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Research Article

Control of a reactive distillation column for methyl acetate system using Aspen Plus

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Abstract
Serious control related problems are encountered in a reactive distillation column due to its very complex process dynamics. In this paper ASPEN PLUS simulation software has been used to control a reactive distillation column for maintaining the product purity at the desired level. System nonlinearity and interactions make direct control of product purity for the high-purity design quite difficult. Introduction of tray temperature control helps in preventing the nonlinearity problem. ASPEN PLUS dynamics extends Aspen Plus steady-state models into dynamic process models, enabling design and verification of process control schemes. A tight and robust control scheme with two levels and one each of pressure, temperature, flow, composition and reflux controllers have been used to maintain the product purity at the desired levels and safely operate the plant at the desired operating conditions.

Keywords
Reactive distillation, Methyl acetate, Control ASPEN PLUS dynamics.

1.Introduction
Reactive distillation is the combination of both separation and reaction in one unit [1-4]. It has been used in a small number of industrial applications for many years, but the last two decades has shown an increase in both research and applications. Distillation is the most desirable process for the separation of multi-component liquid mixture [4]. Combining reaction with distillation as is done in reactive distillation offers significant economic benefits, especially for reversible reactions. Steady-state design and open loop dynamics have been discussed in a large number of research articles. Whereas, only a small number of papers discuss the closed loop control of reactive distillation columns or the interaction between design and control [1].

Process flow sheet and the type of reactions occurring in the column influences the appropriate control structure to be incorporated. Process nonlinearity, complex interactions between vapour-liquid equilibrium and chemical kinetics makes control of a reactive distillation column very difficult.

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The first step in designing a decentralized control system is to choose the set of controlled and corresponding manipulated variables, i.e. the control structure.

The appropriate control structure for a system depends on the flow sheet and on the type of reactions occurring in the column.

2.Steady state design in ASPEN PLUS
The reaction considered in this work is the esterification reaction of methanol and acetic acid yielding methyl acetate and water.

$$CH_3COOH + CH_3OH \leftrightarrow CH_3COOCH_3 + H_2O$$

First of all, ASPEN PLUS steady state file is prepared which is then converted to dynamic mode for implementation of the closed loop control scheme.

RADFRAC (B1 block) model is selected from ASPEN PLUS model library. Selection of feed stage is an important factor for product purity [Dohare et al, 2011][5].Stage location is fixed by performing sensitivity analysis on ASPEN PLUS. The B1 block, as shown in *Figure 1* has 39 stages with stage 1 being the condenser, stages 2-3 being the rectification section, followed by the reactive section with stages 4-37, the stripping section consisting of stage number 38, with stage 39 being the reboiler. Pure Acetic Acid and Methanol, each with flow rates of 50 kmol/hr (0.013889 kmol/sec) and temperature 25°C are fed to stages 4 and 37 respectively of the B1 block.UNIQUAC is selected as the base method for our system. A reflux ratio of 1.5 and a condenser pressure of 1 atm are used with the stage pressure drop being equal to 0.01 atm. B6 and B7 pumps, each with a discharge pressure of 11 atm releases the streams to valves B2 and B3 each with a discharge pressure of 10.8 atm.

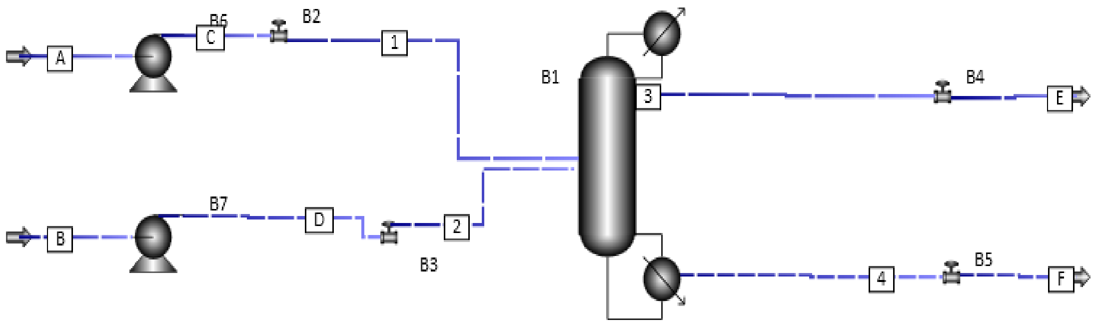

Figure 1 Flowsheet for the process

As can be seen from *Figure 2*, a very high purity (mole fraction = 0.985) of methyl acetate is obtained from the distillate stream and a water mole fraction of 0.976 is obtained from the bottoms stream.

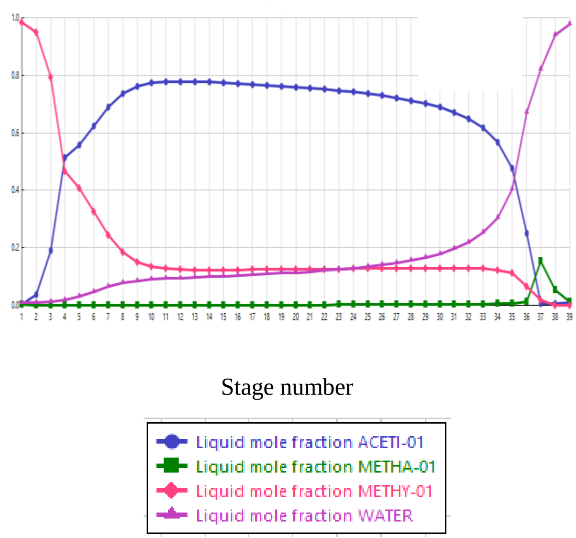

Figure 2 Stage wise composition profile for all components

This steady state file is then converted to ASPEN Dynamics file. A detailed mathematical dynamic model of reactive batch distillation column is formulated for methyl acetate synthesis and presented in terms of differential and algebraic equations (DAEs) [Patel et al., 2007][2]. These DAEs are solved by the in-built ASPEN algorithm to obtain the detailed column dynamics.

3.Control scheme

Seven controllers, with two levels and one each of pressure, temperature, flow, composition and reflux controllers are used. *Figure 3* shows the control structure in which only one composition is controlled (the column internal composition).We have used the B9 controller for this purpose. A dead time of 0.1 min has been added before the controller.

A controller gain of 1.5625 and an integral time of 11 min has been used for proper controller functioning. Flow controller, B8 has been used to maintain the acetic acid flow at the desired level. Temperature in the stripping section is controlled by manipulating the reboiler heat duty using B11 controller as shown in *Figure 3*.

A controller gain of 3 and a rest time equal to 3 min has been used in this controller. This temperature controller maintains bottoms purity at or above its specified value by keeping light components from dropping out the bottom with the heavy product component. The set point of the temperature controller must be set high enough to make sure the bottoms purity is at or above its specification value under worst-case conditions. A reflux ratio control scheme (B12 controller) is used, wherein a controller gain 1.5625 and reset time of 11 min is used and it is manipulated with the flowrate of the distillate stream. The reflux ratio is set high enough to maintain desired distillate purity under worst case condition. Two level controllers, B1Drum LC and B1 Sump LC, each with controller gain equal to 2 and integral time equal to 9999 min has been implemented. Since, a level controller does not require a very tight control; this high value of integral time will nullify the integral action of these two controllers. A pressure controller (B1CondPC) is used to maintain the top pressure of the column at the desired level by manipulating the condenser duty. Relay feedback test has been used to find out the ultimate gain and reset time for the controllers used, which is then implemented in Tyreus-Luyben tuning method to find the suitable gain and integral time for the different controllers.

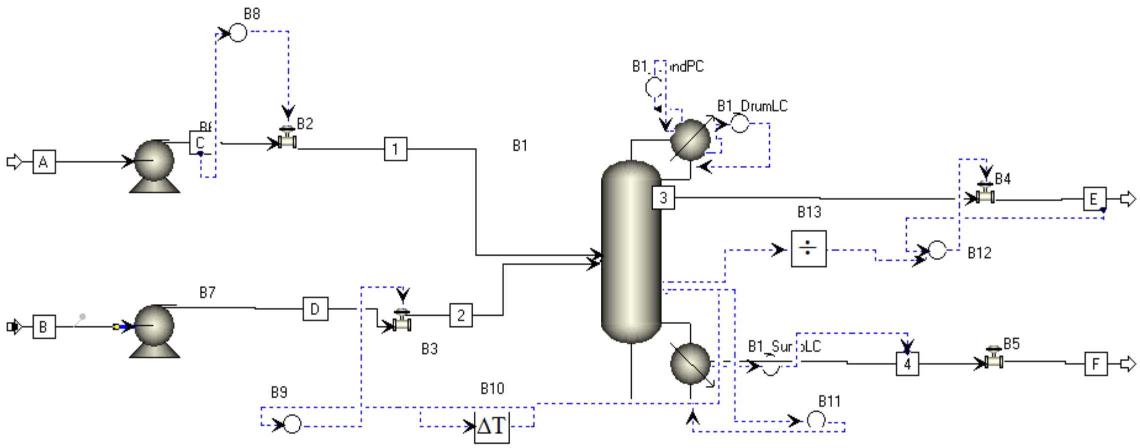

Figure 3 Control structure for methyl acetate system

4.Results and discussion

The response of the closed loop control structure due to set point disturbances is shown in *Figure 4* below.

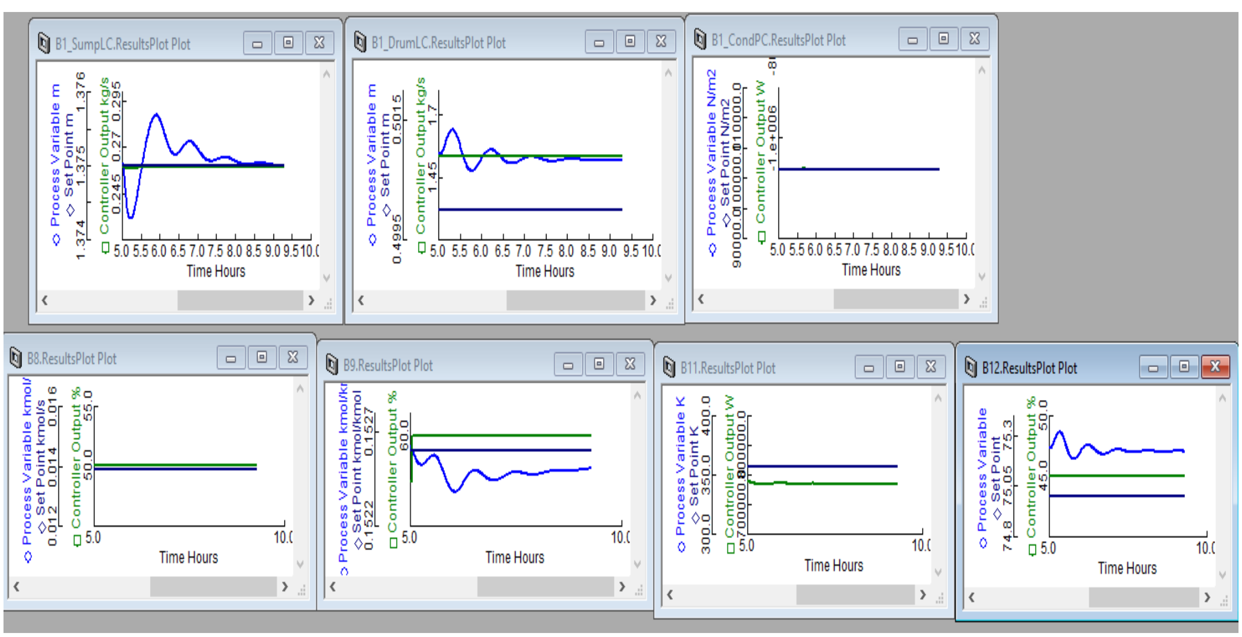

Figure 4 Response of different controllers after a set point change in input methanol feed stream temperature (298.15+3) ˚C at 5.01 hrs

We have considered regulatory problem with changes in temperature in the methanol feed stream. Firstly, a disturbance in feed temperature is introduced in the methanol feed stream at time = 5.01 hrs. The response of the different controllers due to a 3°C increase in temperature is monitored. The control system implemented is seen to neutralise the disturbance after a certain time. As we don't require a very tight control for the level controllers, it may be allowed to operate within the limits as shown in the figure. B8, B9 and B1 Condenser pressure controllers are seen to effectively counterbalance the disturbance.

Next, a disturbance in feed temperature is introduced in the methanol feed stream at time = 3.07 hrs. The response of the different controllers due to a 3°C decrease in temperature is monitored. The control system incorporated neutralises this disturbance and makes the system stable as can visualised from *Figure 5* below.

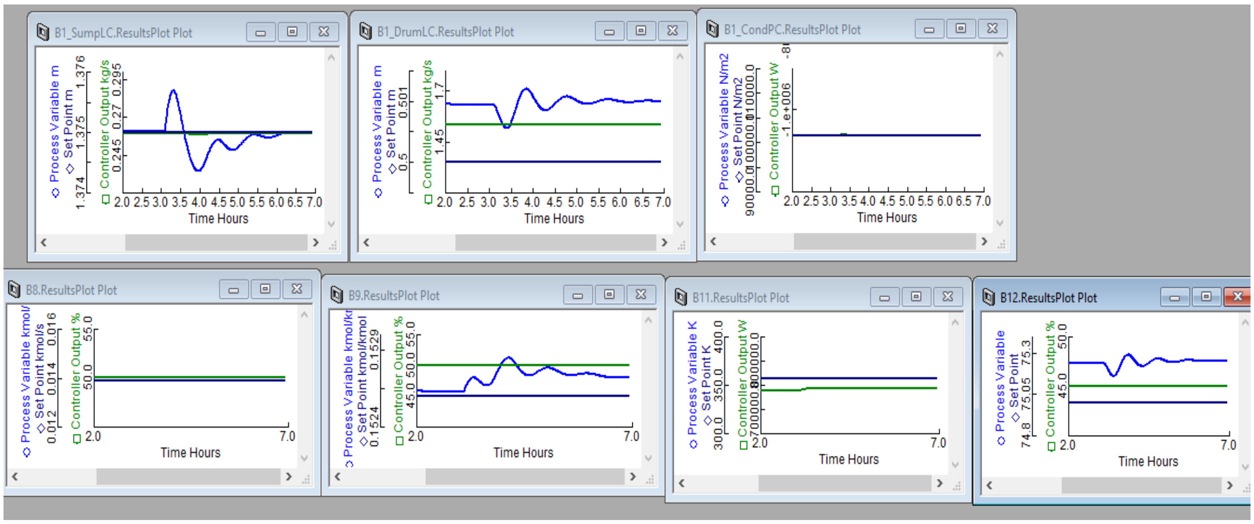

Figure 5 Response of different controllers after a set point change in input methanol feed stream temperature (298.15-3) ˚C at 3.07 hrs

5.Conclusion

In this paper, we have studied the design and control of a reactive distillation column for methyl acetate system. The control structure implemented provides effective control even for high purity requirement scenario. Interaction within loop can be reduced by controlling an internal composition and one temperature. Controlling an intermediate tray temperature in lieu of product purity diminishes the nonlinearity, even for high-purity purity levels. There is no direct control of product compositions, so the temperature controller set point and the reflux ratio must be set to handle worst-case conditions. The major drawback associated with these linear controllers is that they do not perform well over the wide range of operating conditions and with large disturbances.

Since most industrial processes exhibit severe nonlinearity, the studies on the use of artificial intelligence techniques such as artificial neural network(ANN),support vector machine(SVM) and fuzzy logic have drawn increasing attention in recent years because of their ability to represent nonlinear systems and their self-learning capabilities[Sharma and Singh, 2014][3]. A lot of issues related to control and on-line operation of a reactive distillation process have not been properly addressed. Further study is required in this field by applying different controllers like more advanced model predictive control to reduce the complexity of the system.

Acknowledgment

None.

Conflicts of interest

The authors have no conflicts of interest to declare.

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