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The Dynamic Simulation of The Benzene and Toluene Distillation Process

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A B S T R A C T

Benzene and toluene are products of petroleum catalytic fractionation and dehydrogenation, which are utilized extensively for industrial applications, including manufacturing polymers, textiles, solvents, and fuel additives. The combination of these two substances creates an azeotropic condition. Therefore, separating benzene and toluene from their mixture necessitates a significant amount of energy and expense. In this study, dynamic simulation modeling of benzene and toluene separation was performed to determine whether the dynamic method is more efficient than conventional distillation. A dynamic analysis was conducted using Aspen HYSYS with numerous assumptions (Peng-Robinson Fluid Package and Transfer Function Block) and operating state settings, a dynamic analysis was conducted (pressure, flow rate, and vapor fraction). The simulation outcomes were analyzed by contrasting treatments with and without dynamic system configurations (sudden and gradual changes in operational parameters for 30 minutes). The simulation findings indicated that the configuration of the stepwise dynamic system might increase the benzene product concentration by 10% moles. Additionally, dynamic system settings substantially impact the concentration of the bottom product

INTRODUCTION

Toluene, benzene, and xylene are the major constituent products of the chemical industry. Benzene and its derivatives, including toluene, are required for the production of a variety of polymers, textiles, solvents, and fuel additives. Benzene and toluene are typically produced through coal tar fractionation and catalytic dehydrogenation of petroleum [1].

Distillation is a technique for separating mixtures with heavy and light components. At the bottom, the light component is separated. Also, the heavier component is split at the top [2]. Benzene and toluene mixtures are often separated by distillation column. Due to their same physical and chemical characteristics, benzene and toluene formed azeotrope when combined (benzene and toluene have boiling points at atmospheric pressure of 353K and 383.6K, respectively). Normal fractional distillation is an inefficient and energy-intensive method for separating these components. In order to efficiently identify benzene derivatives from toluene, it is important to develop a novel approach [3].

The separation efficiency of benzene-toluene mixtures has been the subject of numerous investigations. Mohapatro et al. [4] used ASPEN Plus to simulate several operating conditions that provided the highest separation efficiency for benzene-toluene mixtures. The study reveals that the production of high-purity benzene might be increased by 1.5 times by consuming 42% more energy [4].

The objective of this study is to investigate the influence of dynamic simulation on separation efficiency. This study simulated dynamic operation using the simplified model. The needed simplified model for transitory process activities is widely recognized. As full-order models, they provide greater computational efficiency [5][6][7]. Optimisation-based control refers to a set of control systems that utilise dynamic plant models to forecast process behaviour and optimize process economic performance while fulfilling operational restrictions. This notion is used in industry by real-time optimization systems that use steady-state models to calculate predictive controller settings for predominantly steady-state continuous processes. The primary control system settings are beneficial [5][8].

METHOD

Aspen HYSYS® process simulation software and the Peng-Robinson Fluid Package were used for the evaluation. The Peng-Robinson formula is represented by Equations 1 and 2[9].

$$P = \frac{RT}{\hat{v}-b} - \frac{a}{\hat{v}(\hat{v}+b)+b(\hat{v}-b)} \quad (1)$$

$$Z^3 - (1-B)Z^2 + (A-2B-3B^2)Z - (AB - B^2 - B^3) = 0 \quad (2)$$

Operating conditions for the feed were P= 3 bar, molar flow = 200 kmol/h, and vapor fraction = 0. To determine the condition and quantity of trays employed in the primary distillation column, the distillation short-cut was required. The acquired parameters are shown in **Figure 1.**

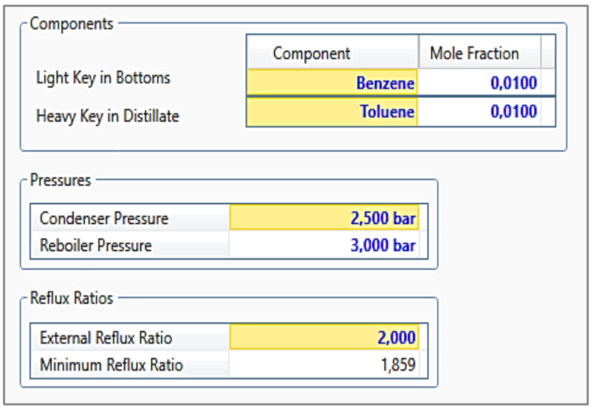

Figure 1. Benzene/ Toluene Distillation Shortcut Parameters

Distillation 1 unit employed a fractionation column equipped with a complete reflux condenser [7]. The distillation shortcut parameters were applied to the distillation model, and the number of trays was changed. Then, adjust the monitor until the distillation column parameters converge. Specifications for the distillation column were listed in **Table 1.**

Table 1. Distillation Column Specifications

Benzene/ Toluene Distillation Column	
Number of Stages	31
Feed Stage	17
Condenser Type	Full Reflux
Pressure Profile	
Condenser Pressure	2,5 Bar
Reboiler Pressure	3 Bar
Condenser Pressure Drop	0,5 Bar
Reboiler Pressure Drop	0,5 Bar
Stream	
Reflux Ratio	±2

The simulation of the process operated in Dynamic Mode, and a Transfer Function Block (TRF) was included to represent changing feed composition. At the Operational Parameters Target, the TRF was linked to the Benzene flow. Changing the value of the PV in Operational Parameters caused dramatic shifts, while Ramp was used for gradual adjustments. The distillation procedure was illustrated in **Figure 2.**

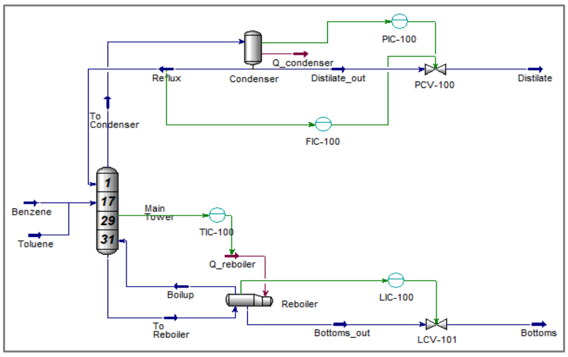

Figure 2. Distillation Process

RESULTS AND DISCUSSION

This simulation was conducted in dynamic mode to analyze the object's development. The condenser and reboiler were configured for Dry Startup. **Figure 3** demonstrated that the condition was nearly constant, with the exception of the bottom flow and liquid percent level-reboiler, due to the uncontrolled operation of the dynamic process. Other variables than bottom flow and liquid percent level-reboiler attained a steady condition after a few minutes of waiting.

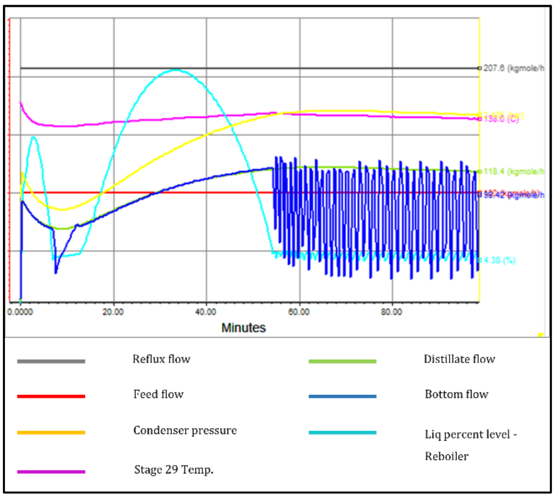

Figure 3. Graphics of the Results of the Dynamics of the Initial Condition to Steady at 0 - 80 Minutes Without Control

As illustrated in **Figure 4**, the bottom flow and liquid percent level-reboiler graphs fluctuated, although the graph alterations tended to be consistent.

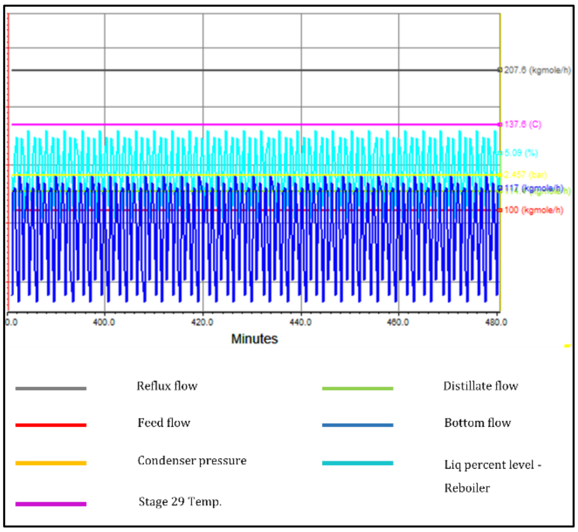

Figure 4. Graphics of the Dynamics of the Steady State Process at 380 - 480 Minutes Without Control

Figures 3 and **Figure 4** demonstrated that the dynamic process lacks control. **Figure 5** illustrates the dynamic process with control. The bottom flow and liquid percent level-reboiler graphs in the figure did not rise and fell like the graphs in **Figures 3** and **4**, but were flat like the graphs for other variables. **Figure 6** illustrated that a dynamic process with control began to approach a steady state after 90 minutes, whereas a process without control reached a steady state around 380 minutes; this phenomenon demonstrated the function of the control system in reducing process disruptions [10].

This control mechanism also influences the energy-use efficiency. The quicker a process reaches steady state, the greater its energy efficiency [11]. Gao et al. [11] determined the energy efficiency of the benzene and toluene separation process under ideal conditions to be 18.47% by simulation. The Liq percent level indicated that the energy efficiency value for this investigation was 4.81%. The value of energy efficiency was reduced due to the dynamic nature of the operating system in this study.

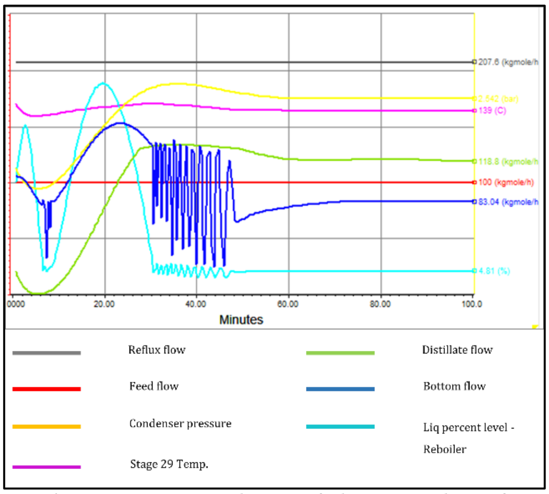

Figure 5. Graphics of the Results of Dynamics Process With Control

In addition, the simulation increased the benzene feed flow rate from 100 kmol/h to 110 kmol/h by utilizing the 'transfer function block' function without a control mechanism. Two strategies were used to make adjustments: abrupt adjustments and 30-minute ramps. This processing method was an example of a situation that frequently arised in industrial practice when searching for the appropriate process control system [12]. The dynamics changes were made at 324 minutes, and the changes can be seen in **Figure 6**.

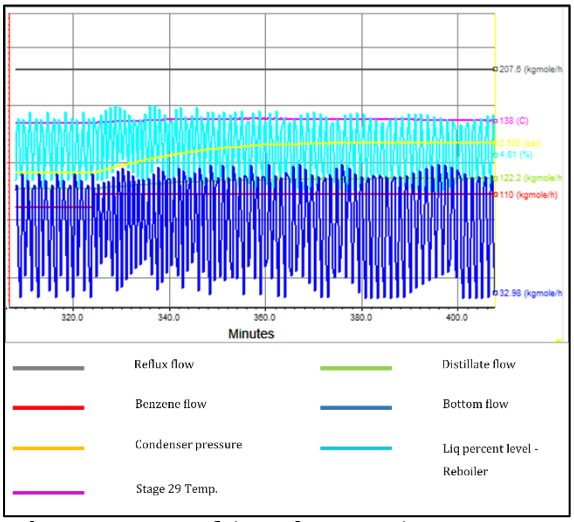

Figure 6. Graphics of Dynamic Response to Changes in the 10%-Mole Benzene Flow Rate Suddenly (Step)

Except for the bottom flow and liquid level reboiler, the other variables in **Figure 6** stay same following the sudden transition. The graph demonstrates that the process control is less effective, leading to an inefficient use of energy [11], which required more time to reach a steady state, as depicted in **Figure 7**.

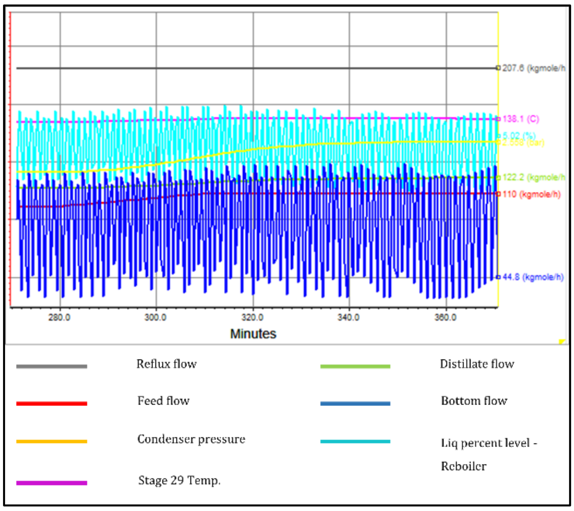

Figure 7. Graphics of Dynamic Response to Changes in the 10%-Mole Benzene Flow Rate in a Ramp for 30 Minutes

Figure 7 shows that all variables except bottom flow and liquid level-reboiler reached a steady state following a ramp shift. **Figure 8** depicted that bottom flow and liquid level-reboiler took longer to reach a steady state. A constant visual response revealed the circumstance.

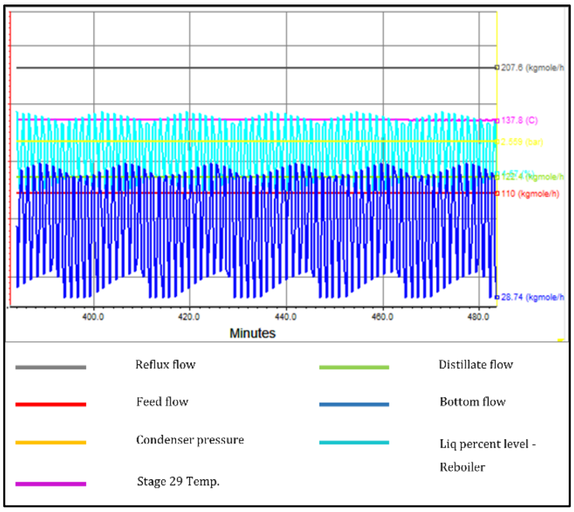

Figure 8. Graphics of Dynamic Response to Changes in the 10%-Mole Flow Rate of Benzene in a Ramp for 30 Minutes at a Steady State

Dynamic conditions can be regulated with the proper process control system, but the time necessary to reach a steady state varied considerably based on the approach employed [3]. Approximately 380 minutes were required to reach the steady state using the ramp method. The method demonstrated that this dynamic process control system requires considerable time to modify a number of variables to a steady state [13]. The circumstance revealed that both the control system and the absence of control had a substantial impact on the product concentration, particularly the concentration of the product at the bottom [3][14][15]. Simulation should be redeveloped with other dynamic techniques, as several sorts of disturbances occur in every industrial process [12][16].

CONCLUSIONS

The dynamics of the change in product concentration as a result of a 10%-mole rise in benzene were analyzed using two methods: sudden changes and changes with a 30-minute ramp. Both procedures were executed with and without a control system. In an uncontrolled system, the profile of the molar flow is flattened, and the liquid level reboiler regularly rises and falls. As with other variables, the shape of the molar flow bottoms and liquid level reboiler was straight in a controlled system.

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