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Subspace model identification and model predictive control based cost analysis of a semicontinuous distillation process

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ABSTRACT

Semicontinuous distillation is a process intensification technique for purification of multicomponent mixtures. 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. In this study, for the first time, a model predictive control (MPC) formulation is implemented on a semicontinuous process to evaluate the associated closed-loop cost. 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. A subspace identification method is adopted to identify a linear, state-space model to be used in the MPC. The first-principals model of the process is then simulated in gPROMS. Simulation results demonstrate that the MPC has reduced the operational cost of a semicontinuous process by about 11%.

1. Introduction

Distillation columns are usually major sources of capital and operating costs in chemical processes (Dunnebier and Pantelides, 1999). 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 (Jana, 2010) and those that consider dividing wall columns that can potentially reduce the capital and operating costs of multicomponent separation (Yildirim et al., 2011). 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 (Adams and Pascall, 2012). The semicontinuous process was first proposed by Phimister and Seider (2000) for ternary mixtures. They compared several features of distillation such as the throughput, flexibility, controllability and investment for continuous, batch and semicontinuous processes. A thorough review of the semicontinuous process can be found in Adams and Pascall (2012) where they compared the performance of semicontinuous process to the conventional continuous configuration for different separations. The semicontinuous process was then extended for n-component mixtures by Wijesekera and Adams (2015a,b).

The essential idea in semicontinuous distillation is to lower the capital costs by purifying n-component mixtures to any desired purities in only one distillation column that is coupled with storage tanks (called middle vessels). Conventionally, n-1 distillation columns are preferred to separate an n-component mixture to any desired purities in a steady-state approach (Fig. 1a). Performing this separation with fewer distillation columns in a steady-state fashion requires taller, more expensive columns with higher operating costs. 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 (Fig. 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

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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
ν	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

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 (Sultana and Kumar, 2012).

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 cost 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.

Pascall and Adams (2013) explored eight PI configurations for the semicontinuous system. 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 (2016) proposed an integrated design and control approach to simultaneously design the structural and operational parameters of the system. 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 the model predictive control (MPC) can likely provide more desirable control for a semicontinuous system. The 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 a dynamic process model for computing the inputs, control of multi-input/multi-output processes and over-arching control objectives are better suited to being achieved via the 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 (2001) studied the MPC control of a binary steady-state distillation column. They compared three control configurations for the system: In the first configuration, the MPC manipulated the reflux and bottoms flow rates to maintain the purities of distillate and bottom streams, respectively, and PI controllers were used for regulatory control of liquid levels in the reflux drum and sump by manipulating the distillate and boil up flow rates, respectively. In the second configuration, the MPC directly controlled all four degrees of freedom of the process 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 performances. In these scenarios, the MPC method could coordinate the input moves for all manipulated variables, whereas in the first configuration the MPC and the 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 setpoints.

The distillate and bottom composition loops in a distillation column usually have high levels of interaction with each other. Barolo and Papini (2000) suggested that the presence of a middle vessel can reduce this interaction and improve the performance of the column. 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.