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Dynamics of Ethyl Benzene Synthesis Using Aspen Dynamics

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ABSTRACT: ***The objective of the study is to generate a plant wide control strategy using Aspen Dynamics for synthesis of Ethyl Benzene process which consists of two CSTRs in series followed by two distillation columns. Steady state simulation has been carried out prior to dynamic simulation using Aspen Plus and exported to Aspen dynamics after providing the required sizing details under flow driven mode. In addition to default controllers, five more controllers are added and the necessary specifications regarding process variable, output variable and set point are specified for each controller. One cascade controller, two ratio controllers, two pressure controllers, four temperature controllers and six level controllers are used in the present study. Controllers are tuned by using Tyreus-Luyben and Ziegler-Nichols controller settings. The response of the whole process is studied for various step disturbances to find the optimal controller parameters and control structure.***

Keywords: Aspen Dynamics, CSTR, Ethyl benzene synthesis, Tyreus-Luyben and Ziegler-Nichols controller settings.

I. Introduction

Ethyl benzene is an important commodity chemical, mostly used in petrochemical industry as an intermediate in the production of styrene. Ethyl benzene is also used as a solvent in inks, rubber adhesives, varnishes, and paints. Production of Ethyl benzene consists of two continuous stirred tank reactors in series, two distillation columns and two liquid recycle streams. The present study is a good example of designing control structure for chemical process plants consisting of multiunit complex process with recycle streams. A multiunit complex process is generally comprised of one or more recycle streams. As the number of recycle streams increase, the complexity of the control increases. The recycle stream directly effects the dynamic behavior of the plant and hence need to be controlled with great accuracy.

The EB process provides a good example of the application of several fundamental principles of designing control structure. If a control strategy is successfully designed for such a complex dynamic behavior of system, similar attempt can be made to design control strategy for more or less complex systems. Selection of appropriate manipulated variables, controlled variables and control loops has been attempted.

In this process two fresh feeds ethylene, benzene and distillate from first column as recycle benzene stream are fed to first reactor. Effluent from first reactor and recycled Di-ethyl benzene coming out from the bottom of the second column are fed into the second reactor. Second reactor converts all the Di-ethyl benzene formed in the first reactor back to ethyl benzene. Effluent of second reactor is fed into first distillation column. Distillate from first column is mostly benzene, which is mixed with the fresh benzene and recycled to the first reactor. Bottoms from first column is fed to second column. Ethyl benzene product leaves as distillate of second column. Bottom is mostly Di-ethyl benzene which is recycled and fed to second reactor.

II. Methods and Methodology

2.1 Steady State Process Simulation:

The first step in simulation is developing the flow sheet by selecting appropriate unit models as shown in fig 3 and 4 by adding the necessary equipment and connect the input and output streams. After inputting specifications as shown in Tables 1 to 3 for streams and blocks and reaction kinetic information shown in Table 4, the flowsheet is simulated under steady state using Aspen One Version 8.1. Property estimation play an important role which effect the results of simulation. Chao-Seader property estimation method has been used in the present study.

Table 1: Input Stream Data

Stream	T (K)	P (atm)	kmol/hr
FRESHBEN (pure benzene)	320	20	630.6
FRESHE (pure ethylene)	320	20	630.6

Table 2: Equipment Parameter Data for reactors

Reactor	T (K)	P (atm)	V (m^3)
CSTR1	434	20	200
CSTR2	432	19	200

2.2 Reaction Kinetics

The following three reactions occur in the process:

$C_2H_4+C_6H_6 \rightarrow C_8H_{10}$…………………… (1)

$C_8H_{10}+ C_2H_4 \rightarrow C_{10}H_{14}$………………… (2)

$C_{10}H_{14}+C_6H_6 \rightarrow 2C_8H_{10}$………………… (3)

Table 3: Equipment Parameter Data for Distillation columns

Variable	Column1	Column2
Calculation type	Equilibrium	Equilibrium
Number of Stages	21	25
Condenser	Total	Total
Reflux Ratio	0.774	1.2
Distillate Rate (kmol/hr)	969.4	630.6
Feed Stage	10	15
Condenser Pressure (atm)	0.3	0.1

Table 4: Reaction Kinetic Parameters

Parameters	k_1	k_2	k_3
k	1.528×10^6	2.778×10^7	1000
E(Cal/mol)	17000	20000	15000

2.3 Dynamic Simulation:

The steady state simulation is converted into dynamic simulation mode by providing additional physical dimensions as shown below in Table 5 under flow driven mode. For reactors, reflux drum and sump a ratio of (L/D) is assumed as 2. The reflux drum and column sump diameter and length are estimated by considering 15 min of holdup for 50% level in it.

Table 5: Equipment Sizing Details

Vessels	Reactors (m)	Reflux Drum (m)		Sump (m)	
		C1	C2	C1	C2
Length	10.0616	5.1084	4.8462	5.7769	5.7195
Diameter	5.0308	2.5542	2.4231	2.8885	2.8598

The primary control objective in the first column is to see that no benzene leaves the column from the bottom. Hence, the temperature in the lower part of the column should be selected to meet this objective. The temperature of 15th stage for the first column and 17th stage for the second column has been selected as the control variable because temperatures are observed to change rapidly from tray to tray around these stages as shown in fig 1 and 2. The sensitive stage temperatures for both the columns are controlled by manipulating reboiler heat input.

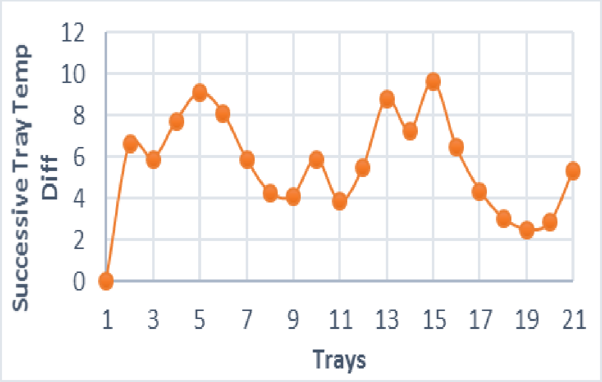

Figure 1: Sensitive Tray Selection for Column C1

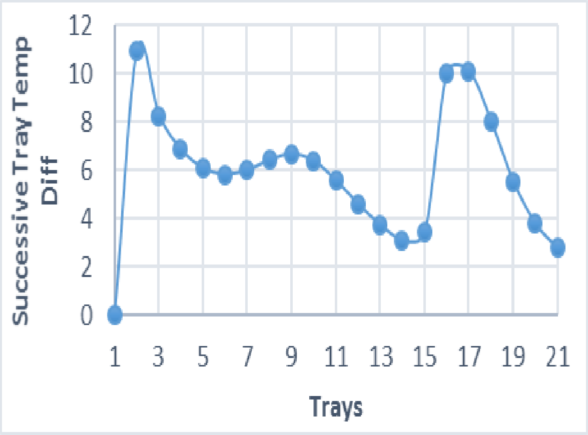

Figure 2: Sensitive Tray Selection for Column C2

Then a reflux-to-feed (R/F) ratio or a reflux ratio is selected to handle feed composition disturbances using ratio controller.

The effect of disturbance in feed composition on "Reflux Rate/Feed rate (R/F)" ratio as well as on "Reflux Ratio (RR)" are shown in the Table 6 for column 1 and Table 7 for column 2. For the same amount of disturbance in feed composition it has been observed that the desired change with respect to R/F is smaller compared to that of RR. Hence R/F has been selected to handle disturbances in feed composition for both columns with details as shown in Table 8.

Table 6: R/F or RR Selection for Column C1

Components	Mole Fraction			% change over range
	Base	10% -ve	10% +ve	
B	0.5102	0.4592	0.5612	--------
EB	0.3354	0.3689	0.3019	--------
DEB	01543	0.1718	0.1368	--------
R/F	0.5106	0.4596	0.5616	19.9714
RR	0.7292	0.8334	0.6454	25.7782

Table 7: R/F or RR Selection for Column C2

Components	Mole Fraction			% change over range
	Base	10% -ve	10% +ve	
B	0.0003	0.0003	0.0003	--------
EB	0.6905	0.6215	0.7596	--------
DEB	0.3092	0.3783	0.2402	--------
R/F	0.6908	0.6217	0.7498	18.5405
RR	0.7886	0.8726	0.7087	20.7781

Table 8: Details of Ratio Controllers used in Distillation

Multiplier	**RFC1**	**RFC2**
Input	Mass flowrate of feed to column1	Mass flowrate of feed to column2
Ratio	0.3228	0.7804
Output	Mass flowrate of Reflux	Mass flowrate of Reflux

Details of manipulated and controlled variables used for controllers are shown below in Table 9.

Table 9: Details of Controllers used.

Controller	Type/ Action	Process Variable	Manipulated Variable
LC1	PI/	CSTR1 Liquid	CSTR1 outlet

	Direct	Level	Flowrate
LC2	PI/ Direct	CSTR2 Liquid Level	CSTR1 outlet flowrate
RFFC	Cascade/ Reverse	Total Benzene Flowrate	Fresh Benzene Flowrate
TCC1	PID/ Reverse	15th Tray Temp. of C1	Reboiler Duty for C1
TCC2	PID/ Reverse	17th Tray Temp of C2	Reboiler Duty for C2

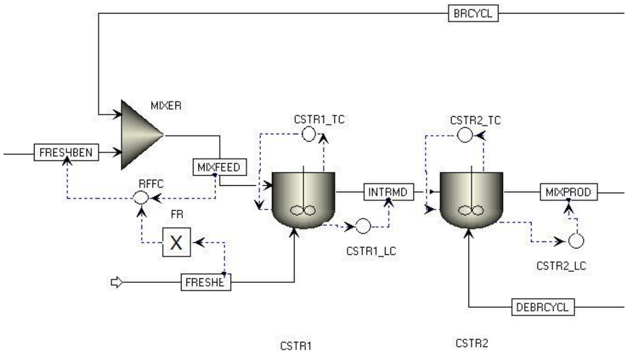

Fig 3: Synthesis flowsheet with control Details (Part A)

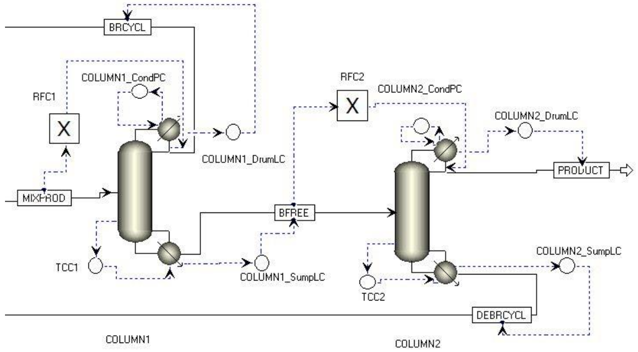

Fig 4: Synthesis flowsheet with control Details (Part B)

III. Results and Discussion

The response of the entire process is summarized in Figs. 5 to 20 with tuned optimal controller parameters from Table 9 by creating the disturbance in fresh Ethylene feed flowrate. As fresh ethylene flowrate is increased (Fig. 5) and decreased (Fig. 13) by 10%, the total benzene flowrate (recycle + fresh) to the rector is adjusted to 2.53 times of fresh ethylene flowrate by manipulating fresh benzene flowrate.

Fig 6 and 14 show change in the level and Fig. 7 and 15 show change in temperature due to change in total input flowrates. Level and temperature are returned to their set points by manipulation of outlet flowrates and cooling duty of reactors respectively. Zero mole fraction of Ethylene in Fig. 8 and Fig. 16 show that complete conversion of Ethylene occurs in first reactor. So recycled diethyl benzene to second reactor is again converted to ethyl benzene as benzene and diethyl benzene concentration in the second reactor is higher. It can be observed that second reactor favors only reaction 3. Due to induced disturbances the compositions of outlet stream has changed which affects the sensitive tray temperature of first column as shown in Fig. 10 and Fig. 18. The effect is confined to the first column itself, the second column sensitive tray temperature remains unchanged. This behavior is due to the reason that first column under any disturbance does not allow the bottom composition to be effected. The Fig. 11 and Fig. 19 show first column is not allowing any benzene slippage from the bottom and Fig. 12 and Fig. 20 show almost negligible variation in the product purity (0.9995+).

Table 9: Tuned controller parameters.

Parameter	LC1	LC2	TCC1	TCC2
Action	Direct	Direct	Reverse	Reverse
Ultimate Period	3.6	1.2	1.2	4.8
Tuning Rule	T-L	T-L	Z-N	Z-N
Integral Time	7.92	2.64	0.6	2.4
Derivative Time	0	0	0.25	0.6
Gain	122.48	125.59	10.83	4.98

3.1 The response of process subjected to 10% increase in fresh feed of ethylene:

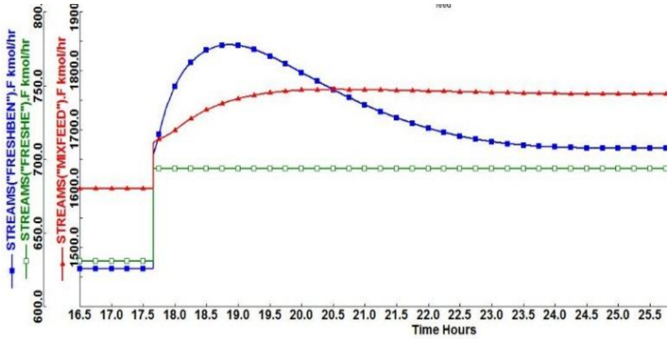

Figure 5: Feed Flows to First Reactor.

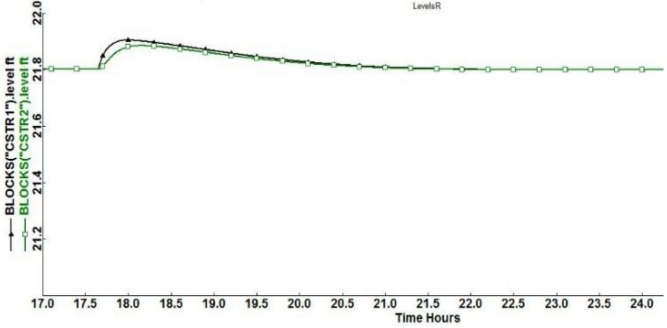

Figure 6: Levels in Reactor.

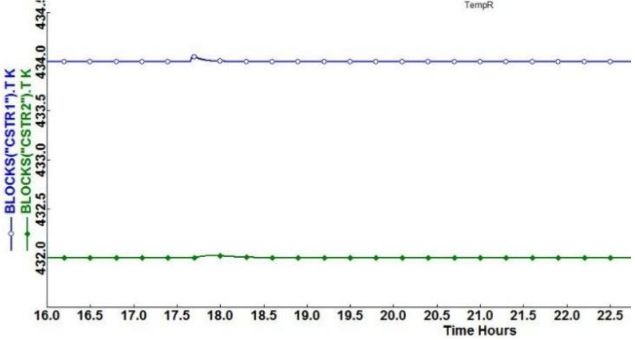

Figure 7: Temperatures in Reactor.

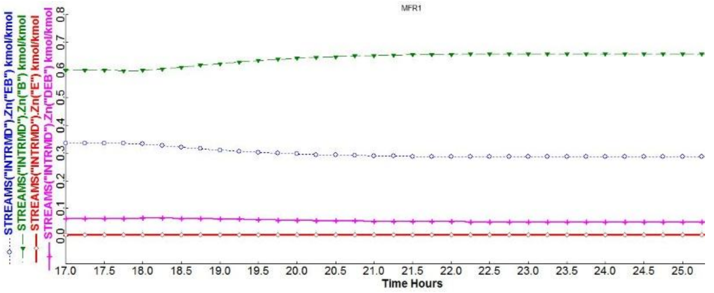

Figure 8: Mole Fractions at Outlet of First Reactor.

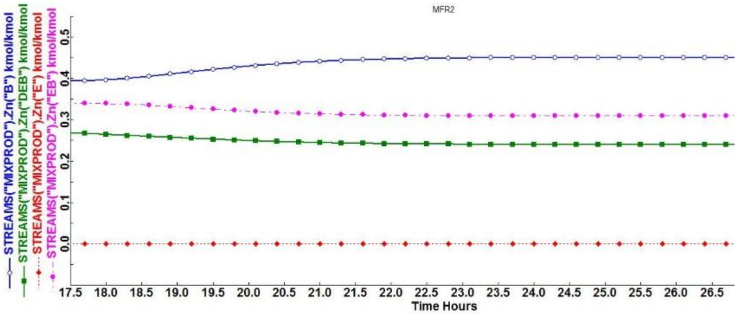

Figure 9: Mole Fractions at Outlet of Second Reactor.

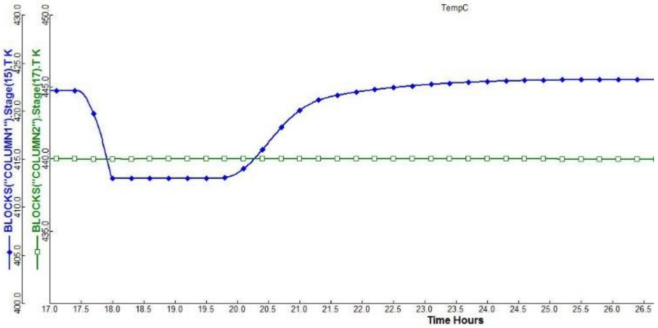

Figure 10: Sensitive Tray Temperatures in Column.

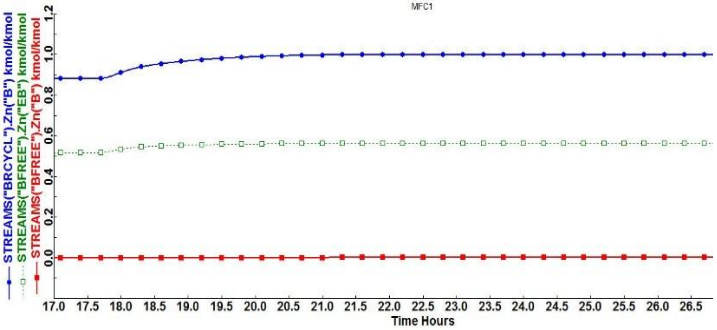

Figure 11: Mole Fractions at Outlet of First Column.

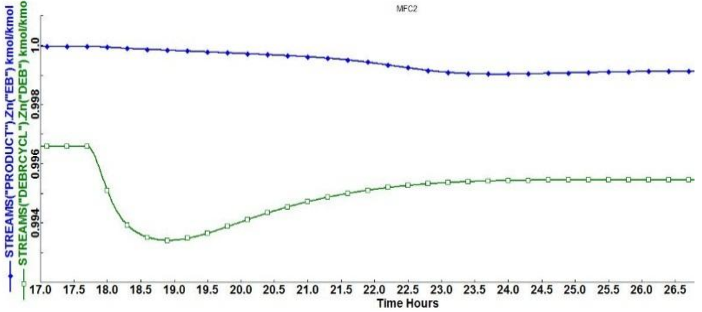

Figure 12: Mole Fractions at Outlet of Second Column.

3.2 The response of process subjected to 10% decrease in fresh feed of ethylene:

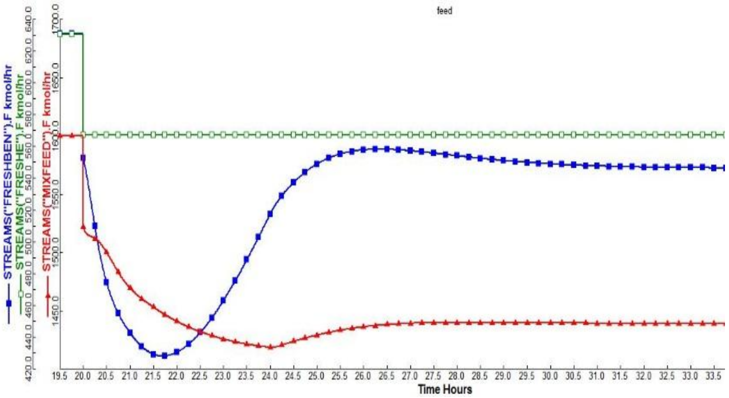

Figure 13: Feed Flows to First Reactor.

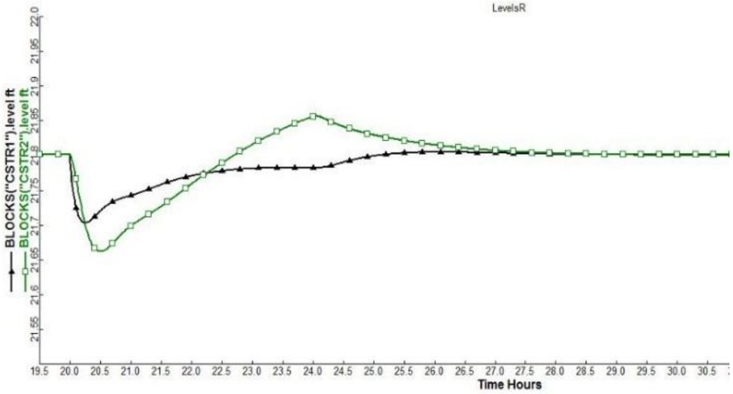

Figure 14: Levels in Reactor.

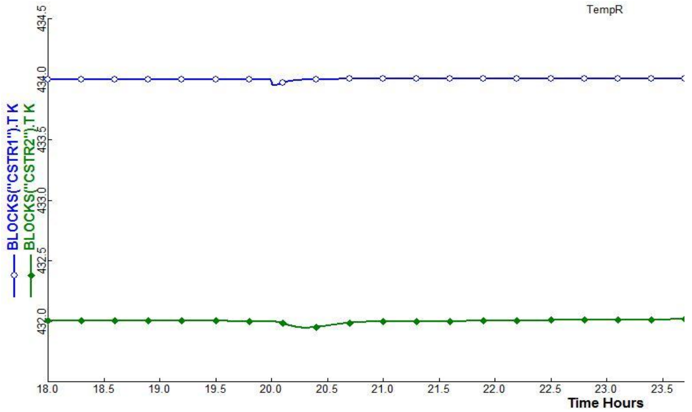

Figure 15: Temperatures in Reactor.

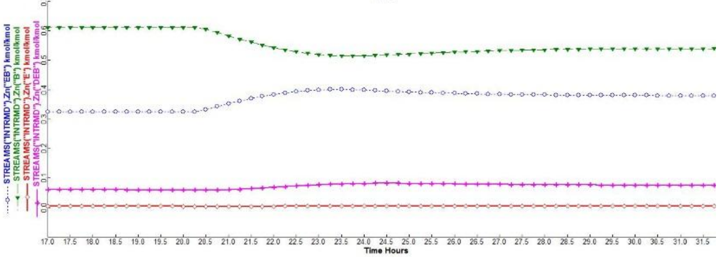

Figure 16: Mole Fractions at Outlet of First Reactor.

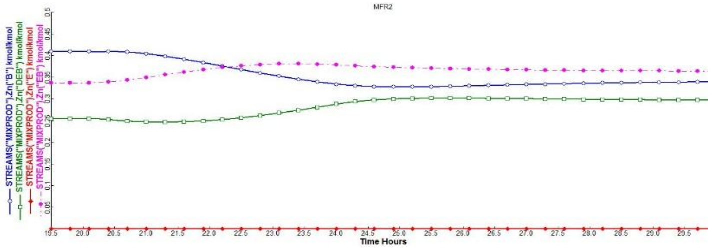

Figure 17: Mole Fractions at Outlet of Second Reactor.

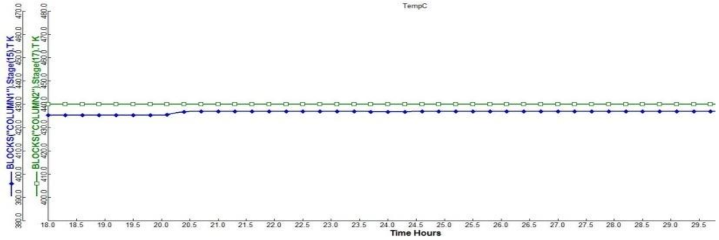

Figure 18: Sensitive Tray Temperatures in Column.

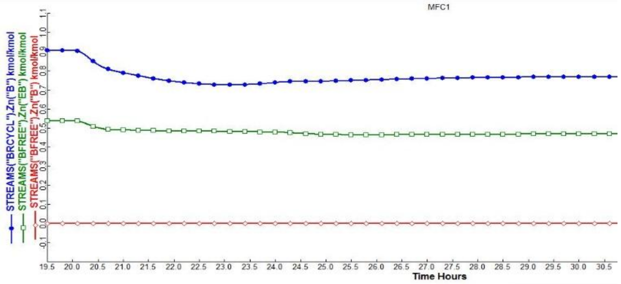

Figure 19: Mole Fractions at Outlet of first Column

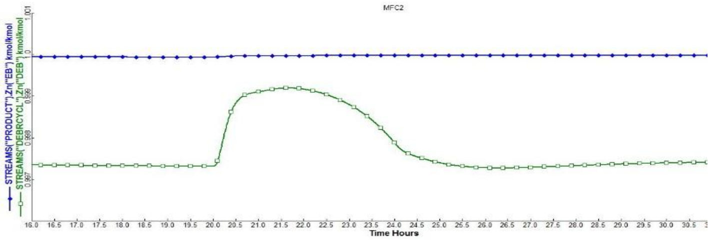

Figure 20: Mole Fractions at Outlet of Second Column

IV. Conclusion

It can be concluded that with tuned controller parameters, the response of the process is better in all the cases irrespective of the type of disturbance.

Out of RR and R/F control structure R/F control structure is found to be better to handle both feed flowrate and composition disturbances to meet desired purity of top products. Hence the selected controllers and their type along with the chosen control strategy is found to be satisfactory.

V. Acknowledgement

Authors are grateful the authority of NIT Warangal for providing facility and technical support.

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