_H is the tray hole diameter, g is the acceleration due to gravity, ρ_L and ρ_V are the liquid and vapour densities, and $u_{\min}$ is the minimum vapour velocity required to prevent weeping. The vapour velocities for the top, middle and bottom stages are calculated for the SwoMV example for the duration of three cycles, and they are well above the minimum velocity, as shown in Fig. 11, and thus there is little danger of weeping.

3.3. *Effect of operational parameters on SwoMV configuration*

During the producing mode, valve V1 opens, V2 closes partially, and the side product is withdrawn. However, the rate at which the intermediate product is collected is a degree of freedom subject to optimization and has a significant effect on the performance of the SwoMV system. For the example shown in Fig. 12, if the side product collection rate is about 1.1 kmol/h,

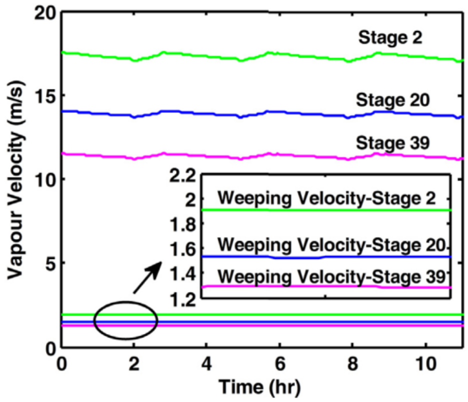

Fig. 11 – Vapour and weeping velocities for SwoMV configuration.

the collection mode takes about 42 min. Alternatively, if the collection rate is higher (for example, initially about 5.2 kmol/h), the collection time is much shorter (only about 15 min). Note that the flow rates are not constant because the flow rate for this fully-open value is purely pressure-driven and a function of the composition of the stream, which changes during the collection mode. Therefore, for a given design, the size of V1 (and therefore the approximate flow rate at which it is withdrawn) is the key parameter of interest.

A range of valve sizes (expressed as the valve coefficient C_v) is considered for V1 as shown for the 45/10/45 example in Fig. 13. Increasing C_v results in a decrease of operating cost per benzene produced and an increase in the benzene production rate up to a C_v of 424 (cm$^{1.5}$ gr$^{0.5}$/(atm$^{0.5}$ s)). This is because with larger product collection rates, there is less mixing of the purified side draw product with the fresh feed. Consequently, this value is chosen as the optimum valve coefficient for V1 for the 45/10/45 case. Valves larger than that are only marginally better in terms of operating costs and product flow rates, but would have much higher capital costs, and so are overall less optimal.

Another parameter that has been studied is the purity of the side stream. In the SwoMV configuration the purity of the intermediate component in the side product fluctuates between the defined upper and lower bounds, and the final product quality would have approximately the average value of those. Fig. 14a shows the mole fraction of toluene in the side stream for three different target product purities, and Fig. 14b illustrates how the side product flow rate changes to meet these specifications. In other words, to yield higher purities, higher recycling rates and subsequently longer non-producing modes are required with diminishing returns.

Finally, in Fig. 15 it is shown that increasing the side stream purity reduces the benzene production rate and increases operating cost per benzene produced as the separation becomes more difficult.

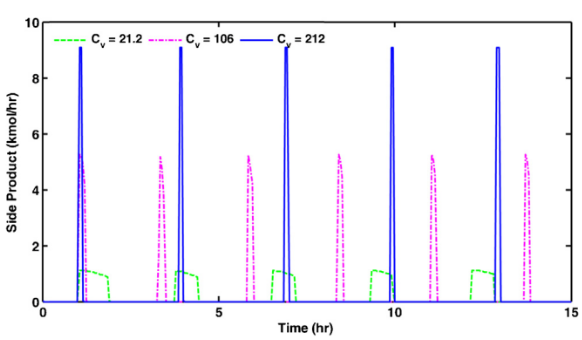

Fig. 12 – Effect of side product removal rate on the performance of SwoMV for the case of feed composition of 45/10/45 mol%.

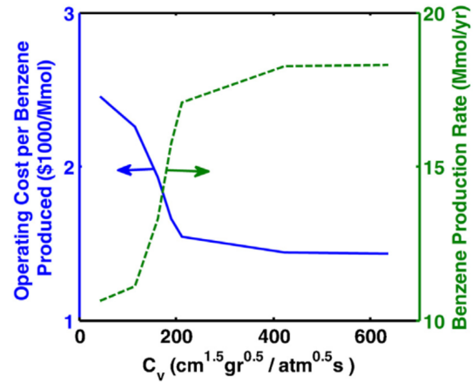

Fig. 13 – Effect of valve V1 coefficient on operating cost and benzene production rate for feed composition of 45/10/45 mol%.

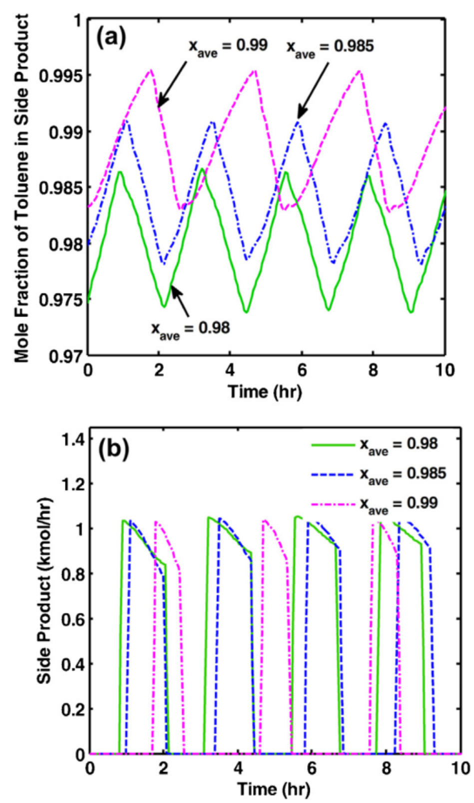

Fig. 14 – Effect of side product purity on the performance of SwoMV for feed composition of 45/10/45 mol%.

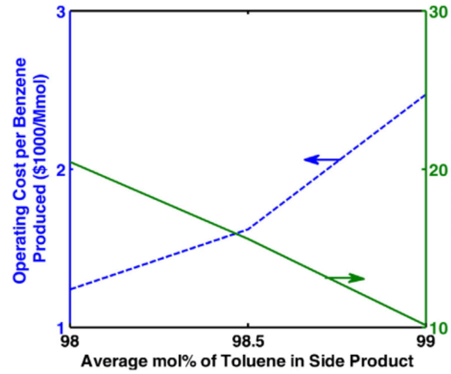

Fig. 15 – Effect of side product purity on the performance of SwoMV for feed composition of 45/10/45 mol%.

3.4. *Effect of feed composition on the profitability of the SwoMV*

To investigate the feasibility and the profitability of the novel proposed SwoMV configuration, three cases with different feed compositions have been studied. The economics of the conventional continuous, conventional semicontinuous, SwoMV and side stream configurations are compared over a production range for a wide feed composition range.

The first case is fresh feed with a composition of 45, 10 and 45 mol% of benzene, toluene and *o*-xylene, respectively. The economic analysis for this case is performed and the results are presented in Fig. 16. The total direct costs of these configurations are shown in Fig. 16a. As expected, the conventional continuous system has higher costs relative to the conventional semicontinuous and the SwoMV due to the presence of two distillation columns. The conventional semicontinuous system has a lower total direct cost with only one column and a middle vessel. However, for higher production rates, the conventional semicontinuous requires the column to have larger diameters relative to the conventional continuous system and also requires larger middle vessels. This ultimately results in higher total direct cost than the conventional continuous system for high overall production rates (above 30 Mmol/year of benzene). The SwoMV has even lower capital costs than the conventional semicontinuous system since it requires only one column and no middle vessels. However, the total direct cost increases sharply with the production rate since the diameter requirements increase even faster with production rate. The same trend is observed for the side stream column, but in this case even larger column diameters are required for the separation which results in a sharper slope of this curve.

The corresponding operating costs are presented in Fig. 16b. The conventional semicontinuous, SwoMV and side stream systems have higher operating costs than the conventional continuous system due to higher reflux and boil up ratios necessary to achieve the desired purities. However, the TAC for the SwoMV system is lower than the conventional continuous, conventional semicontinuous and side stream systems as shown in Fig. 16c for production rates below about 20 Mmol/year of benzene. Overall, for low to intermediate production rates, SwoMV is the most economical configuration, and the conventional continuous system is the most economical for high flow rates. For low flow rates in particular, the TAC savings of the SwoMV system over the conventional continuous one is significant (up to 30%).

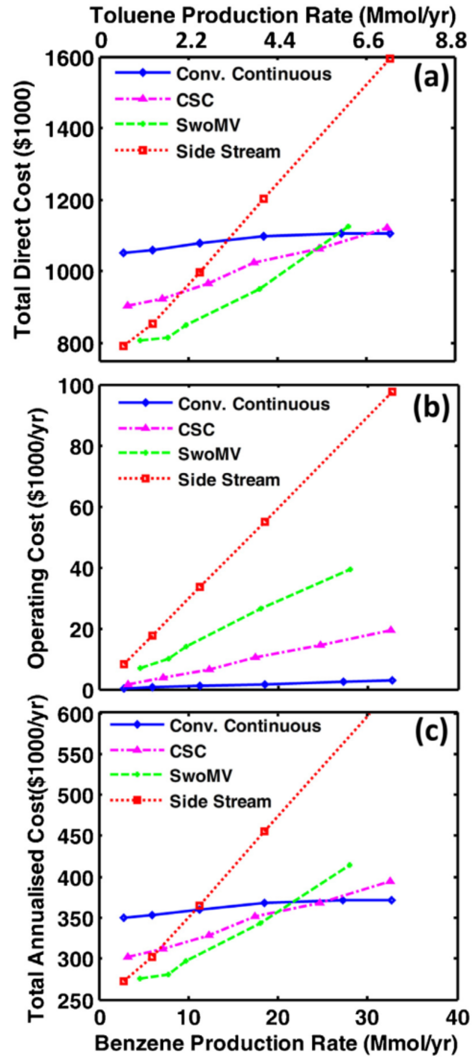

Fig. 16 – Economic evaluations for feed composition of 45/10/45 mol% of BTX. On each subplot, the bottom *x*-axis corresponds to the benzene production rate, and the top *x*-axis corresponds to the toluene production rate.

The second case study uses an equimolar feed composition with 33, 33 and 34 mol% of BTX, respectively. The economic evaluation is shown in Fig. 17. Again, the same basic trends are observed, except that the total direct cost of SwoMV is lower than the other systems over a wider range of benzene production. This is because less recycle is required to bring the MV from 33% to 99 mol% than from 10% to 99 mol%. Therefore, the distillation column in the SwoMV designs do not have to be quite as large, which results in relatively lower direct costs.

The operating cost of SwoMV in this case (Fig. 17b) is approximately the same as the conventional semicontinuous and higher than the conventional continuous system where the side stream column has remarkably higher operating costs than the other configurations. The TAC in Fig. 17c shows that SwoMV is always more profitable than the conventional semicontinuous and side stream systems for purification of this feed composition, and more profitable than the conventional continuous system for flow rates below 60 Mmol/year of benzene.

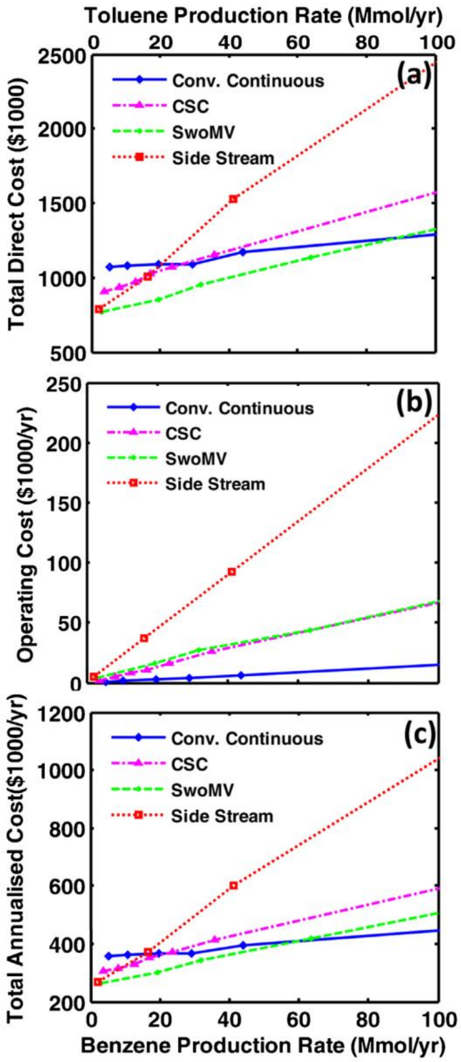

Fig. 17 – Economic evaluations for feed composition of 33/33/34 mol% of BTX.

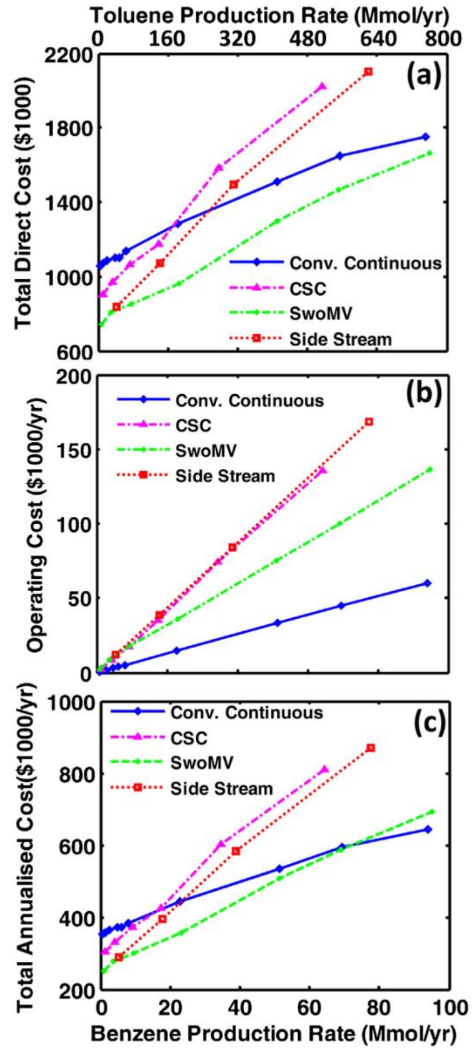

Fig. 18 – Economic evaluations for feed composition of 10/80/10 mol% of BTX.

A third case study is for an intermediate-rich feed composition of 10, 80, and 10 mol% BTX, respectively. The total direct costs of the SwoMV for this case (Fig. 18a) is even lower than the conventional semicontinuous as explained before (less recycling is required). As discussed earlier, the single side stream column configuration is only suitable for intermediate-rich feed compositions since lower vapour boilups are required to obtain the product purities. Therefore, for this case the side stream column has slightly lower direct cost than the conventional semicontinuous system but still has higher cost than the SwoMV configuration. More importantly, the operating cost of SwoMV for this case is lower than the conventional semicontinuous and side stream systems (Fig. 18b). The reason for this is that in the conventional semicontinuous system a large portion of the feed (80 mol%) needs to be recycled which adds to the operating costs of the system. Finally, for this case SwoMV is a better choice than the other systems and has a lower TAC over an even wider range of production rates (below 70 Mmol/year of benzene or equivalently 560 Mmol/year of toluene, see Fig. 18c).

To summarize, the economic comparison of the SwoMV and a single distillation column with a side stream (without any recycling) shows that the SwoMV configuration can reduce the operating and the capital costs of the separation and is therefore a superior configuration. The novel SwoMV concept looks very promising from an economic perspective for a variety of potential applications. Overall, SwoMV tends to be better for applications with lower production rates. The SwoMV system is especially attractive for systems with higher concentrations of the intermediate component in the fresh feed, since it economical at even much larger scales. Interestingly, the conventional semicontinuous system is the opposite and is more attractive for systems with low concentrations of the intermediate component in the fresh feed. However, for our particular example, the conventional semicontinuous was rarely ever more economical than SwoMV.

One additional potential advantage to the SwoMV system over the conventional semicontinuous system is that it better integrates with systems where the feed is produced upstream in a continuous manner. In conventional semicontinuous systems, a second intermediate storage tank (not considered in this analysis) would be needed to link to an upstream process if that upstream process is continuous. For the SwoMV case, the flow rate variation of the feed is much smaller and so any upstream buffer tank required would also be much smaller. However, the difference may not be significant in many cases, as operation and safety requirements might require buffer tanks regardless.

4. Conclusion

Conventional semicontinuous separation is a relatively new configuration for performing ternary separation in one distillation column (where in conventional continuous systems two columns are typically required). Previous studies have shown the applicability of semicontinuous processes for separation of several chemical mixtures. This study extends the applicability and improves the performance of such systems by proposing a novel configuration called semicontinuous without middle vessel (SwoMV).

Unlike the conventional semicontinuous system, the SwoMV configuration does not use a middle vessel, nor does it require charging and discharging modes of operation, thus saving on capital and instalment costs. Therefore, SwoMV not only reduces the total direct costs of the system but also facilitates the retrofit of available distillation columns for ternary purification. Furthermore, the new configuration improves the conventional semicontinuous system by reducing the operating costs for a range of feed compositions and extending the economically optimal range of production.

The separation of BTX is selected as a case study to investigate capabilities of the SwoMV configuration. However, it should be noted that the SwoMV concept should work for any non-azeotropic ternary mixture with sufficiently different relative volatilities. In this study, the column and the proper controller system are designed for the BTX separation application. The economics of SwoMV is compared to conventional continuous, conventional semicontinuous and single side stream column systems for three cases of feed compositions applied to a wide range of process scales. The results show that the total annualized cost of SwoMV is generally lower than the other configurations for the range of production rates studied. For example, for the purification of feeds with a higher proportion of intermediate components, SwoMV has lower TACs than the conventional semicontinuous system for a wider range of production rates, and also has lower operating costs. For instance, for production of 515 Mmol/year of toluene, SwoMV has 42% less total direct cost, 45% less operating cost and 43% less total annualized cost relative to the conventional semicontinuous configuration and also has expanded the economical production range of conventional semicontinuous system by 44.5%. This result helps to extend the range of applicability for semicontinuous approaches. Furthermore, SwoMV also outperforms the single side stream column for all feed compositions and has a lower operating and direct costs.

Finally, the novel SwoMV configuration is a suitable ternary separation technique for processes such as pharmaceutical products, biofuels and specialty chemicals, where typically the production rate is low. Future studies should focus on application of SwoMV configuration to other processes to demonstrate its performance relative to conventional continuous and semicontinuous systems as well as determine the optimum column parameters via dynamic optimization to further improve the economics of this process. In addition, since the system is control driven, improvements in the control system would have a considerable effect on the performance of the system. To the best of our knowledge, only PI control has been used in all proposed semicontinuous system processes. Therefore, the use of model predictive controllers in semicontinuous processes is an area of future research.

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Chapter 3

Integrated design and control of semicontinuous distillation systems utilizing mixed integer dynamic optimization

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Integrated design and control of semicontinuous distillation systems utilizing mixed integer dynamic optimization

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ABSTRACT

Semicontinuous distillation systems are notoriously difficult to design and optimize because the structural parameters, operational parameters, and control system must all be determined simultaneously. In the past 15 years of research into semicontinuous systems, studies of the optimal design of these systems have all been limited in scope to small subsets of the parameters, which yields suboptimal and often unsatisfactory results. In this work, for the first time, the problem of integrated design and control of semicontinuous distillation processes is studied by using a mixed integer dynamic optimization (MIDO) problem formulation to optimize both the structural and control tuning parameters of the system. The public model library (PML) of gPROMS is used to simulate the process and the built-in optimization package of gPROMS is used to solve the MIDO via the deterministic outer approximation method. The optimization results are then compared to the heuristic particle swarm optimization (PSO) method.

1. Introduction

Process intensification techniques promise to reduce the number of unit operations, the size of the equipment required and also to boost the efficiency of the plant. One example of a process intensification technique is the semicontinuous distillation system, introduced to reduce the total annualized cost (TAC) of distillation systems for purification of ternary mixtures (Phimister and Seider, 2000a). However, recent research in the area has generalized the application of the semicontinuous system to the purification of n components (Wijesekera and Adams, 2015). Therefore, where conventionally n-1 2-product distillation columns are required for purification of n components, in the semicontinuous system only one column is used along with n-2 simple storage tanks which are called middle vessels. The purification of all components is then achieved in a cyclic, dynamic manner. This substitution significantly cuts the capital costs and consequently the TAC of the system at intermediate throughputs.

Traditionally, three component mixtures are purified to the desired purities in a continuous, steady state approach using two distillation columns (Fig. 1a). However, the same separation can be achieved in one distillation column using the semicontinuous system, in a dynamic manner (Fig. 1b). In this configuration, the middle vessel is initially charged with the fresh feed and the liquid is continuously fed to the column. A side stream from the distillation column is recycled back to the middle vessel. As the light and heavy key components are removed from the system in the distillate and bottom streams, respectively, the intermediate component is concentrated in the middle vessel. When the desired concentration of the intermediate component is achieved in the middle vessel, this tank is discharged, collecting the third product and subsequently, the middle vessel is charged with the next batch of fresh feed and a new cycle begins.

Several studies over the last 15 years have proved the economical superiority of semicontinuous system over the conventional continuous system for low to intermediate production rates (Adams and Pascall, 2012). This makes the semicontinuous separation technique desirable for biofuel and pharmaceutical production plants which usually have decentralized, low production facilities (Bowling et al., 2011). Also, one advantageous of the semicontinuous system is its flexibility in purifying mixtures with variation in initial feed composition which can be the case for bio-based chemicals (Niesbach et al., 2013).

The semicontinuous system is dynamic and during the cycle, the flow rate and composition of the feed to the column change significantly. Therefore, the determination of the best feed stream and side draw locations as well as the number of stages are critical for an economical design. These parameters affect both the total direct cost (which is the cost of equipment, piping, civil, instrumentation, electrical, paint and others) and the operational cost of the

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Nomenclature

CT^T	Conditional trays on top
CT^M	Conditional trays in the middle
CT^B	Conditional trays on bottom
ET^T	Eliminated trays on top
ET^M	Eliminated trays in the middle
ET^B	Eliminated trays on bottom
D	Middle vessel diameter
H	Middle vessel height
k	Gain
y_1	Binary variable
y_2	Binary variable
w_1	PSO parameter
w_2	PSO parameter
τ	Reset time

system. Furthermore, the dimensions of the middle vessel are another design parameter considered, because total holdup affects cycle time, and liquid height affects flow rates due to hydrostatic pressure head. For example, Adams and Seider (2009a) studied the total cost per production rate as a function of the middle vessel volume. They showed that as the middle vessel hold-up increases, the cycle time of the semicontinuous system increases because longer time is required to purify the mixture utilizing a fixed column diameter. On the other hand, fewer charging and discharging are required that reduces the operating cost of the system. However, the total direct cost increases for bigger middle vessels. Therefore, the middle vessel size is a design decision variable. Standard vertical storage tanks are sold at discrete heights and diameters, therefore these parameters were considered as integer variables in the optimization.

Moreover, the system is control driven and the selection of a proper control structure and its tuning parameters are critical to the performance and efficiency of the system. These parameters have direct influence on the operating cost of the system. Pascall and Adams (2013) investigated eight different proportional integral (PI) control structures for a semicontinuous system. They identified the best control configuration that can effectively maintain the purities of the distillate and bottom streams while successfully rejecting disturbances in the fresh feed composition. Even if the control configuration is chosen a priori, its tuning parameters are a critical design decision because they significantly impact the performance, efficiency, stability, and cost of the system.

Due to the dynamic nature of the system, designing the semicontinuous system for an arbitrary mixture based on the available design heuristics (Adams and Seider, 2009b) is a tedious and time consuming procedure which usually results in suboptimal configurations. Also, the integrated design and control of these systems have not been studied thoroughly in previous works because of the complexities of the system. Previous optimization attempts were limited to a subset of continuous decision variables and had expensive computational times (Adams and Seider, 2008a). For example, Pascall and Adams (2013) reported 40CPU days were required for optimization of only the tuning parameters of the semicontinuous system by linking Aspen Dynamics and VBA and implementing the particle swarm optimization (PSO) method.

Due to these complexities, a sequential design paradigm was the major approach for designing the semicontinuous system in previous studies. In this aforementioned method, the design parameters of the system are fixed initially and then the control structure is designed. Next, the control parameters are tuned to achieve a desirable system performance (i.e., minimizing the integral square error (ISE) of distillate and bottom purities from their set points). However, it has been shown for continuous systems that this sequential approach usually results in suboptimal designs (Georgiadis et al., 2002) and sometimes results in conflicts between economical design parameters and dynamic controllability of the process (Luyben, 2004). A similar result was found for semicontinuous systems as well (Adams and Seider, 2008a).

In other process synthesis problems, integrated design and control methods are commonly used to resolve these issues. Yuan et al. (2012) reviewed the available methodologies for simultaneous design and control problems. They have classified the optimization based simultaneous design and control methods to the: controllability index approach, mixed-integer dynamic optimization (MIDO) approach, robust theory based approach, embedded control optimization approach, and intelligence based approach. In the following section, these methods are briefly introduced.

The controllability index approach defines the objective function as the minimum process steady state economics, and then controllability indicators such as relative gain array, condition number, disturbance condition number or the integral error criterion are defined to quantify the dynamic performance of the system. However, in this method, the lack of a distinct correlation between the controllability index and the economic cost and the linearity assumptions might result in suboptimal solutions (Ricardez-Sandoval et al., 2009a).

The next method is the MIDO approach in which the continuous variables determine the design parameters and the operating conditions of the system where the discrete variables correspond to decision making in the flowsheet such as determination of number of units and stages, control structure, or the existence/nonexistence of streams or process units. Two general approaches are available

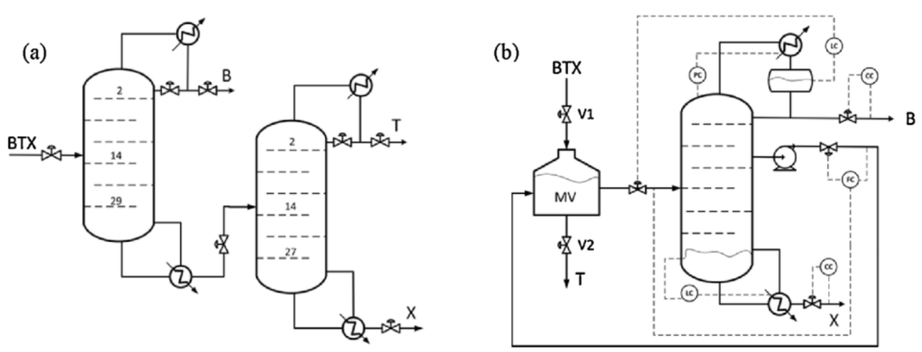

Fig. 1. Schematic of the (a) conventional continuous and (b) semicontinuous configuration for benzene, toluene and *o*-xylene (BTX) separation[1].

[1] Reprinted from Chemical Engineering Research and Design, 93, Meidanshahi, V., Adams II, T.A., A new process for ternary separations: semicontinuous distillation without a middle vessel, 100–112, 2015, with permission from Elsevier.

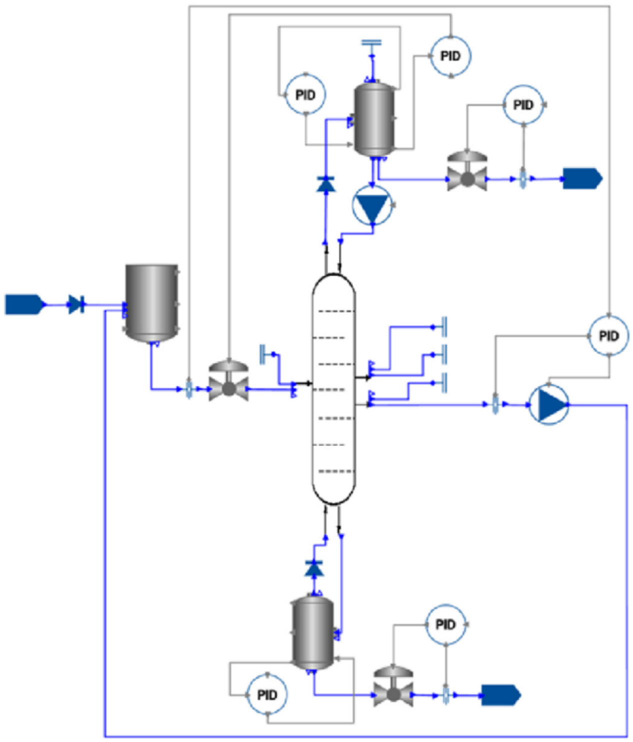

Fig. 2. Semicontinuous system simulated in gPROMS using its PML.

to solve MIDO problems: simultaneous and sequential methods. In the simultaneous method both the controlled and state variables are discretized and the problem is converted to solving a big MINLP problem (Flores-Tlacuahuac and Biegler, 2007). In the sequential approach the problem is solved successively using outer approximation, generalized Bender's decomposition or branch and bound methods (Bansal et al., 2002).

In the robust theory based approach a constrained nonlinear optimization problem is formulated and the worst scenarios are identified via robust stability and performance measures such as Lyapunov theory and structured singular value analysis (Ricardez-Sandoval et al., 2009b). In order to reduce the size of the problem, in the embedded control optimization based method, the design and control variables are separated and the problem is solved in two sub-problems (Malcolm et al., 2007). Finally, the intelligence based approach uses the heuristic methods such as particle swarm optimization, genetic algorithm and Tabu search to solve the optimization problem (Exler et al., 2008). More recently, the incorporation of advanced model based controllers such as model predictive control (MPC) integrated with design has also been studied (Sakizlis et al., 2004; Bahakim and Ricardez-Sandoval, 2014).

In this work, a framework is presented to take advantage of the capabilities of the equation oriented software, gPROMS V4, to be able to obtain an optimum semicontinuous design for any arbitrary ternary mixture in a reasonable amount of computation time. The presented methodology implements MIDO to simultaneously integrate the design and control aspects of the semicontinuous system. The public model library (PML) of gPROMS was used to model the system and its imbedded deterministic outer approximation optimization solver was used to solve the resulting MIDO. Subsequently, gPROMS was linked to Matlab using the gO:MATLAB feature of gPROMS and the MIDO was also solved using the heuristic PSO optimization method for the purposes of comparison. The results are then compared to the previous “best known” version of the system which was sequentially designed using the previously best known methods. As a case study, the separation of a near ideal mixture of benzene, toluene and *o*-xylene (BTX) was considered.

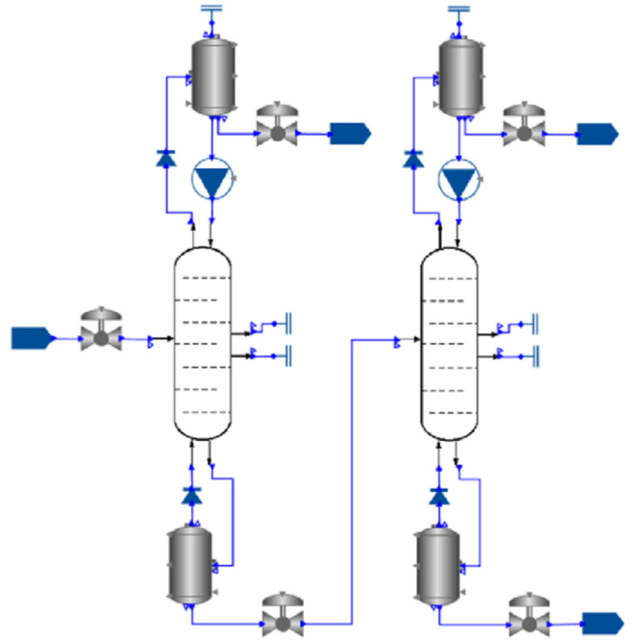

Fig. 3. Schematic of continuous system model in gPROMS.

2. Process modeling

2.1. Semicontinuous process

In previous semicontinuous distillation studies, a sequential design approach was employed. In this approach, first the number of column stages is selected. An initial guess for the number of stages can be obtained from the conventional continuous configuration for the separation of the mixture. The selected number of stages for the semicontinuous system usually lies in-between the number of stages in one of the columns of continuous distillation and the total number of stages in both columns. Next, the locations of the feed and side streams are selected such that the energy consumption of the system is minimized. A good starting point to determine these locations is to select the feed and side draws that result in the minimum operating cost of the column in a hypothetical the steady state mode. Subsequently, other design parameters of the system such as the middle vessel and reflux drum sizes are determined based on available design heuristics for the system (Pascall and Adams, 2013). Afterwards, the control structure for the system is designed and the control parameters are tuned to get the desired performance of the system, i.e., the integral square error of the purities of the distillate and bottom streams are minimized while ensuring the required purity of the intermediate component in the middle vessel at the end of the cycle.

The details of such sequential method used to design a semicontinuous system for the purification of benzene, toluene, *o*-xylene (BTX), can be found in Meidanshahi and Adams (2015). They used Aspen Plus Dynamics to simulate several combinations of number of stages, and feed and side draw locations for the semicontinuous column in order to find a near optimal structure with the lowest total annualized cost. This approach is quite time consuming (months) and cannot guarantee local optimality of the solution.

In this work, the design decision variables are the number of stages of the semicontinuous column, the best locations of the feed

Table 1
Design parameters for a 2 ft. diameter distillation column for BTX semicontinuous system.

Number of trays	Feed tray	Side tray	Condenser pressure (bar)	Middle vessel height (m)
38	23	13	0.37	6

Table 2
Controllers parameters for a 2 ft. diameter distillation column for BTX semicontinuous system.

Distillate purity controller		Bottom purity controller		Reflux drum level controller		Sump level controller		Side draw controller		Column pressure controller	
k	τ	k	τ	k	τ	k	τ	k	τ	k	τ
1	1000	1	700	1	1000	0.5	1000	0.1	1000	0.1	1000

k is the gain and τ (sec.) is the reset time.

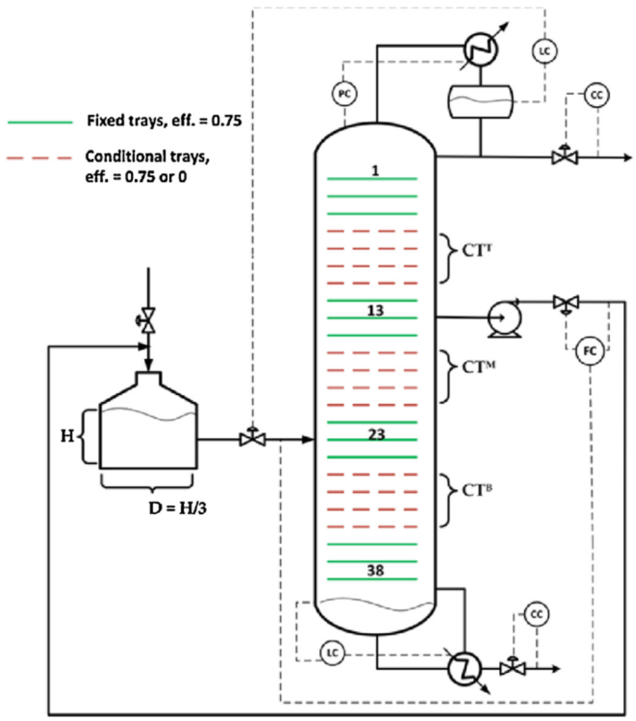

Fig. 4. Continuous decision variables for the semicontinuous system are tuning parameters of controllers and cycle time. Integer variables are ET^T, ET^M and ET^B (number of eliminated trays on top, middle and bottom sections, respectively) and H (middle vessel height).

and the side streams, and the middle vessel size. Although the column diameter is also a design parameter, in this study, the column diameter was fixed at three different values of 2, 4 and 8 ft. while all other design parameters are optimized for each case. The column diameter was fixed because it is the most influential parameter that influences the throughput of the process. To simplify the problem, the control structure was chosen in this work to according to the recommendation of Pascall and Adams (2013) which was shown to have excellent performance in terms of maintaining desired purity setpoints and rejecting disturbances. In this control structure, the purities of the distillate and bottom streams are controlled by manipulating their respective flow rates. The reflux drum and sump levels are controlled by the feed flow rate to the column and the reboiler heat duty, respectively. The column pressure is controlled by the condenser heat duty and finally the ideal side draw control is used to determine the flow rate of the side stream (Fig. 1b). The ideal side draw control strategy was implemented, which is based on mass balance and manipulates the side stream flow rate such that flow rate of the side draw leaving the column be equal to the flow rate of the intermediate species in the feed (Adams and Seider, 2008b). The tuning parameters of PI controllers are considered as decision variables in the optimization problem as well. Consequently, the resulting problem is a mixed integer dynamic optimization. The charging and discharging rates of the middle vessel are design variables. Commonly, these rates are chosen such that the charging and discharging modes of the semicontinuous system constitute only about 3–15% of the total cycle time (Phimister and Seider, 2000a, 2000b), and thus only influence a small percentage of the total operating cost. Furthermore, including them in a formal optimization problem is not trivial since charging and discharging modes operate with different dynamics and cause discrete events which cause difficulty for many dynamic optimization solvers. As such, they are not included in this work and only the processing mode of the semicontinuous system is considered in the optimization problem. The problem of including discharging and charging modes in the optimization is left to future work.

Although Aspen Plus Dynamics provides rigorous distillation column models and the system can be rapidly prototyped and simulated in this environment, it is not suitable for MIDO of semi-continuous system for the following reasons. First, the structural parameters of the system such as middle vessel dimensions cannot be changed and optimized in Aspen Plus Dynamics due to technical difficulties associated with the initialization procedure, which requires external software (Aspen Plus) to be used in the workflow. Secondly, the built-in optimization toolbox in Aspen Plus Dynamics uses successive quadratic programming which is not suitable for MIDO problems. Finally, the application of heuristic optimization methods using an Aspen Plus Dynamics simulation as a black-box objective function has been shown to be moderately effective, but with a significant computational time (on the order of a cpu-month) (Pascall and Adams, 2013).

Therefore, the gPROMS software was chosen to simulate the system due to its capabilities both in modeling the superstructure of the system and its MIDO algorithms. The semicontinuous system was simulated in gPROMS V4 using its PML as shown in Fig. 2. PML provides first principle models for the basic unit operations. One advantage of PML is its ability to be used with other equation-oriented user-defined models. The gPROMS V4 academic version does not have a model for a distillation column but it can be modeled by using a "*column-section*" model (which is the material, energy, and fugacity balance equations for a tray section) and two flash drums acting as the condenser and the reboiler. In this work, the column-section model of gPROMS was modified to accommodate the optimization requirements. The modifications will be discussed later in Section 3.1.

The following parameters and variables were specified in order to reduce the degrees of freedom of the model to zero:

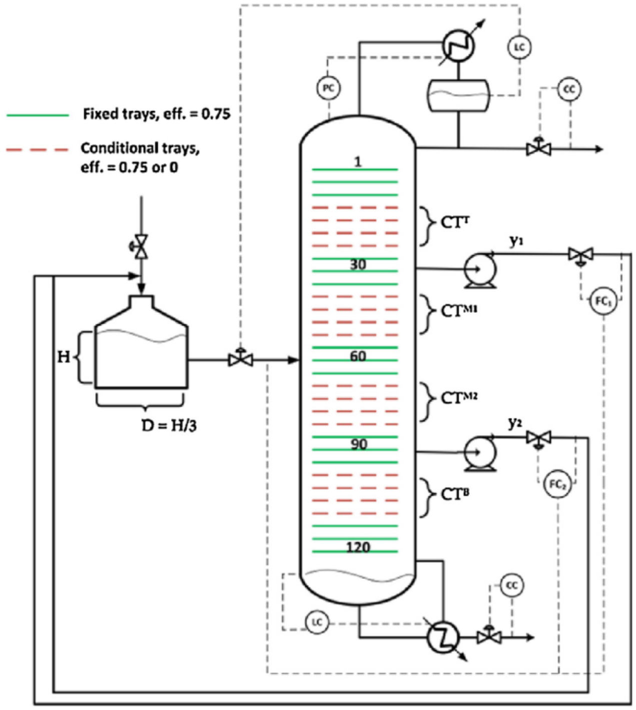

Fig. 5. Schematic of the super structure for the MIDO.

- The number of column trays.
- The feed and the side stream locations.
- The condenser pressure. In this work, the pressure was selected such that cooling water could be used in the condenser.
- The stage pressure drop and corresponding reboiler pressure. In this work, 689 Pa/stage was used (Luyben, 2006).
- In PML, the number of special trays (trays with external addition or withdrawal of mass) must be defined which is 2 in the case of semicontinuous system (a feed and a side tray).
- The configurations of PI controllers and the set point for the purities of the distillate and bottom streams.
- The column diameter, which determines the production range of the system.
- The Murphree tray efficiencies, which were set at 75% for each tray.
- The middle vessel height and diameter (an aspect ratio of 3 was used).

In the first part of this study, the design and control parameters for the BTX system were adopted from Meidanshahi and Adams (2015) and are presented in Table 1 and Table 2, respectively. This configuration was chosen as the base case because it was the best (lowest cost) known configuration in the open literature. The base case was then used as the initial guess for optimization to see how the method presented in this work can improve the system economics and control. However, for semicontinuous systems in general, it can be difficult to find a set of design parameters that result in a feasible operating cycle, let alone an efficient and economic one. Therefore, the proposed design and optimization method is generalized in the second part of the study. The general method allows one to obtain an optimal configuration for a ternary mixture with little to no prior knowledge of feasible design parameters of the system.

Table 3
PSO parameters.

Number of particles	Initial particle distribution	W_1	W_2	Maximum iteration	Number of runs
30	Latin Hypercube	2.8	1.3	100	5

2.2. Continuous process

To compare the economics of the optimized semicontinuous system, the continuous system for purification of BTX was simulated and optimized in gPROMS as well. The continuous system consists of two distillation columns. The direct sequence separation is considered which means that benzene is recovered in the distillate stream of the first column and the toluene and *o*-xylene are separated in the distillate and bottoms of the second column, respectively. Ling and Luyben (2009) reported the optimum configuration for this system which is used as the base case in this work for optimization using OA and PSO methods. In their design, the first column has 28 trays with the feed entering at tray number 13. The condenser pressure is at 0.37 bar so that cooling water can be used in the condenser. The second column has 26 trays. The feed tray is 13 and the condenser pressure is 0.13 bar. Purification of an equimolar mixture of BTX to products with the purity of 98 mass% is considered in this work. The schematic of the continuous system model in gPROMS is shown in Fig. 3.

3. Optimization

To determine the optimum structural parameters of the distillation column, the method proposed by Javaloyes-Antoín et al. (2013) was used. In this method, the column is considered as sets of fixed and conditional trays that may or may not exist. Their existence is determined by their tray Murphree efficiencies. A Murphree efficiency of 0.75 means that the tray exists and a Murphree efficiency of zero means the tray is inactive and can be eliminated. On inactive trays, the net effect in the simulation is that vapor and liquid just pass by each other with no mass transfer. In this way the total numbers of stages as well as the relative positions of the feed and side trays are determined. The value of 0.75 was chosen based on rate based simulations used in the prior work (Meidanshahi and Adams, 2015). One disadvantage to this method is that, for dynamic simulations, the tray holdups are still present in the column and affect the residence time and the balances. However, in this work, each candidate solution presented by the optimizer was re-simulated using the proper number of trays (without any inactive trays), and it was found that there was only very minor differences in column performance, trajectories, and cost. Therefore, this approach was found to be quite suitable for optimization purposes.

The base case structure is shown in Fig. 4. The column has four sets of fixed trays at the top, bottom and at the locations of the feed and side streams. This results in three sets of conditional trays at the top (CT^T), middle (CT^M) and bottom (CT^B) of the column. Three integer variables of ET^T, ET^M and ET^B were defined to indicate the number of eliminated trays from the top, middle and bottom sections, respectively (e.g., $0 \leq ET^T \leq CT^T$). Defining the inactive trays in this manner avoids the non-unique solutions. It means that eliminating the first and the third tray in a CT gives the same solution as eliminating the second and the fourth tray in that set (Javaloyes-Antoín et al., 2013). The elimination of trays in each section determines the relative location of feed and side trays and the total number of trays required.

The objective function was to minimize the total annualized cost (TAC) per annual processing rate of the feed (Eq. (1)). A payback period of 3 years was considered in this work which is reasonable

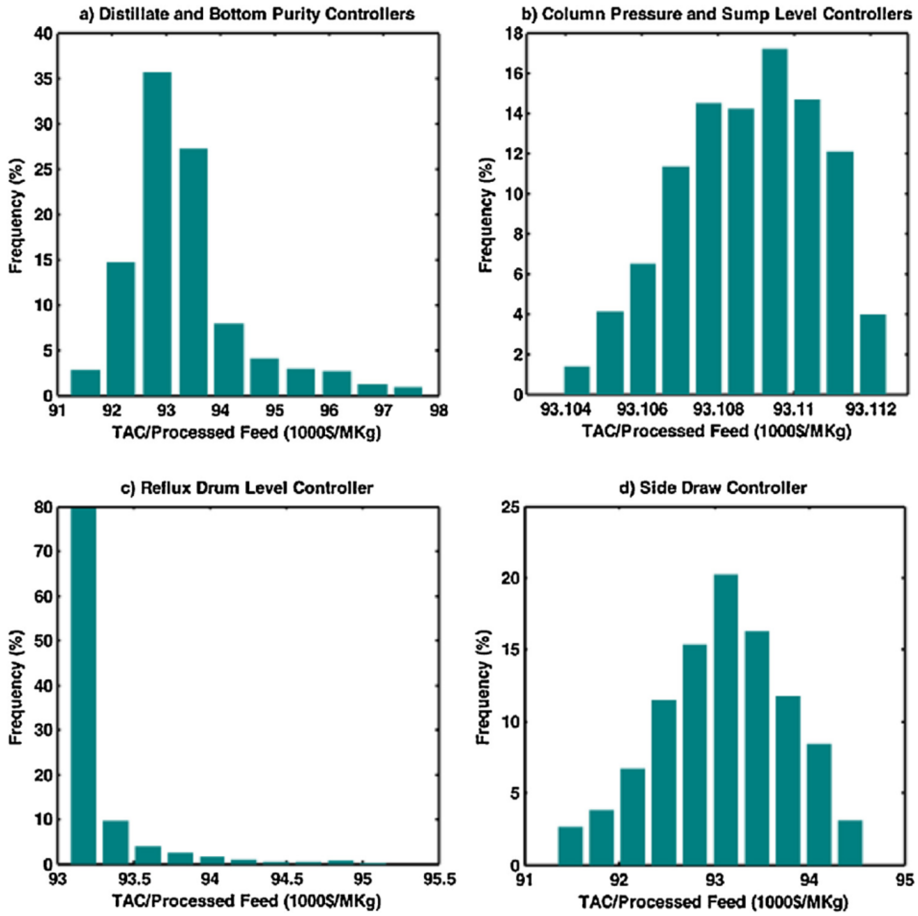

Fig. 6. Sensitivity analysis of the controllers tuning parameters.

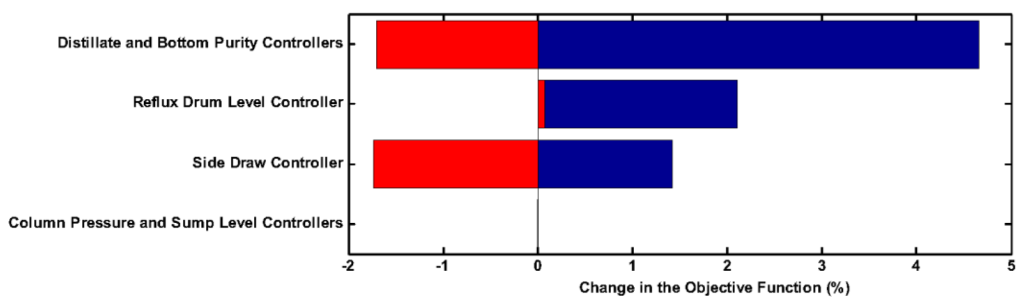

Fig. 7. Tornado plot showing the percentage of objective function change from the perturbation of different controller tuning parameters.

for small scale production plants and has been used in other studies (Luyben, 2010). The operating costs were calculated considering only the utility costs of steam and cooling water according to the method discussed in Towler and Sinnott (2012). Pump costs were neglected because they were trivially small. The cost of the system was calculated using the equations reported in Seider et al. (2009). The optimization problem was subjected to the constraints shown in Eqs. (2)–(6). The time average purity of the distillate and bottom streams by the end of the cycle should be equal or higher than the required purities for these two streams. To achieve on-aim purities for these two streams, better control systems, such as model predictive control, are required which is the subject of our future work. In this study, time average purities were considered with the idea that the products will be pooled later. Furthermore, the desired purity of the intermediate component in the middle vessel should be achieved by the end of the cycle and is another constraint. Also, the liquid levels in the condenser and column sump should be maintained in a desirable range.

$$\text{Min}: \left(\frac{\text{Total direct cost}}{\text{Paybackperiod}} + \text{Annual Operating Cost}\right) / \text{Annual processing rate of feed} \tag{1}$$

$$\text{Average purity of benzene in the distillate stream} \geq 98\ \text{mass\%} \tag{2}$$

$$\text{Average purity of } o\text{-xylene in the bottom stream} \geq 98\ \text{mass\%} \tag{3}$$

Table 4
Optimization results for conventional continuous system.

Production rate (Mkg/year)		3.93		19.95		99.79		Ling & Luyben design, (2009)
		OA	PSO	OA	PSO	OA	PSO	
Column 1	ET^T	0	5	0	4	0	3	–
	ET^B	0	7	0	7	0	4	–
	Reflux ratio	1.64	3.01	1.88	3.1	1.99	2.42	1.87
	Reboil ratio	1.01	1.36	1.88	1.42	1.12	1.17	0.96
	Opt. feed location	13	8	13	9	13	10	13
	Opt. no. of trays	28	16	28	17	28	21	28
Column 2	ET^T	0	6	0	4	0	5	–
	ET^B	0	6	0	7	0	3	–
	Reflux ratio	1.78	3.01	1.98	3.01	2.01	2.89	1.53
	Reboil ratio	1.75	2.59	1.88	2.99	2.2	2.25	1.54
	Opt. feed location	13	7	13	9	13	8	13
	Opt. no. of trays	26	14	26	15	26	18	26
Objective function (k$/Mkg)		135.9	117.9	31.6	27.1	7.2	6.3	–
CPU time (min)		26	112.5	1.16	99.9	15	160.1	–

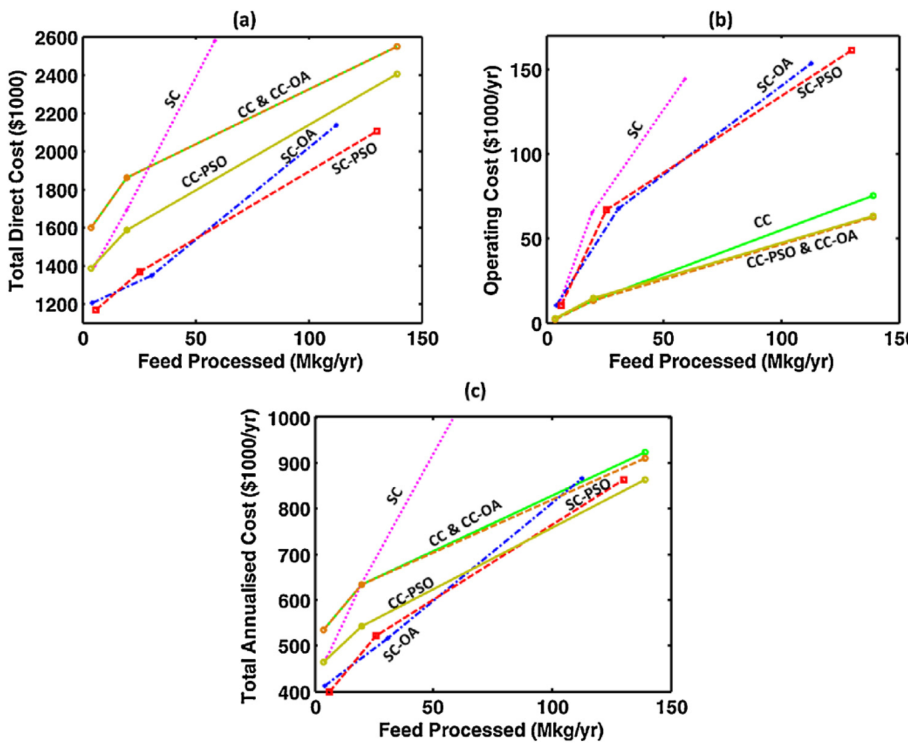

Fig. 8. Economic analysis for the semicontinuous (SC), conventional continuous (CC) and their optimum designs using OA and PSO methods.

$$\text{Purity of toluene in the middle vessel by the end of cycle} \geq 98\ \text{mass\%} \tag{4}$$

$$0.1 \leq \text{condenser liquid level fraction} \leq 0.9 \tag{5}$$

$$0.3 \leq \text{sump liquid level fraction} \leq 0.8 \tag{6}$$

To solve the resulting MIDO, the deterministic outer approximation (OA) method and the heuristic particle swarm optimization (PSO) method were employed and the results are compared in the next section.

In this work composition controllers were used to maintain distillate and bottom streams' purities. The implementation of temperature inferential controllers instead of composition analyzers have been studied in previous work (Pascall and Adams, 2013) and was shown to be feasible, practical, and to perform similarly to composition analyzers. In other words, at the early design phase, composition analyzers can be used since they are much easier to implement and then later substituted with temperature inferential controllers. Also, a near-ideal mixture is chosen in this work to present the methodology, however, in previous studies, it is shown that the semicontinuous systems can be implemented successfully for non-ideal and azeotropic mixtures (Adams and Pascall, 2012). Therefore, the optimization based approach presented here can be applied to design those systems as well.

3.1. Outer approximation with a known base case

The MIDO problem was solved using the gPROMS optimization toolbox. To solve the MIDO, gPROMS uses a sequential method with control vector parameterization and single shooting. In this method, the control variables are discretized and the problem is converted to a mixed integer nonlinear problem (MINLP). The state variables are determined by integrating an initial value problem. To solve the resulting MINLP, gPROMS employs the outer approximation with equality relaxation and augmented penalty method (OA/ER/AP). In this method first binary variables are relaxed and an initial NLP problem is solved. Then a master problem is formulated by linearizing the objective function and the constraints around the obtained solution to set up an MILP. The integer variables are obtained from the solution of the MILP. Then, in the next step, the integer variables are relaxed and a NLP problem is solved to obtain a solution which satisfies the Karush–Kuhn–Tucker (KKT) conditions. The last two steps are repeated until the stopping criterion is met. For details of OA/ER/AP method, refer to Viswanathan and Grossmann (1990). The OA/ER/AP is guaranteed to obtain the globally optimal solution if the optimization problem is convex. This is usually not the case in many engineering problems. However, the augmented penalty (AP) strategy employed in the algorithm increases the probability of obtaining a global solution. Nevertheless, local optimality is guaranteed within an optimality gap (which in this work was a relative error of 0.001).

In order to solve the optimization problem in gPROMS, the decision variables should be defined as "variables" in the model and they should be "assigned" initial values in the process entity. This means that model parameters cannot be selected as decision variable in the optimization toolbox. Therefore, the column-section model of PML was modified for optimization purposes. The three variables ET^T, ET^M and ET^B were added to the model and the Murphree efficiency variable was modified so that it can be varied for each tray. A series of "*if*" statements were added to the model to change the value of Murphree efficiencies based on the values of ET^T, ET^M and ET^B.

Another feature of the optimization toolbox is that any schedule specification in the process is ignored during the optimization and no tasks are executed. Therefore, the cycle time of the semicontinuous system should be set so that the equations are integrated for that fixed time horizon. But since the cycle time is a function of structural and control parameters of the system, and its value is unknown beforehand, it can be considered as a decision variable in the optimization. However, bounds on the cycle time should be defined to prevent excessively long cycles or failed cycles that will never complete. To find an initial guess for the lower bound on the cycle time, all conditional trays were set inactive and the cycle time was computed. The lower bound was then set to a smaller value than that. For the upper bound, based on experience with the system, a large value was selected. The bounds were loosened if the optimization results landed on the bounds. Furthermore, an initial feasible starting point is required for the optimization and the model should be robust for the range of the decision variables.

3.2. PSO with a known base case

Particle swarm optimization is a heuristic, population based optimization algorithm which is proposed by Kennedy and Eberhart (1995). This optimization method does not require any gradient information and can easily be implemented. Although the method cannot guarantee the optimality of the results, it usually can improve the objective function of the problem and give a better design for the system. Hence, this technique has become popular between researchers especially when only a black box model of the system is available.

In this method, a number of particles are placed in the search space of decision variables either randomly or based on Latin Hypercube (the latter is used in this study). Each particle evaluates the objective function and the constraints. Then, based on the best solution found by each particle and other particles, the particle movements are calculated for the next iteration using a weighted combination of the particle's personal best known location and the best known location found by the group as a whole, plus some stochastic influences. At first, the search space is explored broadly but coarsely, and toward the end the particles hone in on a small region of the search space and explore it in more detail. The algorithm terminates when all of the particles have converged to within some small neighborhood, or when a maximum number of iterations or solution time has been reached. The details of the algorithm can be found in Poli et al. (2007). Adams and Seider (2008b) suggested some heuristics on the selection of PSO parameters for semicontinuous systems. The values used in this study are listed in Table 3.

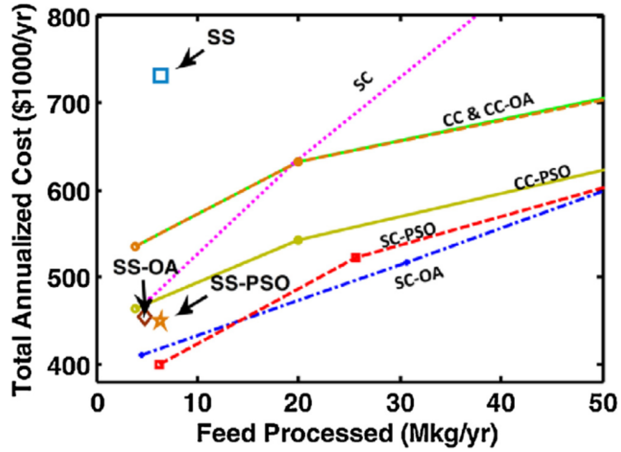

Fig. 9. Economic analysis for the superstructure design (SS).

To implement PSO, the gO:MATLAB feature of gPROMS was used. gO:MATLAB creates an encrypted file of the process model in gPROMS which can be called as a function in MATLAB. Then within MATLAB, the PSO code generates the values of decision variables which are sent to that function, the process is simulated, and finally the values of the objective function and the constraints are sent back to MATLAB.

It should be noted that, the height of the middle vessel is a decision variable. This variable is also used in one of the initial condition equations to compute the initial mass hold up of the middle vessel (it is assumed that at the beginning of the cycle the middle vessel is charged to 90% of its height). Therefore, changes in the value of this decision variable in the optimization problem change the initial condition of the system. When the system was optimized with the OA toolbox in gPROMS, the system was reinitialized after each minor optimization iteration which subsequently modifies the initial condition values of the system. However, this was considered when implementing PSO by having a "*reinitial*" command after updating the decision values to ensure that the initial conditions were reinitialized to the new values.

Discrete variables were modeled as continuous variables with rounding applied, and a penalty function is used to account for the constraints. A weighting factor of 10^{10} was considered for all constraints in the penalty function. Each PSO optimization study was repeated 5 times using different randomly-generated Latin Hypercube as the initial locations of the particles, and the best obtained result is reported.

3.3. Superstructure approach: when no base case is available

In previous sections, the MIDO framework was used to optimize a known structure for purification of a ternary mixture in an

Table 5
Optimization results for the 2 ft. column.

		Lower bound	Upper bound	OA result	PSO result
Integer variables	ET^T	0	5	5	2
	ET^M	0	7	7	6
	ET^B	0	5	5	2
	Middle vessel height	4	8	6	4
Continuous variables	$k^{\text{Distillate purity}}$	0.01	20	6.55	7.1
	$\tau^{\text{Distillate purity}}$	10	10,000	10,000	8585.6
	$k^{\text{Bottom purity}}$	0.01	20	8.95	11.14
	$\tau^{\text{Bottom purity}}$	10	10,000	10,000	9976.5
	$k^{\text{Reflux level}}$	0.01	10	1.16	1.45
	$\tau^{\text{Reflux level}}$	100	2000	1098	1018.5
	$k^{\text{Side draw}}$	0.01	5	0.12	0.119
	$\tau^{\text{Side draw}}$	100	2000	500	506.5
	Cycle time	79,000	100,000	94,012	20,230
Objective function (k$/Mkg)				91.1	64.4
Opt. side draw location				13	16
Opt. feed stream location				16	20
Opt. number of stages				26	33

Table 6
Optimization results for the 4 ft. column.

		Lower bound	Upper bound	OA result	PSO result
Integer variables	ET^T	0	5	5	4
	ET^M	0	7	7	7
	ET^B	0	5	5	5
	Middle vessel height	4	8	5	5
Continuous variables	$k^{\text{Distillate purity}}$	0.01	20	0.13	5.1
	$\tau^{\text{Distillate purity}}$	10	10,000	99.9	5578.2
	$k^{\text{Bottom purity}}$	0.01	20	11.45	11.97
	$\tau^{\text{Bottom purity}}$	10	10,000	10,000	10,000
	$k^{\text{Reflux level}}$	0.01	10	0.79	0.8
	$\tau^{\text{Reflux level}}$	100	2000	500	743.1
	$k^{\text{Side draw}}$	0.01	5	0.11	0.047
	$\tau^{\text{Side draw}}$	100	2000	500	733.56
	Cycle time	8000	100,000	8000	9575.2
Objective function (k$/Mkg)				16.8	20.3
Opt. side draw location				13	14
Opt. feed stream location				16	17
Opt. number of stages				26	27

Table 7
Optimization results for the 8 ft. column.

		Lower bound	Upper bound	OA result	PSO result
Integer variables	ET^T	0	5	4	1
	ET^M	0	7	7	5
	ET^B	0	5	4	5
	Middle vessel height	4	8	7	7
Continuous variables	$k^{\text{Distillate purity}}$	0.01	20	4.54	1.14
	$\tau^{\text{Distillate purity}}$	10	10,000	1000	5578.1
	$k^{\text{Bottom purity}}$	0.01	20	4.31	11.97
	$\tau^{\text{Bottom purity}}$	10	10,000	1000	10,000
	$k^{\text{Reflux level}}$	0.01	10	1.2	0.85
	$\tau^{\text{Reflux level}}$	100	2000	667.86	743.1
	$k^{\text{Side draw}}$	0.01	5	0.01	0.047
	$\tau^{\text{Side draw}}$	100	2000	500.01	733.5
	Cycle time	5000	100,000	5977.8	5171.7
Objective function (k$/Mkg)				7.6	6.6
Opt. side draw location				14	17
Opt. feed stream location				17	22
Opt. number of stages				28	32

attempt to find a better design and control for that structure. In this section, however, the objective is to extend the methodology to design a semicontinuous system for an arbitrary ternary mixture where no a priori information about the structure of the system is available.

The idea is to obtain an optimum configuration starting from a general superstructure configuration and let the optimizer find the best design and control parameters. The superstructure considered is shown in Fig. 5. An upper bound of 60 trays above and 60 trays below the feed was specified, and later testing confirmed that these bounds were sufficiently large because they were not active in the optimal solution. Two side streams were considered for the column, one above and one bellow the feed at tray locations of 30 and 90, respectively, meaning that an upper bound of 30 trays could exist between the feed the side draw. Only one of these side streams should be selected in the final design and this is determined by two binary variables added to the model namely y_1 and y_2 assigned to these streams such that:

$$y_1 + y_2 = 1 \tag{7}$$

Therefore, y_1 is another binary decision variable in the optimization. These variables can also be defined as Special Ordered Sets variables in gPROMS which defines them as a set of binary variables that only one of them can have a non-zero value.

In this configuration, there are four sets of conditional trays and consequently four integer variables at the top (ET^T), above the feed (ET^{M1}), bellow the feed (ET^{M2}) and at the bottom of the column (ET^B). The rest of the decision variables are the same as the base case optimization problem.

3.4. Continuous process optimization

The conventional continuous process was also optimized with both the OA and the PSO for the sake of economical comparison with the optimized semicontinuous system. The decision variables for the continuous system were conditional trays above and below the feed stream, and the reflux and reboil ratios for each column, giving 8 decision variables in total. The objective function was to minimize the TAC subject to the following constraints:

$$\text{Benzene purity in the distillate stream of the first column} \geq 98\ \text{mass\%} \tag{8}$$

$$\text{Toluene purity in the distillate stream of the second column} \geq 98\ \text{mass\%} \tag{9}$$

$$o\text{-Xylene purity in the bottom stream of the second column} \geq 98\ \text{mass\%} \tag{10}$$

4. Results and discussion

4.1. Continuous process

The design of Ling and Luyben (2009) is used as the base case for the optimization. To optimize the structural parameters of the conventional continuous configuration shown in Fig. 1a, ten conditional trays were considered above and below the feed stream of the two distillation columns. Also, the reflux and reboil ratios of both columns were decision variables. Lower and upper bounds of 0.1 and 10 were selected for these parameters. A multi-start approach was used for the OA method to start the optimization from different starting points based on the Latin Hypercube method. The best obtained optimization results for the conventional continuous system are reported in Table 4 for three different production rates. For each production rate, PSO found a better design with fewer numbers of stages. The OA method was stuck at a local optimum with no tray elimination and the only improvement in the TAC was achieved by reducing the operating costs. The economic results are shown in Fig. 8 in Section 4.3.

4.2. Sensitivity analysis for semicontinuous system

Before optimizing the semicontinuous system, a sensitivity analysis was performed to investigate the impact of each controller tuning parameters on the objective function. The semicontinuous system has six PI controllers which results in twelve decision variables (gains and reset times). The sensitivity analysis will determine if the number of decision variables can be reduced by eliminating the tuning parameters of the controllers which have minor effect on the objective function. This will decrease the computational time of the optimization problem.

To this end, a Monte Carlo analysis was used. In this method, the gain and the reset time of each controller were perturbed by 20% from the base case values in a uniform distribution and the histogram of the objective function is plotted in Fig. 6. The controllers with similar effects are grouped together, for brevity. As expected, the tuning parameters of the distillate and bottoms purity controllers have a considerable effect on the objective function since they affect the cycle time of the process and therefore the production rate of the system. On the other hand, the column pressure and sump level controllers have the least effect on the objective function. The reflux drum level and side draw controllers strongly impact the flow rate of feed to the column and the side stream withdrawal rate, respectively, which also affects the cycle time of the system and are consequently important design variables. It also appears that the reflux drum controller settings are at some local optimum.

The tornado plot of the sensitivity analysis is shown in Fig. 7, which shows the objective function variation (as a percentage change) resulting from a perturbation of each tuning parameters by ±20%, with all other parameters held at the base case values. It is clear that the column pressure and sump level controllers have negligible effect on the objective function and they can be eliminated as decision variables from the optimization problem.

4.3. Base case optimization of the semicontinuous system

Initially, five conditional trays were considered in top, middle and bottom sections of the base case design (Tables 1 and 2). The OA and PSO optimization results for the base case for three column diameters (corresponding to different production rates), showed zero tray elimination in the top section of the columns (ET^T's were zero). Since this variable was at the bound, 5 more conditional trays were added to the top section of the base case and the optimization was repeated. The modified base case configuration had 43 trays with side draw and feed stream locations at tray 12 and 28, respectively.

The optimization results for the modified base case structure are reported in Table 5 for the 2 ft. column. The upper bounds on the conditional trays are the maximum number of trays that can be eliminated in each section and the system is still feasible. Furthermore, the lower bound on the cycle time should be selected such that the problem stays feasible even with the maximum number of tray eliminations, otherwise the OA method fails. The column pressure and sump level controllers are omitted from the optimization (as discussed in the sensitivity analysis) to simplify the problem. The OA results show that the ET's are placed on the bounds. Further attempts to increase the upper bounds resulted in the infeasible problem. On the other hand, the PSO landed on a design with much shorter cycle time which increases the production rate.

The corresponding results for the 4 ft. and 8 ft. columns are reported in Table 6 and Table 7, respectively. The OA method is very sensitive to the initial starting point. Very different local optimums can be obtained by changing the starting point. The advantage of the PSO over the OA method is the independency of the method to the initial values of decision variables and also the ability to jump over infeasible regions. However, very similar results are obtained with both methods.

The economic analysis is shown in Fig. 8. In this figure, SC is the base case design for the semicontinuous system, SC-OA is the obtained optimum design for the SC using OA, SC-PSO is the optimum design for the SC using PSO, CC is the conventional continuous design, CC-OA and CC-PSO are the optimum designs for the CC using OA and PSO, respectively. Fig. 8a shows the total direct cost versus the production rate. The total direct cost of the SC system increases rapidly over the CC for higher production rates since larger column diameters are required to process the feed in one column. The cost

Table 8
Optimization CPU times (min).

	2 ft. column	4 ft. column	8 ft. column
OA	27	14.7	7.9
PSO	289.6	207.15	376

Table 9
Superstructure optimization results for the 2 ft. column.

		Lower bound	Upper bound	OA result	PSO result
Integer variables	CT^{T}	0	26	16	14
	CT^{M1}	0	26	26	24
	CT^{M2}	0	26	26	26
	CT^{B}	0	26	20	20
	Middle vessel height	4	8	7	6
	y_1	0	1	1	1
Continuous variables	$k^{\text{Distillate purity}}$	0.01	20	1.12	9.34
	$\tau^{\text{Distillate purity}}$	10	10,000	1980	5000
	$k^{\text{Bottom purity}}$	0.01	20	1.57	7.14
	$\tau^{\text{Bottom purity}}$	10	10,000	2000	4361.9
	$k^{\text{Reflux level}}$	0.01	10	1.1	2
	$\tau^{\text{Reflux level}}$	100	2000	1200	1462.9
	$k^{\text{Side draw 1}}$	0.01	5	0.01	0.6
	$\tau^{\text{Side draw 1}}$	100	2000	500	800
	$k^{\text{Side draw 2}}$	0.01	5	0.01	0.62
	$\tau^{\text{Side draw 2}}$	100	2000	500	809
	Cycle time	70,000	500,000	110,922	71,779.2
Computational CPU time (min)				25.9	1567.5
Objective function (k\$/Mkg)				75.1	76.1
Opt. side draw location				14	16
Opt. feed stream location				18	22
Opt. number of stages				32	36
“True” cycle time				138,170.8	65,518.6

of the CC and CC-OA designs are the same since they have the same structural parameters (all ETs are zero in Table 4). However, CC-PSO has a lower total direct cost due to the elimination of a couple of trays in each column section (Table 4). Although the direct cost of the SC base case is higher than the best obtained design for the conventional continuous system (the CC-PSO design), both optimum designs for the SC (SC-OA and SC-PSO) have lower direct cost than the CC-PSO for the whole range of studied production rate.

Fig. 8b shows the operating costs of these designs for different production rates. SC system generally has a higher operating cost than the CC system due to its cyclic nature. However, optimization has reduced the semicontinuous operating costs especially for higher production rates. For production rate of 60 Mkg/year the operating cost of the optimum semicontinuous system has shrunk by one third. This is generally due to better tuning parameters for the control system which shortens the cycle time and decreases the utility consumption. For the conventional continuous system, both PSO and OA have slightly reduced the operating costs of the CC system.

Finally, Fig. 8c shows the TAC for these designs. The SC base case is only more economical than the CC and the CC-OA for low production rates (up to 20 Mkg/year). However, the SC-OA and SC-PSO have improved the TAC considerably. For instance, for the production rate of 60 Mkg/year the TAC of SC has reduced from 1000 k\$/year to 650 k\$/year (about 35%). Also, the optimum SC designs have expanded the economical production rate from 20 Mkg/year to 60 and 90 Mkg/year for SC-OA and SC-PSO, respectively. This is 2 and 3.5 times increase in the economical production rate for the semicontinuous system with respect to the CC-PSO.

The computational times of both OA and PSO methods are shown in Table 8. The OA method has lower CPU times than the PSO method as suspected. However, the OA method requires a substantial amount of time to find a good initial point to use for the optimizer, which has to be achieved through trial and error, and this human time is not included in the table. However, the PSO method was more robust because it can often avoid terminating in a local optimum and can handle infeasible points gracefully.

4.4. Superstructure optimization

The optimization results for the superstructure are presented in Table 9 for the 2 ft. distillation column. The upper bounds on the conditional trays are selected such that with maximum tray elimination, the structure remains feasible. The y_1 variable determines the side stream location. In this case, y_1 is equal to one which means the side stream is above the feed. This result is consistent with the heuristically-determined base case design for the semicontinuous system from the previous study.

Also in Table 9 the computational CPU times for the OA and PSO methods are reported which shows a significant difference between them. The computational time for simulating the superstructure is higher than the base case due to the higher number of trays in the superstructure case. During the optimization, although a bunch of these trays become inactive and they do not participate in the mass transfer, their liquid hold up dynamics will be accounted in the simulations which result in both a higher computational time and also inaccuracy associated with the predicted cycle time for the system. Therefore, the cycle times reported in Table 9 for the 2 ft. column is much longer than the corresponding results for the base case design reported in Table 5.

To obtain the “true” cycle times and economic results, the optimum designs must be simulated with the actual number of trays. The structures obtained from OA and PSO methods are slightly different but the TACs of the two locally optimum designs are close to each other and are shown in Fig. 9 as the diamond and star points, respectively. The largest possible column with all 120 trays (shown as a square in Fig. 9) has a high TAC and the optimizations have resulted in designs which are close to the base case design.

Therefore, it can be concluded that the MIDO can be successfully implemented to achieve a close to optimal design for semicontinuous system for any arbitrary ternary mixture. This approach can reduce the tedious, time consuming procedure of designing the system by sequential approach. Although not attempted in this work, the obtained designs using the superstructure approach can then be used as an initial guess for a second stage optimization with the inactive trays eliminated. The reason for the two stage optimization for the superstructure is that the high number of inactive trays in the simulations during the optimization will result in a slightly different system dynamic. Therefore, by eliminating those trays in the second optimization stage a more realistic optimum result will be obtained, but will nevertheless be very close to the first stage result.

5. Conclusion

In this work, a simultaneous integrated design and control methodology is proposed to design a semicontinuous distillation system for a ternary mixture. This is advantageous over previously developed methods because the simultaneous method captures the dynamics of the system in the design stage and also significantly reduces the time required for designing a close to optimal solution compared to the sequential approach. Mixed integer dynamic optimization using the outer approximation method was shown to find similar solutions as particle swarm optimization when the system was modeled in gPROMS using its PML library.

The OA method was considerably faster when good initial guesses were provided, but very sensitive to the initial guesses. Many initial guesses resulted in failure of the OA algorithm, and finding good initial guesses a priori for semicontinuous systems in general is very difficult. Therefore, a superstructure method was proposed which uses an excessively large distillation column as an initial guess with possible side draw locations both above and below the feed. It was found that both the PSO and OA methods found very similar solutions using this approach, and those solutions could then be used as the initial guess for a more rigorous optimization approach with either PSO or OA. However, because the OA approach is much faster at both of these stages, it is recommended for use whenever possible. Nevertheless, since both OA and PSO always found similar solutions and neither one consistently found better design than the other, the PSO is recommended for use where OA methods are not available, as is sometimes the case in other commercial simulation software.

For future work, it is suggested that the charging and discharging modes of operation be included in the simulation and the optimization of the system. The key parameters of those modes are the rate at which the tanks are filled or discharged. Generally, faster is better in terms of cycle time, but the costs of this have not previously been considered, so there is some optimal policy which is currently unknown.

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Chapter 4

Subspace model identification and model predictive control of semicontinuous distillation process

The content of the following chapter is **submitted** to the following peer-reviewed journal for publication consideration:

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Subspace Model Identification and Model Predictive Control of Semicontinuous Distillation Process

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Abstract

Semicontinuous distillation is a process intensification technique for purification of multicomponent mixtures. The process dynamically separates a multicomponent mixture to desired purities using only one distillation column, which is integrated with one or several storage tanks. The system works in stable cycles, each consisting of charging the tanks, processing the mixture and discharging the tanks. The system is control-driven and thus the control structure and its tuning parameters have crucial importance in the operation and the economics of the process. So far, in all previous studies of the system, only multi-loop proportional integral (PI) controllers have been used for this highly nonlinear, multivariable, constrained process with high variable interactions. In this study, for the first time, the implementation of model predictive control (MPC) on a semicontinuous process is studied. As such, the ability of this more advanced control strategy to improve the operability and economics of a semicontinuous case study is examined. A cascade configuration of MPC and PI controllers is designed in which the setpoints of the PI controllers are determined via a shrinking-horizon MPC. The objective is to reduce the operating cost of a cycle while simultaneously maintaining the required product qualities by the end of the cycle. A subspace identification method is adopted to identify a linear, time invariant, state-space model to be used in the MPC. The first-principals model of the process under the proposed control scheme is then simulated in gPROMS. Simulation results demonstrate that the MPC has reduced the operational cost of the semicontinuous process by about 11% by changing the operational policy of the process to achieve the separation in a shorter cycle time.

Keywords:

Semicontinuous distillation; Model predictive control (MPC); Cascade MPC with PI; Subspace identification; Dynamic distillation; gPROMS

4.1 Introduction

Distillation columns are usually major sources of capital and operating costs in chemical processes [1]. Unsurprisingly, reducing these costs has been the driving force for intensive research on process intensification techniques aimed at the mitigation of these major costs. Among such studies are those that consider heat integration configurations aimed at reducing the operating costs of the process [2] and those that consider dividing wall columns that can potentially reduce the capital and operating costs of multicomponent separation [3]. Semicontinuous distillation is another intensification technique that has been shown effective in reducing the total annualized cost (TAC) of processes with low to intermediate throughputs [4]. The semicontinuous process was first proposed by Phimister and Seider [5] for ternary mixtures and was extended for n-component mixtures by Wijesekera and Adams [6]-[7].

The essential idea in semicontinuous distillation is to lower the capital costs by purifying n-component mixtures in only one distillation column that is coupled with storage tanks (called middle vessels). Conventionally, n-1 distillation columns are required to separate an n-component mixture in a steady-state approach (Figure 1a). Alternatively, the same purification can be achieved dynamically with semicontinuous system. In this configuration, n-2 middle vessels are integrated with a single distillation column (Figure 1b).

A typical semicontinuous cycle proceeds as follows: Initially, the middle vessels are charged with fresh feed. Each middle vessel feeds the column and a side stream of the column is recycled back to it. During the processing mode, the lightest and the heaviest components, in terms of boiling points, are removed from the distillate and bottom streams of the distillation column, respectively. Each intermediate component is concentrated in a middle vessel based on its relative volatility. The most volatile intermediate component is concentrated in a middle vessel that receives the side stream from a tray closer to the column's condenser, and the heaviest intermediate component is accumulated in a middle vessel that receives the recycle from a tray closer to the reboiler of the column. When the desired purities of all intermediate components are achieved in each of the middle vessels, the processing mode terminates and the vessels are discharged. The products are collected before the middle vessels are refilled with fresh feed, marking the end of one cycle.

By omitting n-2 distillation columns, the semicontinuous system lowers the capital cost of a given separation process and consequently the TAC of the process. Being a compact and less expensive configuration, semicontinuous distillation is thus a desirable candidate for low-throughput processes such as biofuel or pharmaceutical processing [8].

Since the dynamic variability of semicontinuous processes is very high, its performance is heavily dependent on its control system. Proper control can shorten the cycle time, increase the production rate and reduce the operating costs of the process, while improper control can disrupt the cycle and even result in instability of the column, leading to safety concerns and economic losses. Despite the obvious importance of semicontinuous control system design, very few studies have examined the use of advanced control techniques to improve the process' performance. So far, only proportional integral (PI) control structures have been implemented on this configuration.

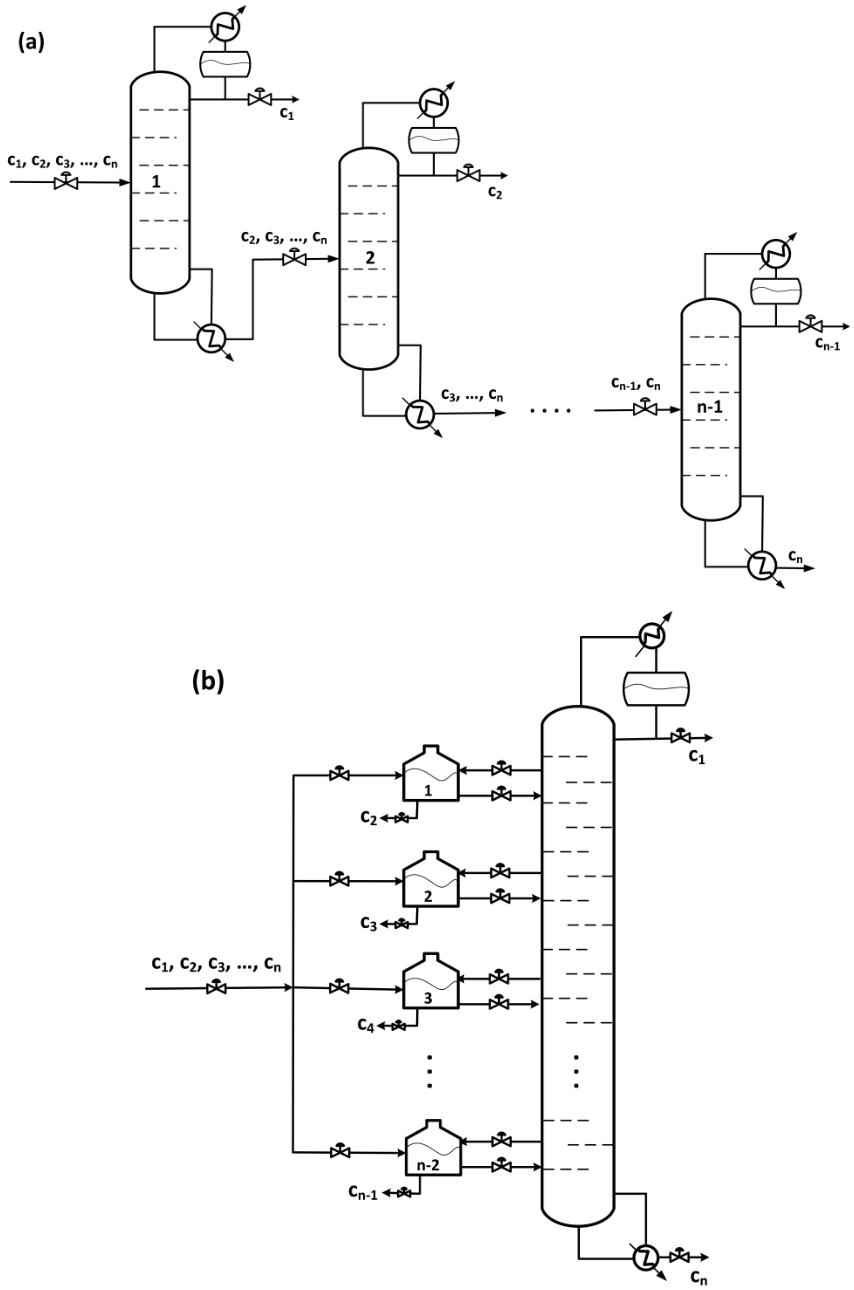

Figure 1- (a) conventional continuous distillation train for purification of *n*-component mixture, (b) the corresponding semicontinuous configuration.

Pascall and Adams explored eight PI configurations for the semicontinuous system [9]. They compared the configurations and evaluated their performances in terms of maintaining product purities and rejecting disturbances in the feed composition. They showed PI control can satisfactorily operate the system. However, the challenge with multi-PI controllers for semicontinuous distillation lies in tuning the controllers' parameters. High interactions between control loops are the main reason. Moreover, regular tuning methods such as Cohen-Coon, Ziegler-Nichols, Tyreus-Luyben and auto-tune rely on the assumption that the process is operating at steady-state. Since the semicontinuous system operates in a purely transient fashion and thus does not have any steady states, these methods cannot be used and a tedious trial-and-error procedure must be utilized.

To address this issue, Meidanshahi and Adams proposed an integrated design and control approach to simultaneously design the structural and operational parameters of the system [10]. In their proposed method, the tuning parameters of the controllers are determined simultaneously with structural parameters (such as feed stream location, number of trays, etc.) in a mixed-integer dynamic optimization problem. Although this method provides a suitable methodology for tuning PI controllers, advanced control strategies such as model predictive control (MPC) can likely provide more desirable control for a semicontinuous system. MPC utilizes a model of the process, which allows it to optimize the inputs to the system to achieve a pre-defined objective (whether it is economic or operational) while considering for process constraints and dynamics. However, in large plants, MPC is not a replacement of proportional integral derivative (PID) controllers, but is rather an addition to it. While PID controllers have been shown to handle single-input/single-output systems effectively and have the benefit of not requiring process models, multi-input/multi-output processes and over-arching control objectives are better suited to being controlled via an MPC method.

There are several literature studies that feature the implementation of MPC on distillation columns. These studies have also investigated the specific way in which MPC is applied, such as whether it should be directly implemented on the column or used in combination with PI control loops.

For instance, Huang and Riggs studied the MPC control of a binary steady-state distillation column [11]. They compared three control configurations for the system: In the first configuration, the MPC controller manipulated the reflux flow rate and the bottoms flow rate to maintain the purities of distillate and bottom streams, respectively, and PI controllers were used for regulatory control of liquid levels of reflux drum and sump by manipulating the distillate and boil up flow rates, respectively. In the second configuration, the MPC controller directly controlled all four degrees of freedom which were the distillate, reflux, boilup and bottom flow rates. In the third configuration, a cascade design was studied in which the MPC was directly manipulating the reflux and bottom flow rates to control the product purities and indirectly controlling the liquid levels by manipulating the setpoints of the PI level controllers. The authors concluded that both the direct and cascade (the second and the third) configurations had desirable performance. In these scenarios, the MPC method could coordinate the input moves for all manipulated variables, whereas in the first configuration the MPC and PI controllers had conflicting input actions to the system, leading to decreased performance. With respect to the performance of the MPC itself, the authors also discussed the advantages and disadvantages of direct versus cascade control configurations.

In the direct configuration, the MPC performed more reliably due to its independence of the PI regulatory level controllers. However, a significant disadvantage of this configuration was that the system could become unstable during step-tests for MPC model identification without the PI regulatory controls in place. The cascade configuration could compensate this shortcoming. High-fidelity models could be obtained with the cascade configuration while the MPC still had the leverage to manipulate the liquid levels by influencing the control input actions to the process via the PI set points.

The distillate and bottom composition loops in a distillation column usually have high levels of interaction with each other. Barolo and Papini suggested that the presence of a middle vessel can reduce this interaction and improve the performance of the column [12]. They proposed a novel configuration called middle vessel continuous distillation column (MVCC) for binary mixtures. In this configuration, the feed stream was fed to the middle vessel, which had a level controller to adjust the feed flow rate to the column. The side stream of the column was recycled back to the middle vessel. The authors showed that the presence of a middle vessel could hydraulically decouple the interaction of the top and bottom composition loops and improve the composition control of the system. In this configuration, the choice of the middle vessel holdup volume and the level controller gain were the main design parameters of the system.

Subsequently, Bezzo et al. studied two MPC configurations of the MVCC [13]. In the first, MPC was directly manipulating the five inputs to the system (distillate, reflux, bottom, boilup and feed flow rates). In the second configuration, the MPC controller manipulated the setpoints of three PI level controllers (controlling the reflux drum, sump and middle vessel liquid levels) while also directly controlling the reflux and boilup ratios. The authors used step tests to find a linear model of the process and implemented the MPC employing the MPC Toolbox of MATLAB. The authors concluded that by using MPC they could use a smaller middle vessel. However, it was also found that the MPC strategy had the same control performances as a properly tuned PI control structure and a proper middle vessel hold up.

On the other hand, Rewagad and Kiss observed outstanding performance of MPC on dividing wall columns compared to PID control [14]. They also addressed the issue of direct or coupled MPC implementation. In the direct configuration, all inputs were computed by the MPC. In the other configuration, two PID controllers were used to control the liquid levels and the MPC was directly manipulating the other inputs to the system. A linearized model of the dividing wall column was used for calculations in the MPC. The authors observed that both MPC configurations showed similar performance and they could successfully lower the integral absolute error (IAE) of overshoots when compared to PID control.

In this study, the implementation of MPC on a semicontinuous system is studied for the first time. Although the total direct cost of the semicontinuous system is lower than a conventional continuous system, its higher operating costs motivate the need for more effective cycle control. The higher operating costs are due to the fact that the side stream is continuously being recycled back to the middle vessel, resulting in losing energy by mixing the purified side stream with the non-purified hold up in the middle vessel. The objective of this work is to investigate if a semicontinuous process can be operated more efficiently and hence with lower operating costs, while still meeting the required product purities. In order to accomplish this objective, a subspace identification technique for batch processes [15] is adopted to identify a linear model of the semicontinuous distillation process and it is used in a shrinking-horizon MPC.

4.2 Simulation environment

The separation of an equimolar ternary mixture of benzene, toluene and o-xylene (BTX) is chosen as a case study for this work. The semicontinuous purification of this mixture requires one middle vessel as shown in Figure 2. In this configuration, the distillate and bottom stream purities are controlled by their respective flow rates. The reflux drum and sump levels are controlled by the feed flow rate to the column and the reboiler heat duty, respectively. Column pressure is maintained by manipulating the condenser heat duty. The flow rate of the side stream is adjusted by a flow rate controller. This control structure was shown to be the most effective multi-PI control loop for semicontinuous system in terms of disturbance rejection and maintaining product purities [9]. Therefore, this control structure was used in the present study for comparison against the proposed MPC alternative.

To simulate the process, gPROMS' process model library (PML) is used. PML provides first-principle models of commonly used process equipment and facilitates the simulation of process flowsheets. For details on simulating the BTX semicontinuous distillation in gPROMS, refer to Meidanshahi and Adams [10]. In the present work, the charging and discharging modes of the semicontinuous cycle are added to the simulation. The sequence of the operational modes is added to the SCHEDULE section of gPROMS. The differential algebraic equations (DAEs) of the system are integrated until the desired purity in the middle vessel is reached. Subsequently, the middle vessel discharge valve is opened to empty the tank until the liquid level reaches about 6% of the tank height. Following that, that valve is closed and the feed stream valve to the tank is opened. The middle vessel is charged with fresh feed up to 80% of its height, thus beginning a new cycle.

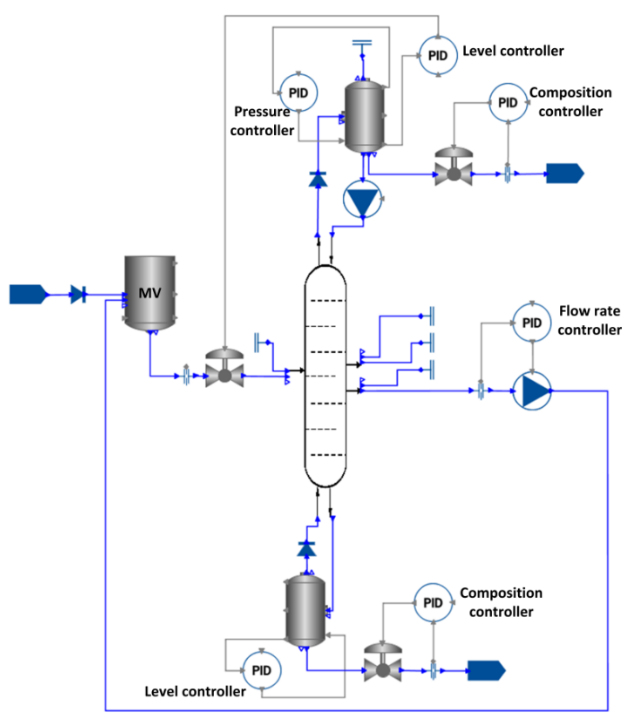

Figure 2- Semicontinuous distillation of BTX, simulated in gPROMS' PML.

4.3 Implementation of MPC on semicontinuous system

MPC can be implemented on a semicontinuous system either directly or cascaded with PI control loops. The direct MPC implementation methodology is shown in Figure 3. In this configuration, the column pressure and the sump levels are left to be controlled by PI controllers to ensure the stability of the process. However, the distillate, bottom, side stream and feed flow rates are directly manipulated by the MPC. The advantages of this configuration are the elimination of PI controllers and their dynamics from the control system. Moreover, this configuration eliminates the need for tedious trial-and-error tuning of the PI controllers. However, the disadvantage of this configuration is that the system is open-loop during the model identification step required for the MPC.

As the pseudo-random binary sequence (PRBS) signals are added to the nominal input trajectories (flow rates in this case), the outputs (composition of the products and constraint variables) deviated away from the closed-loop trajectories. Even with small PRBS amplitudes, the deviation was found to be significant which resulted in poor model identification. Without the ability to identify a high-fidelity predictive model, the direct MPC implementation configuration was ruled out for this study.

With the direct MPC methodology ruled out, the cascade MPC configuration becomes the next best option for the proposed semicontinuous system (Figure 4). In this configuration, PI controllers ensure stability of the process. Also, during the model identification tests, the system remains in closed-loop. In this cascade configuration, the MPC adjusts the setpoints of the distillate and bottoms composition, side stream flow, reflux drum level, and sump level controllers.

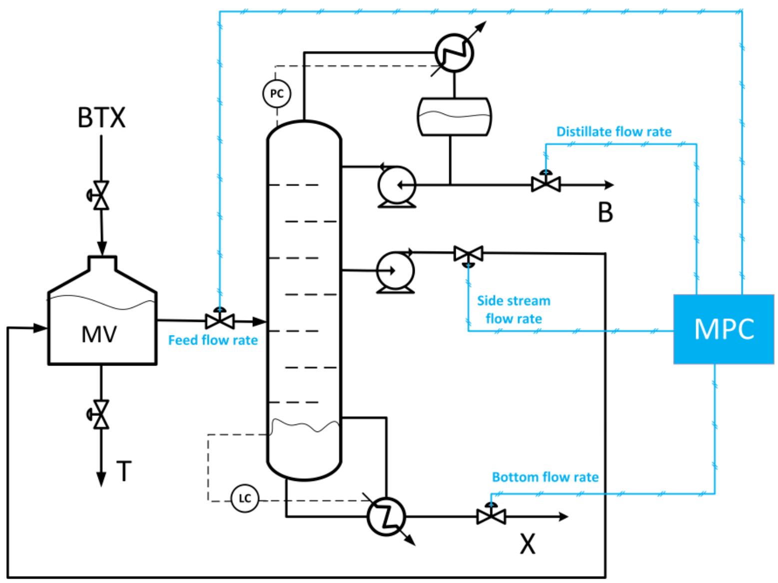

Figure 3- Direct MPC implementation on a semicontinuous system.

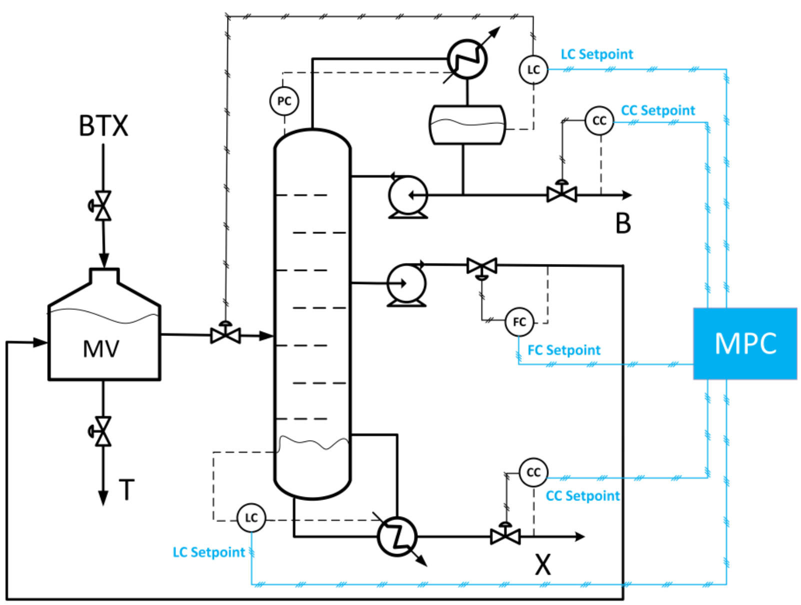

Figure 4- Cascaded MPC with multi-PI loops.

The column pressure controller setpoint is not considered as an input determined by the MPC since the column is designed to operate at the lowest possible pressure such that inexpensive cooling water could be used as the utility in the condenser. Further reducing the pressure would require the use of refrigerants, which are significantly more expensive.

The methodology presented by Corbett and Mhaskar for controlling batch processes is adopted here [15]. They presented a subspace quality model predictive control (SQMPC) to obtain the desired product qualities by batch termination. The subspace identification method was used to identify a data-driven linear model of the process. Then they built a quality model which related the states and the inputs of the system to the quality variables. Quality variables were defined as process variables that are required to meet a desired specification by the end of the cycle or the batch.

Having the process linear model and the quality model, the objective of the proposed shrinking horizon SQMPC was to reject disturbances in the batch initial condition and to track setpoint changes such that by the end of the batch product specifications were met. The main thrust of SQMPC is described next.

Consider a general dynamic process of the form:

$$\dot{\boldsymbol{x}} = f(\boldsymbol{x}, \boldsymbol{u}) \tag{1}$$
$$\boldsymbol{y} = g(\boldsymbol{x}, \boldsymbol{u}) \tag{2}$$
$$\boldsymbol{q} = h(\boldsymbol{x}, \boldsymbol{u}) \tag{3}$$

where $\boldsymbol{x}$ is the state variable, $\boldsymbol{u}$ is the input, $\boldsymbol{y}$ is the output and $\boldsymbol{q}$ is a vector of quality variables. The nonlinear functions describing the dynamics of the system are denoted by f, *g* and *h* and are nonlinear functions relating the outputs and the quality variables, respectively, to the states and the inputs. Quality variables are defined as a subset of outputs that are required to meet a desired specification by the end of the cycle. They can be measured or unmeasured outputs of the process. In the work of Corbett and Mhaskar, the quality variables were unmeasured and a data driven model was developed to predict them during the batch [15].

A full cycle of a semicontinuous process consists of charging, processing and discharging modes of operation. To simplify the control problem and avoid considering the charging and discharging phases in the MPC, a model is identified only for the processing mode of the system and the MPC is implemented only during that mode of operation. During the charging and discharging of the middle vessel, the MPC is turned off and the setpoints of all controllers are reset to their nominal values during the transitions. After recharging the middle vessel for the following cycle, the MPC is turned on again.

To design the MPC for semicontinuous system, it should be noted that the control system of the process should satisfy the following objectives:

1) The time-averaged purities of the distillate and bottom streams should meet the required specifications for these streams by the end of the processing mode.
2) The desired purity of the intermediate component in the middle vessel must be achieved by the end of the processing mode.

3) The purification is performed in the shortest possible cycle time which results in increasing the total production rate and also reducing the operating cost of the process.
4) The column pressure and liquid levels in the reflux drum and the sump, respectively, are maintained at or close to their nominal values during the cycle to ensure stable operation.
5) Weeping and flooding should be avoided in the column during the cycle.

Therefore, the quality variables of the semicontinuous system are chosen to be the middle vessel purity (q_1), the average purities of distillate (q_2) and bottom (q_3) streams, and the operating cost (q_4). The product purities are set by design specifications and are required to be obtained by the end of the processing mode of the semicontinuous cycle. The time-averaged purities of distillate and bottom streams are computed via the following equations:

$$q_2 = \frac{\int_0^{t_f} F^{dis} \times x_B^{dis}}{\int_0^{t_f} F^{dis}} \tag{4}$$

$$q_3 = \frac{\int_0^{t_f} F^{bot} \times x_X^{bot}}{\int_0^{t_f} F^{bot}} \tag{5}$$

where F is the flow rate of distillate and bottom streams and x is the composition of the main component in those streams. The average purities are integrated from the beginning of the processing mode until the end of it (t_f). The operating cost is also chosen as a quality variable since it is desired that the system operates with minimum energy consumption by the end of cycle. The operational cost is the cost of utilities in the condenser and the reboiler and is computed via Eq. 6. The costs of utilities (v_1 and v_2) are computed based on the method available in Towler and Sinnott [16].

$$q_4 = v_1 \int_0^{t_f} Q_{condenser} + v_2 \int_0^{t_f} Q_{reboiler} \tag{6}$$

The output measurements (y) of the semicontinuous system considered in the MPC are the reflux drum and sump liquid levels and the vapour velocities at top and bottom of the column (tray numbers 5 and 20, respectively). These measurements are needed to set operational constraints on the process to be considered in the MPC calculations to guarantee safe operation and avoid weeping and flooding of the column during the cycles. Furthermore, in this work, it is assumed that the measurements of the quality and output variables are available free of measurement noise during the cycle. The inputs to the system ($\boldsymbol{u}$) are the setpoints of controllers as shown in Figure 4. The *f*, *g* and *h* functions are the first-principle DAEs of the process which are simulated in gPROMS.

The next step is to identify a discrete, time invariant, linear, state-space model. This model is employed in the suggested shrinking-horizon MPC, to predict the quality and the output variables during the cycle. In the following section, the procedure for identifying the model is discussed.

4.4 Subspace model identification

MPC computes future input moves to the process based on the provided model of the process. Therefore, the model should be both descriptive of the process dynamics and simple enough to allow for reasonable computation times of the optimization problem. Step-test identification methods cannot be used for a semicontinuous system due to the lack of any steady-state conditions of the process, which are required to identify process gains and time delays. Linearizing the nonlinear distillation column model is another option. In this method, multiple linear models are constructed along the process trajectory. These models are then combined into one global model to describe the whole cycle, utilizing proper weighting factors [17].

However, the subspace identification method is an alternative approach which can identify one linear model for the whole cycle and eliminate the need of weighting factors [18]. This method is chosen to identify the linear model in this work. This data-driven method is based on gathering the input-output trajectories of the process and constructing a linear model [19]. Corbett and Mhaskar expanded the method to apply to batch processes with varying batch length [15].

To adopt the Corbett and Mhaskar technique for the semicontinuous system, PRBS signals are added to the five inputs of the system (distillate and bottom composition controller setpoints, side stream flow rate setpoint, reflux drum and sump liquid level controller setpoints). The magnitudes of the PRBS signals are chosen to be significant enough to be able to identify the correlation between the inputs and the outputs. However, larger magnitudes result in poorly identified models.

Given the input and output trajectories of the process, the subspace identification method determines the A, B, C and D matrices of the state space model:

$$\tilde{\boldsymbol{x}}(k+1) = \boldsymbol{A}\,\tilde{\boldsymbol{x}}(k) + \boldsymbol{B}\,\boldsymbol{u}(k) \tag{7}$$

$$y(k) = \boldsymbol{C}\,\tilde{\boldsymbol{x}}(k) + \boldsymbol{D}\,\boldsymbol{u}(k) \tag{8}$$

in which $\tilde{\boldsymbol{x}}$ is the vector of subspace states which are different from the true states of the system. Therefore, a Luenberger observer should be deigned to obtain the true value of the states during the cycle. It was found that forcing the matrix $\boldsymbol{D}$ to zero for the present application resulted in a better model. Sampling time (k) is considered to be one minute in this work which is in the order of process time scale. The identified model captures the dynamics of the PI controllers. However, it should be noted that the PI controllers should be tuned to have fast responses toward setpoint changes. This remark will be discussed more in section 6.2.

4.5 SQMPC

Once the linear model is obtained, the values of quality and output variables can be computed during the cycle and their terminal values can be predicted by the end of cycle. To do so, the values of the true process states at each sampling time and the future input trajectories to the process should be known. To obtain the true values of the states, a Luenberger observer is initialized at the beginning of the cycle. As the process measurements become available, the observer is updated until the output predictions converge to the measured outputs. After the observer convergence, the model predictions are initialized. The quality variables are computed at the end of the processing mode via the following equations:

$$\tilde{\boldsymbol{x}}(k_f) = \boldsymbol{A}^{k_f-k}\tilde{x}(k) + \left[\boldsymbol{A}^{k_f-k-1}\boldsymbol{B} \quad \boldsymbol{A}^{k_f-k-2}\boldsymbol{B} \ \ \dots \quad \boldsymbol{B}\right]\boldsymbol{v}(k) \tag{9}$$

$$\boldsymbol{v}(k) = [\boldsymbol{u}(k),\ \ \boldsymbol{u}(k+1),\ \ \dots,\ \ \boldsymbol{u}(k_f - 1)]' \tag{10}$$

where k is the current sampling time and the k_f is the final sampling instance. $\boldsymbol{v}$ is the candidate input trajectory to the process. Subsequently, the quality variables can be readily computed as:

$$\boldsymbol{q}(k_f) = \boldsymbol{C}\,\tilde{\boldsymbol{x}}(k_f) \tag{11}$$

Therefore, by having the predictions of the quality variables at the end of the cycle, the following MPC objective function can be computed and the future input trajectories to the process is optimized at each sampling time via a quadratic optimization problem:

$$\min_{\boldsymbol{u}} \ \ \left(\boldsymbol{q}(k_f) - \boldsymbol{q}_d\right)'\boldsymbol{M}\left(\boldsymbol{q}(k_f) - \boldsymbol{q}_d\right) + \ \Delta\boldsymbol{v}(k)'\,\boldsymbol{P}\,\Delta\boldsymbol{v}(k) \tag{12}$$

Subject to:

$$\boldsymbol{q} = \boldsymbol{C}\ \left(\boldsymbol{A}^{k_f-k}\tilde{x}(k) + \left[\boldsymbol{A}^{k_f-k-1}\boldsymbol{B} \quad \boldsymbol{A}^{k_f-k-2}\boldsymbol{B} \ \ \dots \quad \boldsymbol{B}\right]\boldsymbol{v}(k)\right) \tag{13}$$

$$\Delta \boldsymbol{v}(k) = [\boldsymbol{u}(k),\ \boldsymbol{u}(k+1),\ \ldots,\ \boldsymbol{u}(k_f - 1)]' - [\boldsymbol{u}(k-1),\ \boldsymbol{u}(k),\ \ldots,\ \boldsymbol{u}(k_f - 2)]' \tag{14}$$

$$\boldsymbol{v}_{min}(k) \le \boldsymbol{v}(k) \le \boldsymbol{v}_{max}(k) \tag{15}$$

$$0.1 \le Reflux\ drum\ and\ sump\ liquid\ level\ fractions\ \le 0.9 \tag{16}$$

$$V^i_{min} \le V^i \le V^i_{max}\ , \qquad i = tray\ number\ 5\ and\ 20 \tag{17}$$

where $\boldsymbol{q_d}$ is the desired values of quality variables at the end of the processing mode. The diagonal matrix $\boldsymbol{M}$ penalizes any deviation from the desired qualities and the diagonal matrix $\boldsymbol{P}$ penalizes the magnitude of input moves. There are hard constraints on the inputs of the process and also on the outputs. The last constraint (Eq. 17) is intended to prevent weeping and flooding during the cycle. V is the vapour velocity and the maximum allowable vapour velocity in the column to prevent flooding and the minimum vapour velocity to prevent weeping of liquid are computed based on equations provided in Mersmann et al. [20].

The gPROMS rigorous first principle model is considered as the process model. The shrinking horizon MPC code is implemented in MATLAB. Therefore, the gO:MATLAB feature of gPROMS is used to link these two software platforms. The inputs to the process are computed in MATLAB and then they are passed into gPROMS, where the outputs of the process are computed and are sent back to MATLAB.

4.6 Results and discussion

The structural parameters of the BTX semicontinuous separation used in this work are listed in Table 1, which are adopted from Meidanshahi and Adams [10]. In that work, the authors optimized the process and found the optimum structural and operational parameters for the system. However, they only considered the processing mode of operation in the optimization problem and did not include the charging and discharging modes. The reported gains for the side stream flow and liquid level controllers are small. When MPC is cascaded with these sluggish underlying PI controllers, it does not respond quickly enough to the setpoint changes instructed by the MPCs, and therefore the MPC changes the operation of the system by only a small amount. As a result, the improvement in the operational cost of the process is small (~1-2% reduction in cost).

Table 1– Semicontinuous design parameters for BTX separation.

Number of trays	Feed tray	Side tray	Condenser pressure (bar)	Middle vessel height (m)	Column diameter (ft.)
26	16	13	0.37	5	4

Another issue is that in this study the MPC is only on during the processing mode of the process and all controllers' setpoints are set back to their nominal values during the discharging and charging modes. Therefore, if the PI controllers are not fast enough to bring the process variables back to the their nominal values, the column will face material imbalance which results in liquid accumulation in the column or dry the column trays and eventually disrupts the operation of the process.

Therefore, the PI tuning parameters are changed to the values reported in Table 2 to avoid the aforementioned issues. Subsequently, the performances of the multi-PI loops and the cascaded MPC with PI controllers are compared. Furthermore, the charging and discharging rates of the middle vessel are designed at lower rates to give the process enough time for transition to the nominal conditions at the beginning of the subsequent cycle.

Table 2– PI controllers tuning parameters.

Distillate Purity controller		Bottom Purity controller		Reflux drum level controller		Sump level controller		Side draw controller		Column pressure controller	
k	τ	k	τ	k	τ	k	τ	k	τ	k	τ
5	40200	5	50251	3	1000	3	1000	3	1000	0.5	1000

k is the gain and τ is the reset time (sec.).

In the following subsections, first the results of model identification are discussed. Subsequently, performance of the MPC strategy on the semicontinuous system is examined in two case studies. The first case study explores the economic benefits of the MPC implementation on the process. The main focus in this case is to reduce the operating cost of a semicontinuous cycle. The second case study examines the capability of the MPC in maintaining product purities in the face of changes in the feed stock composition.

4.6.1 Subspace model

As it is mentioned earlier, the linear model is identified only for the processing mode of the operation. A database of input-output trajectories of the process is generated to build the model. The database contains the nominal PI trajectories as well as the data gathered from exciting the process by adding PRBS signals to the setpoints of PI controllers. No open-loop data is collected in the database since it adversely affected the accuracy of the identified model.

Twenty percent of the database is used in model validation and the rest in training the model. The main parameters of the subspace identification method that should be determined are the number of states and the number of Hankel matrix rows. These parameters are chosen such that the sum square of errors of model predictions and process output measurements are minimized. These values for the identified model are 12 states and 14 Hankel rows.

Figure 5 illustrates the prediction capabilities of the identified linear model. In this Figure the model predictions of the quality variables are compared to the corresponding process measurements. For the first fifty sampling instances, the Luenberger observer is in closed-loop and is updated with process measurements until the observer converges and the true values of states are obtained. Subsequently, the observer is turned off and model predictions are started with the obtained states from the observer. The inputs to the process are fed to the identified model and the quality variables are computed. Figure 5 shows that the identified model can predict the quality variables with decent precision.

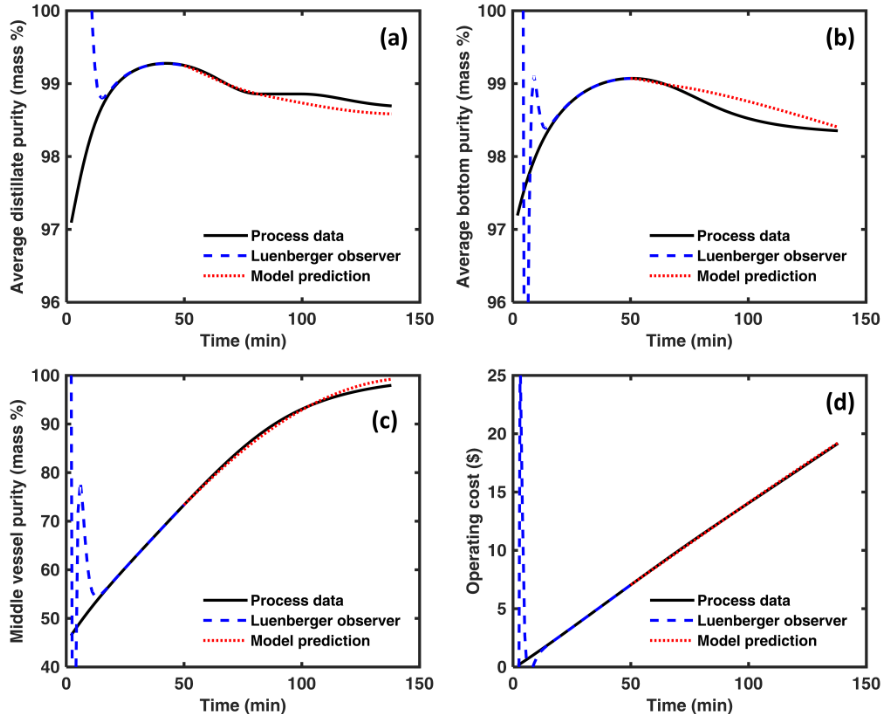

Figure 5- Comparison of the process quality variables measurements with the corresponding model predictions.

4.6.2 Case 1: Cost improvement

The emphasis of this case study is to explore the possibility of improving semicontinuous economics by implementing the MPC on the process. The goal here is to reduce the operating costs of the system while maintaining all product purities. To apply the MPC to the process, first the desired values of the quality variables that are required to be achieved by the end of the processing mode should be set.

It should be noted that it takes a couple of cycles before the semicontinuous process converges to stabilized cycles. Therefore, in this work, the first ten cycles of the process with PI control are discarded and the nominal PI trajectories are considered from the eleventh cycle. The time-average purities of the distillate and bottom streams by the end of the processing mode of the eleventh cycle are 98.6 and 98.8 mass%, respectively. These are selected as the desired final quality variable values. The other quality variable is the middle vessel purity and its desired final value is set to be 98 mass%. Finally, the last quality variable is the operating cost of the process. The terminal value of this variable is not known beforehand and it is desired to be minimized. Therefore, any small value can be selected for it. In this work, it is set to be 80% of the operating cost of the process with PI control configuration.

The tuning parameters of the MPC, namely the ***M*** and ***P*** matrices, are tuned manually to obtain the best performance of the process. The chosen values for the diagonal elements of the ***M*** matrix are presented in Table 3. The values in this Table are the weights on the purity of the middle vessel (m_1), the average purities of the distillate (m_2) and bottom (m_3) streams and the operating cost (m_4). In regards with the ***P*** matrix, the penalty values of 100 are considered for the distillate and bottom setpoints moves and 10 for the rest of the input moves.

Table 3–Tuning parameters of the MPC for case 1.

m_1	m_2	m_3	m_4
50	50	50	1000

Figure 6 shows the PI controllers' setpoints during five full cycles of the semicontinuous system with PI-only and cascaded MPC control. During the discharge and recharge of the middle vessel the inputs are set back to the nominal values. Subsequently, the nominal inputs are implemented to the system until the observer converges (about 20 sampling times). After the convergence of the observer, the model predictions are started and the MPC is turned on.

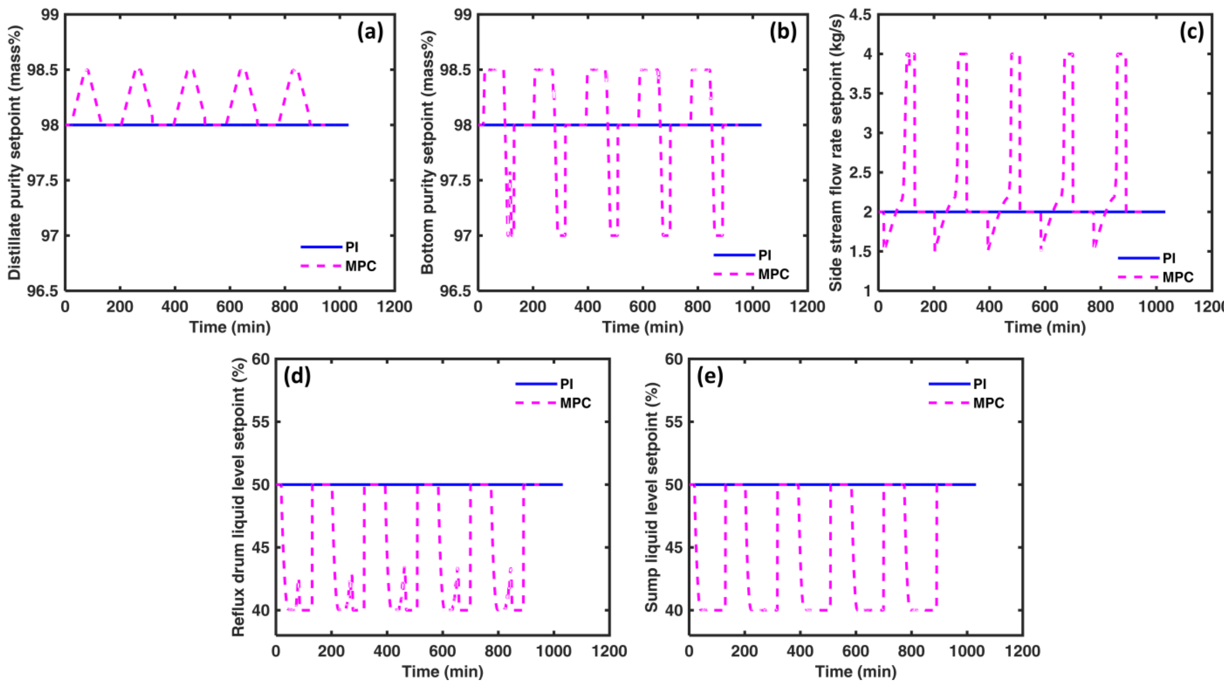

Figure 6- The PI controllers' setpoints in the PI-only and cascaded MPC control over the course of five cycles.

The quality variables are shown in Figure 7. For the closed-loop system under the PI controller alone, higher product purities (than the setpoints) are observed during the cycles (Figure 7a and 7b) which result in unnecessarily higher operating costs. This is a result of the underlying PI composition controllers being unable to regulate to the setpoint (see Figure 11b and 12b), which in turn results in taking more cycles before stable cycles are established. The cycles will eventually stabilize if no disturbances are considered to the system. Figure 7 shows the cycles from the 11th until the 15th cycles. The MPC is implemented starting in cycle 11, which is time zero in this work.

Figure 7a, 7b and 7c show the average purities of the distillate and bottom streams and middle vessel purity, respectively. The MPC has obtained the desired product purities for these quality variables by the end of the processing modes. It has also stabilized the cycles and has cancelled the effect of the PI controllers that tend to increase the purities in each cycle. This is promising that the MPC can compensate the deficiencies of the imperfect tuning parameters of the PI controllers to some extent.

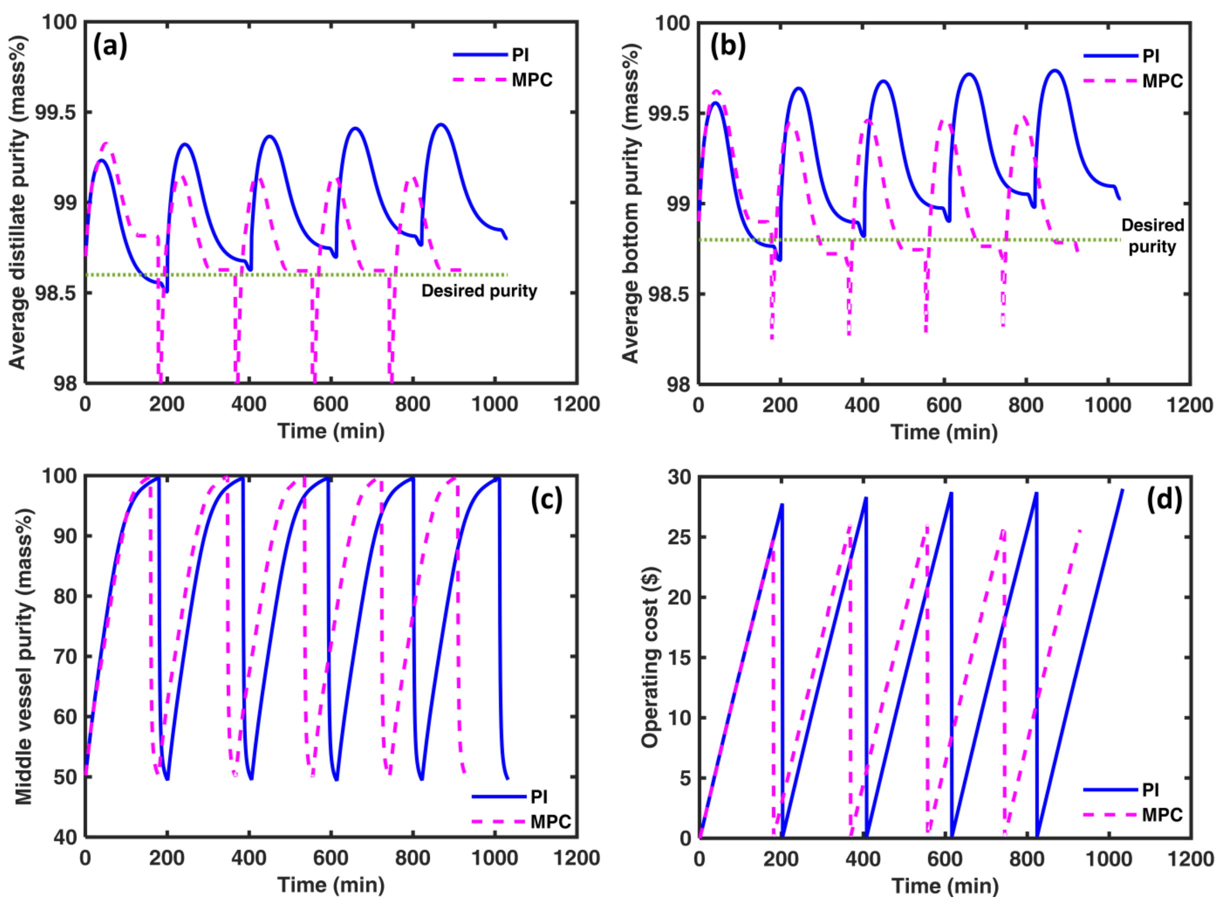

Figure 7- Variation of quality variables during five cycles.

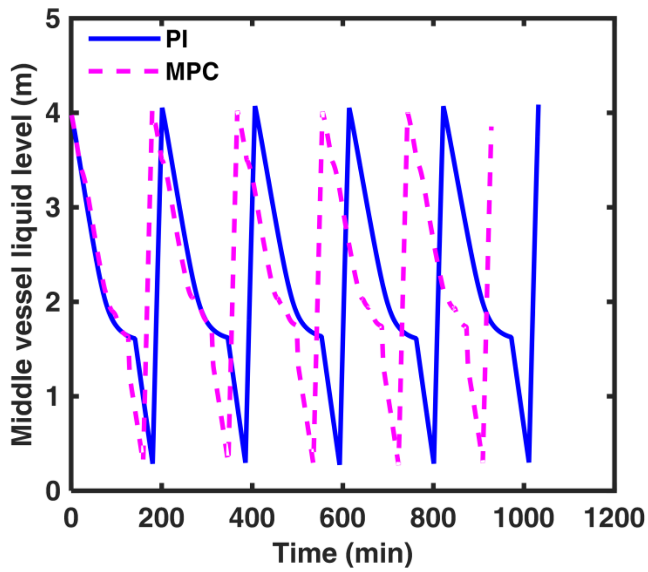

Figure 8- Liquid level in the middle vessel during semicontinuous cycles.

Figure 7c shows the middle vessel purity and it illustrates that the MPC cycles are 10% shorter than the multi-PI control configuration. The liquid level profile in the middle vessel during the cycles is shown in Figure 8. Finally, the operating cost of the process is shown in Figure 7d. The MPC has reduced the cost by 11.7% per cycle. This cost improvement is slightly due to avoiding the over purification of the products in each cycle and mainly due to a better operational policy that the MPC has computed for the semicontinuous process. Figure 7d shows that the operating cost is essentially a linear function of time. Therefore, the MPC has reduced the cost by changing the operation of the process such that the separation can be achieved in a shorter cycle time.

The major improvement in the operation of the system achieved by the MPC is by changing the side stream flow rate profile during the processing mode of the system. Two main policies for controlling the side stream flow rate have been utilized in previous studies for semicontinuous processes. The first policy is to maintain a constant side stream flow rate by having a flow controller on the stream with a fixed setpoint. This was found to be the most economic for the system and therefore used in this study. The second policy is the ideal side draw control strategy [21]. In ideal side draw control the flow rate set point of the side stream is adjusted by a cascade control which continually updates the set point to be equal to the amount of intermediate component entering the column via the middle vessel. With this control policy the side stream flow rate usually increases during the processing mode and hits a plateau by the end of that mode.

However, the MPC has found a better policy for side stream control which shortens the process' cycle time. To explain the new policy, Figure 9 zooms in to the first full cycle of the semicontinuous process. The nominal PI and the MPC trajectories are shown to illustrate how the MPC has changed the operation of the system. The cycle starts from the processing mode and the vertical lines show the beginning of the charging and the discharging modes of the process for the MPC trajectories. Since the MPC cycles are 10% shorter than the PI control configuration, the charging and discharging times are not at the same times for these two control configurations.

As shown in Figure 9a, at the beginning of the processing mode, the purity of the intermediate component (toluene) in the side stream is lower than its specification (98 mass %). During this period the MPC reduces the flow controller setpoint (Figure 9b) to withdraw less liquid from the column (Figure 9c). As this purity reaches the desired specification (around minute 90), the setpoint of the side stream flow controller is increased sharply and put on its upper bound (Figure 9b). Consequently, the side stream flow rate is increased rapidly to its maximum flow rate (Figure 9c).

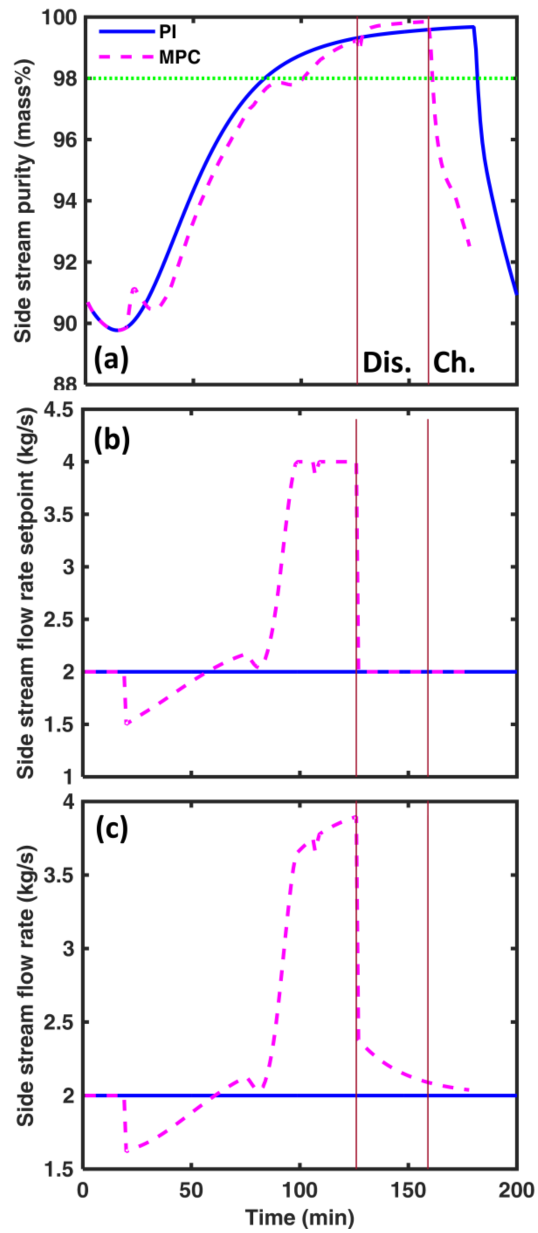

Figure 9- (a) Side stream purity, (b) controller setpoint, and (c) flow rate. The vertical lines corespond to the beginning of the discharging (Dis.) and charging (Ch.) modes of the process in the MPC configuration only.

Recycling the side stream which is pure to the desired purity back to the middle vessel at the highest rate and feeding the tanks hold up at a higher rate back to the column has resulted in shortening the cycle time. Figure 9a shows that after the side stream purity has reached the desired specification, the profile has a higher slope with the MPC control than with PI control.

At the beginning of the discharging mode the setpoint is brought back to the nominal value (Figure 9b). Figure 9c shows that the PI flow controller is fast enough to bring back the side flow rate to the nominal value without any oscillation by the end of the cycle. This is why faster PI controllers are more desirable in the MPC implementation. Another advantage of the MPC control policy is that by the end of the cycle, the purity of the side stream is higher than its corresponding value in the PI control system which results in a shorter subsequent cycle time.

It is interesting to mention that the side stream flow rate profile that the MPC has computed is similar to the semicontinuous without middle vessel (SwoMV) configuration suggested by Meidanshahi and Adams [22]. The authors suggested that the semicontinuous process can achieve the same separation without the necessity of the middle vessel with lower operational and direct costs. In the SwoMV configuration, there is no side stream withdrawal until the purity of the stream reaches above the desired specification. The MPC results show similar trend for the side stream flow rate.

Figure 10 shows the setpoint, the measurement and the manipulated variable of the reflux drum liquid level controller. In PI control configuration, the setpoint is set at 50% to keep the reflux drum level half full during the cycle. As the distillate flow rate decreases during the cycle (Figure 11c), the liquid level goes up in the reflux drum (Figure 10b). Therefore, the PI controller reduces the feed flow rate to the column (10c). Consequently the column is not working at its maximum capacity by the end of the cycle. However, MPC has fixed this drawback. In the MPC configuration, the reflux drum level setpoint is decreased and is set it to the lower bound during the processing mode (Figure 10a).

Initially, the reflux level jumps up since the distillate flow rate is increasing in that period (Figure 11c) which results in a dip in the feed flow rate to the column at about minute 20 (Figure 10c). However, as the distillate flow rate decreases during the cycle, the level goes down to the specified setpoint and therefore by the end of cycle the MPC can increase the feed flow rate to the column (Figure 10c). This increase in the feed flow rate occurs at about the same time as the MPC has increased the side stream flow rate to the column. These two synchronized effects result in shorter cycle time and lower operating cost.

Due to the decrease in the feed flow rate to the column at the beginning of the MPC cycle, the distillate stream purity has increased slightly (Figure 11b) and therefore the distillate flow rate is increased slightly during the processing mode (figure 11c). However, although loose tuning parameters are chosen for the distillate composition controller, changes in the setpoint resulted in distillate flow rate oscillations. Especially, just before the beginning of the discharge mode, there is a short pick in distillate flow rate which is just at the same time that the feed flow rate to the column is at its maximum flow rate. This resulted in significant drop in the purity of the distillate stream during the discharging mode in the MPC configuration (Figure 11b), noting though that the distillate flow rate during this time is nearly zero and so the net effect on cumulative product quality is small. The MPC has tried to slightly increase the distillate composition controller setpoint to compensate for the purity drop in the discharging mode. The same behaviour is also observed in the bottoms composition controller as shown in Figure 12.

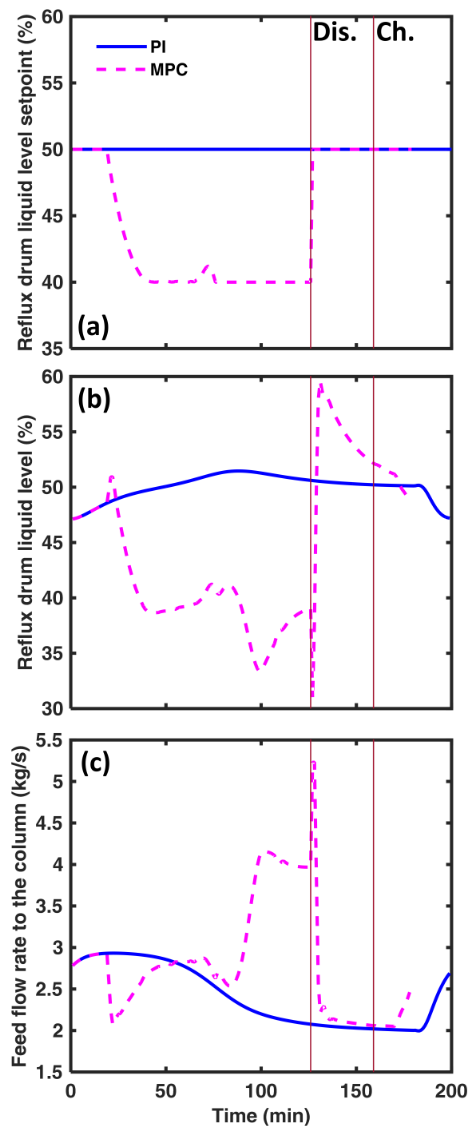

Figure 10- (a) Reflux drum's level controller setpoint, (b) level measurement, and (c) the manipulated variable (feed flow rate to the column).

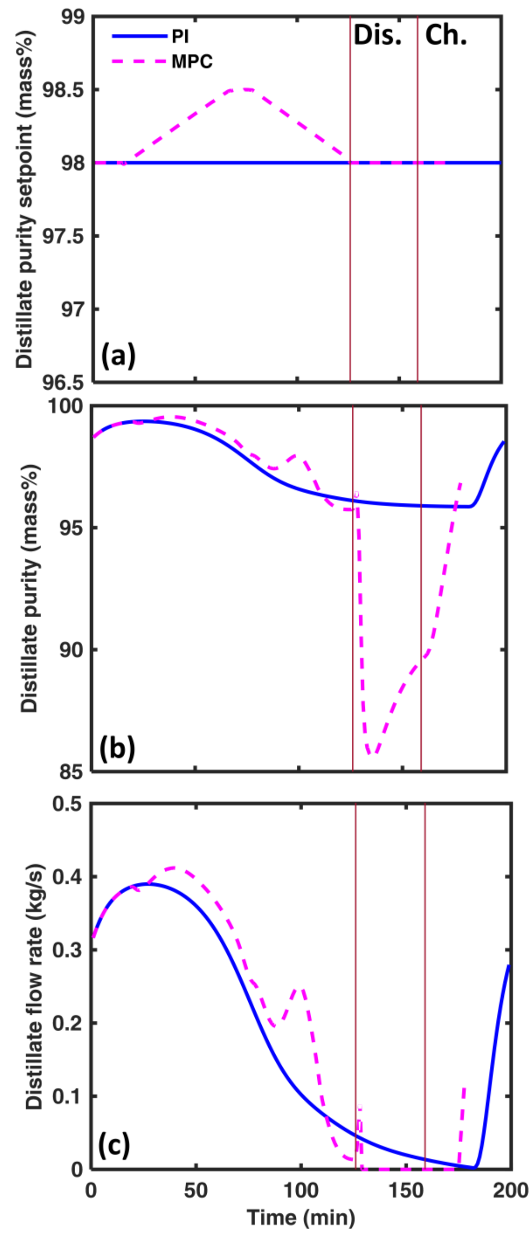

Figure 11- (a) Distillate composition controller's setpoint, (b) measurement and (c) manipulated variable.

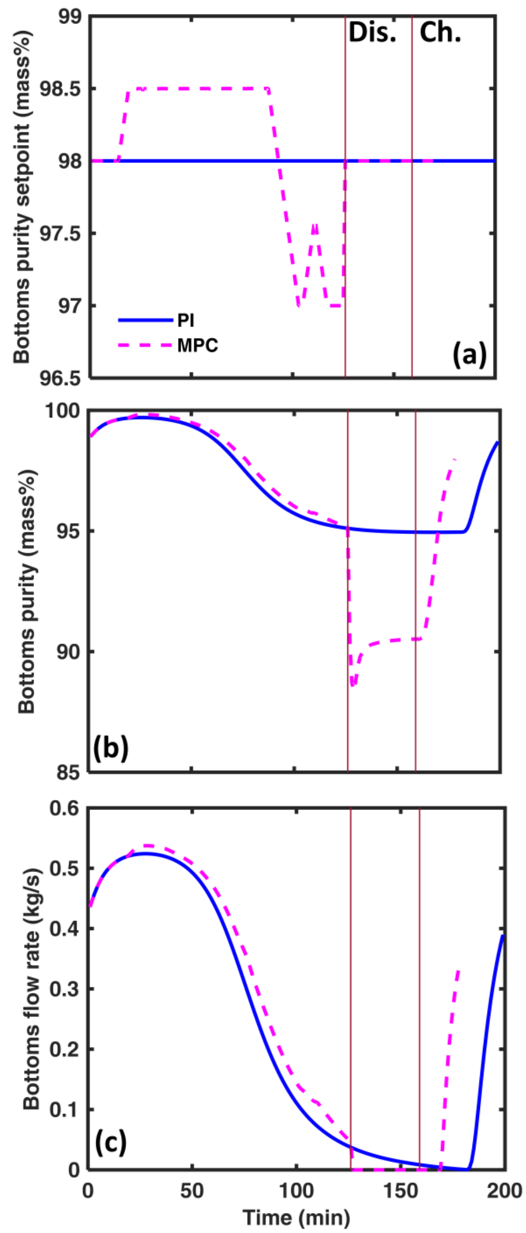

Figure 12- (a) Bottoms composition controller's setpoint, (b) measurement and (c) manipulated variable.

The changes in the sump's level are shown in Figure 13. The setpoint is decreased to the lower bound. It is interesting to notice that this PI controller has a rather quick response to setpoint changes and the process variable follows the setpoint tightly. However, this fast response has resulted in a sharp increase in the reboiler heat duty at the beginning of the discharging mode as the liquid level is brought back very fast to its nominal value.

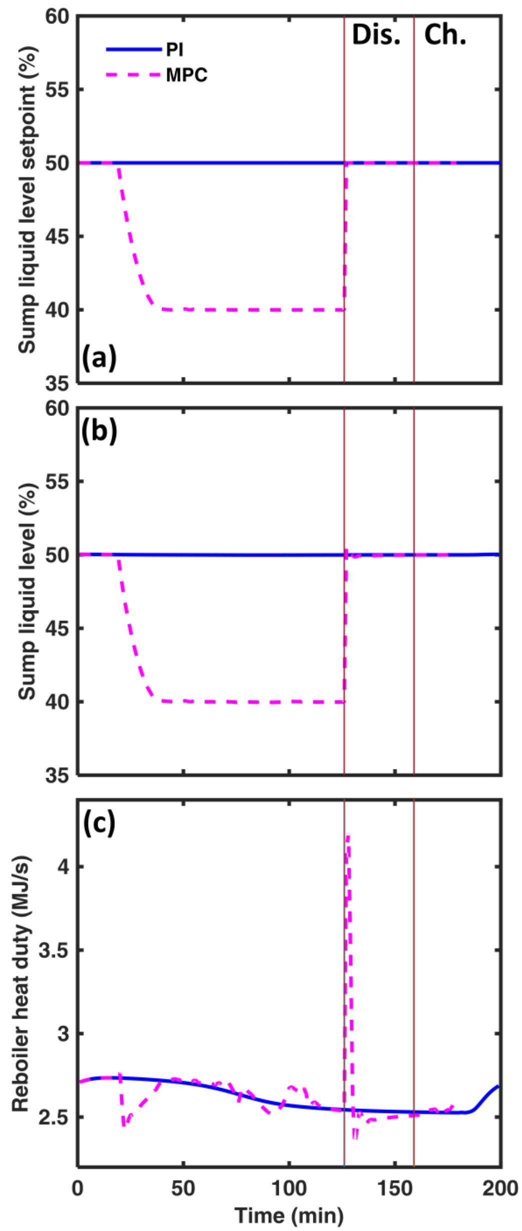

Figure 13- (a) Sump liquid level controller's setpoint, (b) measurement and (c) manipulated variable.

It is important to note that the distillation model assumes that the reboiler system hardware is actually capable of delivering a rapid but brief spike of this magnitude. If this were not obtainable in reality, the system would take longer for the sump liquid level to return to 50% full but the general trends would be the same.

The manipulated variables of the PI controllers which are the distillate, bottoms, feed and side stream flow rates are plotted in Figure 14 during the five cycles of the semicontinuous system under the two control strategy studied in this work. Figure 14a and 14b show that has the MPC has stabilized the cycles faster. Where in the PI control configuration the distillate and bottoms flow rates are gradually shrinking, these profiles look more stable with the MPC control.

Finally, in order to ensure that the process is safe and stable, operational constraints are considered in the MPC. These constraints are shown in Figure 15. Figure 15a and 15b shows the liquid levels in the reflux drum and sump, respectively. These figures show that the levels are kept in the desired ranges (10-90% of the vessel heights) during the cycles. Figure 15c and 15d show the vapour velocities at top (tray number 5) and bottom (tray number 20) of the column, respectively. The vapour velocities are kept in between the limits to avoid weeping and flooding of the column throughout the cycles. The spikes at the end of the processing modes in the vapour velocity profiles are due to the sharp increase in the reboiler heat duties and consequently increased vapour flow rate in the column. However, the vapour velocities are still slightly below the maximum allowable velocity.

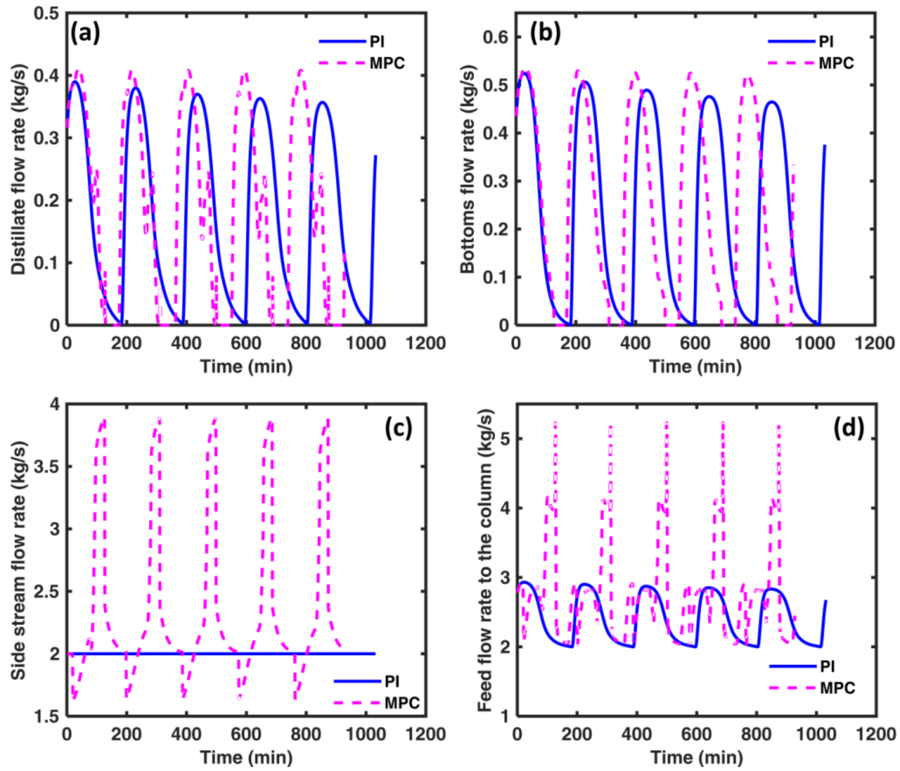

Figure 14- Manipulated variables of the PI controllers during the five cycles of multi-PI and cascaded MPC with PI control configurations.

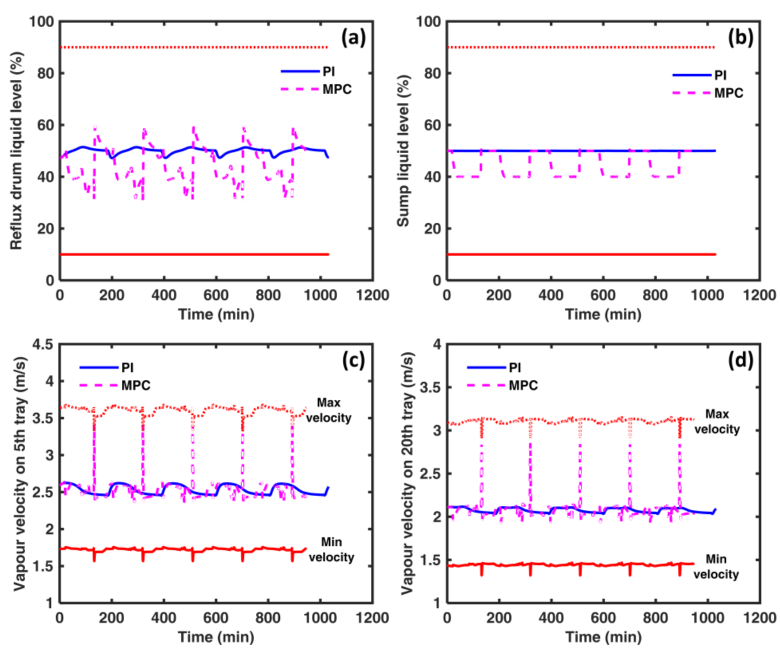

Figure 15- Operational constraints on the process.

For the last remark, it should be noted that MPC calculation time at each sampling instant is fairly shorter than the sampling time of the process. This ensures the applicability of the method to the process. One advantage of the SQMPC method is its fast computational time at each sampling instance. The optimization problem is formulated as a convex, quadratic programming problem which can be solved fast while guaranteeing optimality of the solutions. The SQMPC computational time at each sampling instance took on average 0.6549 seconds in this study (with minimum calculation time of 0.0296 seconds and maximum 11.34 seconds, on a 3.4 GHz, Intel, Core i7, 64-bit machine). This computational time is smaller than the sampling time of the process which was 60 seconds and ensures applicability of the method on the process.

4.6.3 Case 2: Change in the initial feed composition

In this case the performance of the MPC with change in the initial feed composition is studied. The linear model and all parameters are kept constant except the M matrix. In this case heavier penalties are considered for the average distillate and bottoms purities as shown in Table 4. In this case, from the second cycle of the semicontinuous process, the mass fraction of the intermediate component is increased by 10%. The responses of the PI and the cascaded MPC control configurations are examined.

Table 4– Tuning parameters of the MPC for case 2.

m_1	m_2	m_3	m_4
50	5000	5000	1000

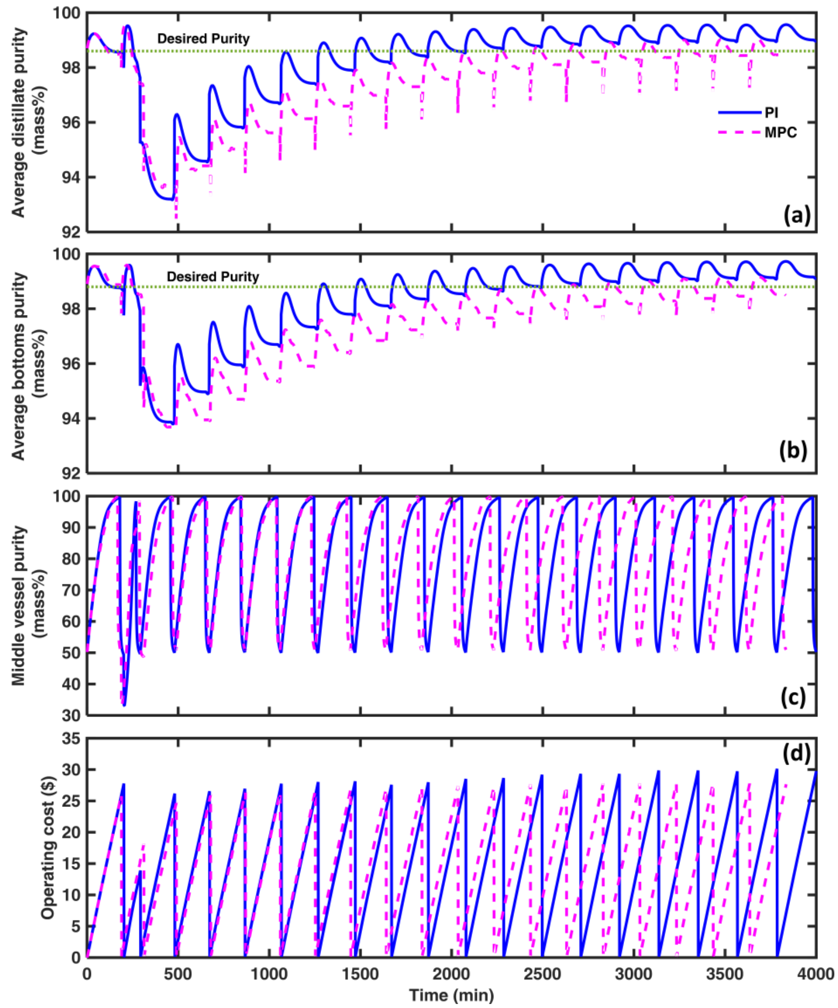

Figure 16- Quality variables profiles for twenty cycles with the feed disturbance condition.

The quality variable profiles are shown in Figure 16. The behaviour of the MPC in handling the change is similar to the PI control. However, the MPC has brought all the product purities close to the desired specifications while having a shorter cycle times and consequently 8.17% lower operational cost per cycle compared to the PI configuration. The corresponding inputs to the system are shown in Figure 17. The MPC input profiles follow the same trend as the previous case study. The importance of this case study is to show that the MPC can handle step changes in the feed stock conditions of the process even without an updated model.

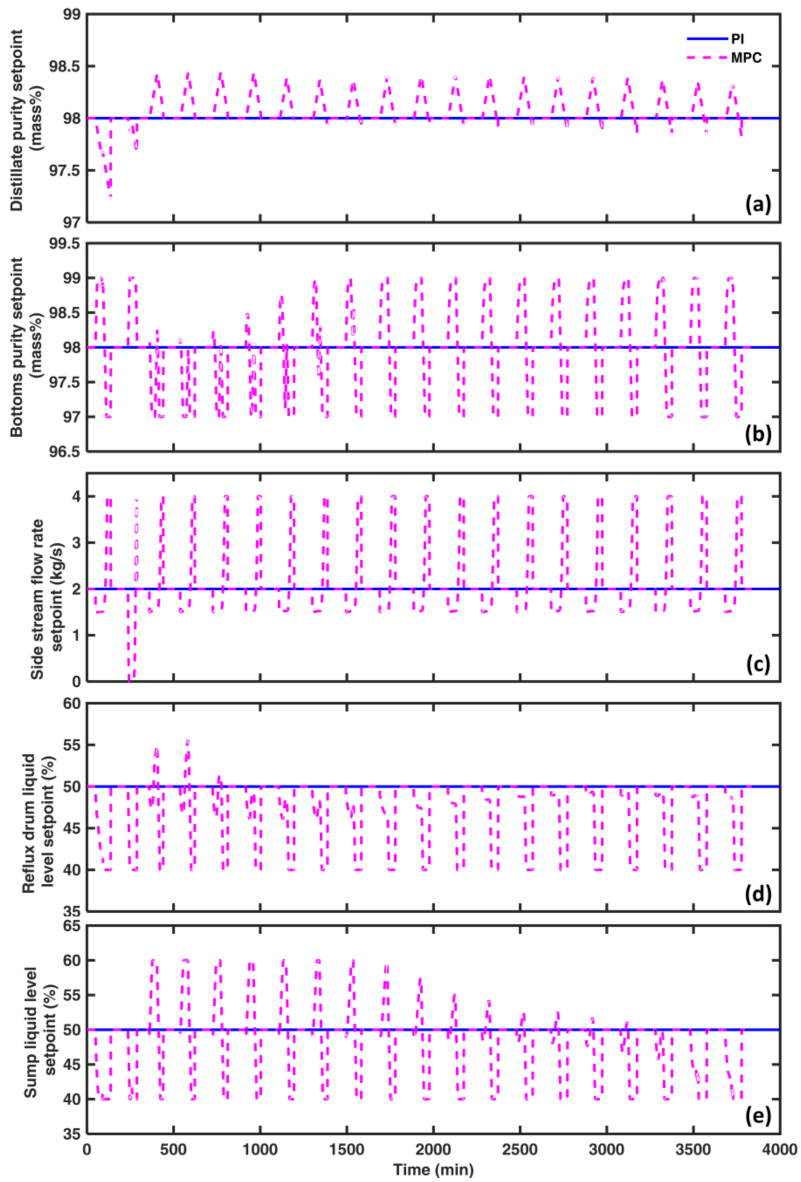

Figure 17- PI setpoints for the studied control configurations with 10% change in the feed stock composition implemented to the process from the second cycle.

4.7 Conclusion

In this study the implementation of the MPC on a semicontinuous system is studied for the first time. The objective of the MPC is to reduce the operational costs of the process while maintaining all product purities. Direct and cascaded MPC configurations are studied and it is concluded that the cascaded MPC with PI control loops is a better configuration for the semicontinuous process. Subsequently, the subspace identification method is adopted to identify a linear, state-space model of the process. It is shown that the model can predict the dynamics of the process sufficiently well for control purposes. Finally, a shrinking horizon SQMPC method is devised to compute the inputs to the process which are the setpoints of the PI controllers. The MPC results show up to 11.7% reduction in the operational cost of the process per cycle. This improvement is the result of 10% reduction in the cycle time of the semicontinuous process with the MPC strategy. Higher cost improvements could potentially be obtained with optimum tuning parameters of the MPC.

In multi-PI control configuration, the distillate and bottoms flow rates decrease during the cycle as the concentrations of light and heavy boiling point components decrease in the middle vessel. Subsequently, the feed flow rate to the column is decreased. Meanwhile, the side stream flow rate is either kept constant or is increased or decreased (depending on the design of the system) during the cycle until the flow rate hits the plateau by the end of the cycle. However, the MPC has changed this operational policy and found a shorter path to purify the mixture.

In the cascaded MPC with multi-PI configuration, the feed and the side stream flow rates are decreased at the beginning of the processing mode. This will reduce recycling at the beginning of the processing mode and will lessen the mixing of the purified side stream with the un-purified middle vessel holdup. Subsequently, as the purity of the side stream reaches the desired specification, the feed flow rate to the column and the side stream flow rate are increased to accelerate the separation. This operational policy computed with the MPC agrees well with the SwoMV configuration which was already shown more economical than the semicontinuous system for a range of operations.

Furthermore, it was observed that the MPC can dampen the effect of the PI tuning parameters and stabilize the process faster. However, the effect of the PI tuning parameters on the performance of the MPC is the focus of future work. Also, it is suggested that the tuning parameters of the PI controllers are included as inputs in the MPC algorithm so they can be adjusted as the cycle proceeds.

Finally, the performance of the MPC is examined for a case with changes in the feed stock composition. It is observed that MPC can maintain its superior performance compared to the PI control configuration in this case as well.

The inclusion of the charging and discharging modes of operation in the MPC is also the subject of ongoing research. This will probably result in better control and economics for the system because the MPC will not have to reset at the start of each cycle, forcing the inputs to return to their nominal values each cycle and requiring the observer to re-converge each cycle. Instead, the information from previous cycles will be carried forward to better inform future cycles.

4.8 Nomenclature

F	Flow rate, (kg/s)
$\boldsymbol{M}$	Penalty matrix on quality variables
$\boldsymbol{P}$	Penalty matrix on input moves
$\boldsymbol{q}$	Quality variable
$Q_{condenser}$	Condenser heat duty, (kJ/s)
$Q_{reboiler}$	Reboiler heat duty, (kJ/s)
t_f	Final time, (s)
$\boldsymbol{u}$	Input variables
$\boldsymbol{v}$	Candidate input trajectory
V	Vapour velocity, (m/s)
v_1	Cost of condenser heat duty, ($/kJ)
v_2	Cost of reboiler heat duty, ($/kJ)
$\boldsymbol{x}$	State variables
$\tilde{\boldsymbol{x}}$	Subspace states
x_B^{dis}	Purity of benzene in the distillate stream, (mass %)
x_X^{bot}	Purity of *o*-xylene in the bottom stream, (mass %)
$\boldsymbol{y}$	Output variables

Abbreviations

DAE	Differential algebraic equation
MPC	Model predictive control
MVCC	Middle vessel continuous distillation column
PI	Proportional integral
PID	Proportional integral derivative
PML	Process model library
PRBS	Pseudo-random binary sequence
SQMPC	Subspace quality model predictive control

4.9 Chapter 4 references

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Chapter 5

Conclusions and recommendations

Semicontinuous separation is a relatively new process intensification technique for performing ternary separations in one distillation column. Previous studies have shown the applicability of the semicontinuous processes for separation of several chemical mixtures. In this thesis project, the economic improvement of the semicontinuous process is targeted by proposing better design, optimum design parameters and more efficient control system for the process. The obtained results can be summarized as follows.

5.1 Design

In the first part of this thesis project the performance of semicontinuous systems has improved by proposing a novel process intensification technique called semicontinuous without middle vessel (SwoMV). The SwoMV configuration does not require a middle vessel, and it also does not have any charging and discharging modes of operation. Therefore, the proposed process can save on capital and instalment costs. Consequently, the SwoMV configuration reduces the total direct costs of the system and also it facilitates the retrofit of available distillation columns for ternary separations.

Furthermore, the proposed configuration reduces the operating cost of the conventional semicontinuous process for a range of feed compositions and extends the economically optimal range of production. The separation of BTX is selected as a case study to examine capabilities of the SwoMV configuration. However, the SwoMV concept can be extended for any non-azeotropic ternary mixture with sufficiently different relative volatilities. In this work, a semicontinuous system is designed for the BTX mixture and the column structure and the proper controller system are designed. An economic analysis is performed and SwoMV process is compared to conventional continuous, conventional semicontinuous and single side stream column systems for three cases of feed compositions applied to a wide range of process scales.

For the range of production rates studied, the results illustrates that the total annualized cost of SwoMV process is generally lower than the other studied configurations. For instance, for purification of intermediate rich feed mixture, the SwoMV has lowered the total direct cost up to 42% and has reduced the operating cost up to 45% which has resulted in up to 43% less total annualized cost relative to the conventional semicontinuous configuration and also has expanded the economical production range of conventional semicontinuous system by 44.5%.

The obtained results show that proposed SwoMV configuration can expand the range of semicontinuous application. Furthermore, the performance of SwoMV is compared with a single side stream distillation column. It is shown that for all studied feed compositions SwoMV has a lower operating and direct costs compared to the side stream column.

Consequently, the novel SwoMV configuration is a suitable ternary separation technique for production of specialty chemicals, where production rates are low. Future studies should focus on application of SwoMV configuration to other processes to demonstrate its performance relative to conventional continuous and semicontinuous systems. Also the MIDO optimization framework and the MPC control system that have been developed in the following chapters should be implemented on the SwoMV configuration to further improve the economics of the process.

5.2 Optimization

In the second part of this thesis project, integration of design and control of semicontinuous processes is studied and a methodology is proposed to design a semicontinuous distillation system for an arbitrary ternary mixture. The proposed methodology is based on a simultaneous design approach which considers the dynamics of the process in the design stage. This is generally more desirable than the previously known sequential design approaches for the semicontinuous process. The proposed method also significantly reduces the required time for designing a close to optimal semicontinuous system.

The mixed integer dynamic optimization (MIDO) is adopted to obtain locally optimum structural and operational parameters of the process. The resulting MIDO problem is then solved by using both the gradient-based outer approximation (OA) method and the gradient-free particle swarm optimization (PSO) methods. It is shown that OA method finds similar solutions to PSO method. The OA method was considerably faster when good initial guesses were provided, but very sensitive to the initial guesses. Many initial guesses resulted in failure of the OA algorithm, and finding good initial guesses a priori for semicontinuous systems in general is very difficult. On the other hand, PSO has higher computational times but it is not that sensitive to initial condition.

Subsequently, the methodology is generalized to a superstructure where no a priori information is available for designing the semicontinuous process. The method uses an excessively large distillation column as an initial guess with possible side draw locations both above and below the feed. It was found that both the PSO and OA methods found very similar solutions using this approach, and those solutions could then be used as the initial guess for a more rigorous optimization approach with either PSO or OA. However, because the OA approach is much faster at both of these stages, it is recommended for use whenever possible. Nevertheless, since both OA and PSO always found similar solutions and neither one consistently found better design than the other, the PSO is recommended for use where OA methods are not available, as is sometimes the case in other commercial simulation software.

For future work, it is suggested that the charging and the discharging modes of operation be included in the simulation and the optimization of the system. The key parameters of those modes are the rates at which the tank is charged or discharged. Generally, faster is better in terms of cycle time, but the costs of this have not previously been considered, so there is some optimal policy which is currently unknown.

5.3 Control

Finally, in the last part of the thesis implementation of the MPC on a semicontinuous system is studied for the first time. The objective of the MPC is to reduce the operational costs of the process while maintaining all product purities. Two configurations are studied. The direct and cascaded MPC configurations are it is shown that the cascaded MPC with PI control loops is a more favourable configuration for the semicontinuous process. The subspace identification method is adopted to identify a linear, state-space model of the process to be used in the MPC. It is shown that the model can predict the dynamics of the process with decent precision. Finally, a shrinking horizon SQMPC method is implemented on the process and the inputs to the process which are the setpoints of the PI controllers are computed. The MPC results show up to 11.7% reduction in the operational cost of the process per cycle. This improvement is the result of 10% reduction in the cycle time of the semicontinuous process with the MPC strategy. Higher cost improvements could potentially be obtained with optimum tuning parameters of the MPC.

The improvement in the economics is due to alteration of the operational policy of the semicontinuous system by the MPC. In the cascaded MPC with multi-PI configuration, the recycling at the beginning of the processing mode is reduced which will result in lessening the mixing of the purified side stream with the un-purified middle vessel holdup. Subsequently, as the purity of the side stream increases and reaches the desired specification, the feed flow rate to the column and the side stream flow rate are increased to accelerate the separation. This operational policy computed with the MPC agrees well with the SwoMV configuration which was already shown more economical than the semicontinuous system for a range of operations.

Furthermore, it was observed that the MPC can stabilize the process faster. However, the effect of the PI tuning parameters on the performance of the MPC is the focus of future work. It is suggested to include tuning parameters of PI controllers as inputs in the MPC algorithm so they can be adjusted as the cycle proceeds.

Finally, feed stock composition change is also studied and performance of the MPC is evaluated for this case as well. It is observed that the MPC can maintain its superior performance compared to the PI control configuration in this case as well.

The inclusion of the charging and discharging modes of operation in the model identification and the MPC is the subject of ongoing research. This will probably result in better control and economics for the semicontinuous process since the MPC will not have to reset at the start of each cycle, forcing the inputs to return to their nominal values each cycle and requiring the observer to re-converge each cycle. Instead, the information from previous cycles will be carried forward to better inform future cycles.

5.4 Final remarks

The contributions of this thesis project and its advancements on the semicontinuous distillation process are summarized in Figure 3. In this figure, the TAC per production rate of a conventional continuous system is shown. A semicontinuous distillation is designed for the same process based on available sequential heuristic design rules in literature. The obtained design parameters are then manually tweaked to get the best design with the lowest TAC. The resulting semicontinuous process has a 14.8% higher TAC per production rate (for an illustrative example) compared to the conventional continuous process as shown in Figure 3 (second bar from the left). The obtained design is then optimized using the proposed MIDO framework in this work. The resulting locally optimum design has 11.5% lower TAC per production rate compared to the conventional continuous process. Finally, the MPC is implemented on the locally optimum semicontinuous process and the cost of the process has reduced by 34.2% compared to the conventional continuous process.

Therefore, this figure shows the effectiveness of the methods developed for and implemented on the semicontinuous process in this thesis. Lower operating cost and consequently TAC are obtained for the semicontinuous distillation process which was the main objectives in this thesis project.

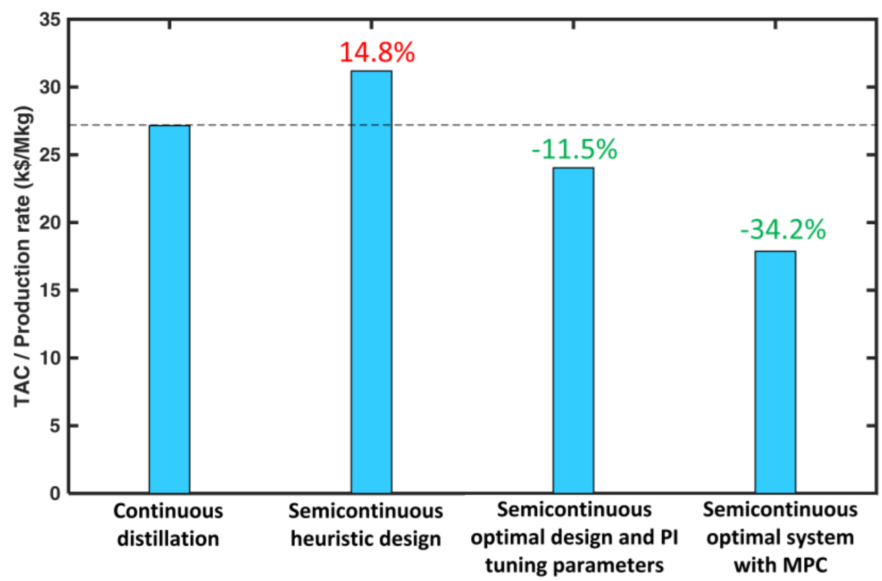

Figure 3- Summery of the contributions of this thesis project on the semicontinuous distillation process.

The End.