

## Dynamics and control of binary distillation column

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### Abstract

The simulation of open loop response of binary distillation column is one of the major fields of study in present industrial revolution. Control of column is a challenging problem and has received considerable attention because of its importance in the process industry. This study provides the information about the simulation of open loop response in binary distillation column which consists of two component mixtures for different plates using Runge-Kutta method in excel. Next, we controlled the top tray(x2) and bottom tray(x10) of tower keeping L and V as the manipulated variable and by disturbing the feed composition we brought back to its original steady state level. The controllers used here is proportional integral derivative controller. We also set the delay of two hours and span of control for the distillation column.

**Keywords:** Binary distillation, Open loop response, Controlling, Proportional Integral Derivative controller

### Introduction

A distillation is the separation or partial separation of a liquid feed mixture into components or fractions by selective boiling (or evaporation) and condensation. A distillation produces at least two output fractions. This fraction include at least one volatile distillate fraction, which has boiled and been separately captured as a vapor condensed to a liquid, and practically always a bottoms (or residuum) fraction, which is the least volatile residue that has not been separately captured as a condensed vapor. Distillation is a unit operation, or a physical separation process, and not a chemical reaction.

### Methods

#### Batch distillation

Batch distillation refers to the use of distillation in batches, meaning that a mixture is distilled to separate it into its component fractions before the distillation still is again charged with more mixture and the process is repeated. This is in contrast with continuous distillation where the feedstock is added and the distillate drawn off without interruption. Batch distillation has always been an important part of the production of seasonal, or low capacity and high-purity chemicals. It is a very frequent separation process in pharmaceutical industry and in wastewater treatment units.

#### Continuous distillation

Continuous distillation is an ongoing distillation in which a liquid mixture is continuously (without interruption) fed into the process and separated fractions are removed continuously as output streams as time passes during the operation. Continuous distillation differs from batch distillation in the respect that concentrations should not change over time. Continuous distillation can be run at a steady state for an arbitrary amount of time. For any source material of specific composition, the main variables that affect the purity of products in continuous distillation are the reflux ratio and the number of theoretical equilibrium stages (practically, the number of trays or the height of packing). Reflux is a flow from the condenser back to the column, which generates a recycle that allows a better separation with a given number of trays. Equilibrium stages are ideal steps

where compositions achieve vapor-liquid equilibrium, repeating the separation process and allowing better separation given a reflux ratio. A column with a high reflux ratio may have fewer stages, but it refluxes a large amount of liquid, giving a wide column with a large holdup. Conversely, a column with a low reflux ratio must have a large number of stages, thus requiring a taller column.

### Binary Distillation

A binary distillation column has two component mixtures with different no of trays plus reboiler and condenser. Two variants of this system are:

An "uncontrolled" column with level controllers for condenser and reboiler, but with no temperature or composition control. The reflux  $L$  and the boil-up  $V$  remain as degrees of freedom.

A "controlled" column with an additional composition controller in the lower column part that manipulates the boil-up rate  $V$ . The uncontrolled system is used to explain the system equations and the reduction procedure. The major modeling assumptions are: Ideal trays, which means that liquid and vapor are in equilibrium at each tray; ideal mixture, which means that the vapor composition  $y$  can be expressed as a function of the liquid composition  $x$  assuming the constant relative volatility

$$y = k(x) = \frac{\alpha x}{1 + (\alpha - 1)x}$$

where,  $\alpha$  is the relative volatility,  $x$  is the mole fraction; constant molar flows, which means that the energy balance is simplified; constant molar hold upon each tray and negligible mass in the vapor phase.

The column has one feed flow  $F$  at tray number  $nF$ .  $zF$  denotes the concentration of the first (light) component in the feed. A liquid flow  $L$  (or  $L + F$  for trays below the feed tray) and a vapor flow  $V$  enter and leave each tray. The condenser and reboiler levels are assumed to be controlled using the distillate  $D$  and bottom flow  $B$ , respectively. For simplicity, perfect level control is assumed, such that  $D = V - L$  and  $B = L + F - V$ . The concentrations in these flows determine the

purity of the distillation products and are therefore the most important output variables in the process. The feed flow rate  $F$  and the feed concentration  $z_F$  can be seen as disturbance variables, and the flows  $L$  and  $V$  are manipulated variables. The main process in binary distillation is that separates a feed mixture stream to two fractions: one distillate and one bottoms fractions (which is known as residue).

### Runge-Kutta method

In numerical analysis, the Runge-Kutta methods are an important family of implicit and explicit iterative methods for the approximation of solutions of ordinary differential equations. These techniques were developed around 1900 by the German mathematicians C. Runge and M.W. Kutta.

### Fourth order Runge-Kutta method

This method is simply a higher order approximation to the midpoint method. Instead of shooting to the midpoint, estimating the derivative, the shooting across the entire interval the Runge-Kutta method, in a sense takes, four steps, shooting across one quarter of the interval, estimating the derivative, and then shooting to the midpoint, and so on. The precise manner in which the method propagates across a time step is done in the optimal way for the four steps. We will not provide a formal derivation of the Runge-Kutta algorithm; instead we will present the method and implement it. The general system of ODEs can be written as,

$$\frac{dx}{dt} = f(t, x)$$

The Runge-Kutta method is defined as:

$$\begin{aligned} K_1 &= \Delta t f(t_n, x_n) \\ K_2 &= \Delta t f\left(t_n + \frac{\Delta t}{2}, x_n + \frac{K_1}{2}\right) \\ K_3 &= \Delta t f\left(t_n + \frac{\Delta t}{2}, x_n + \frac{K_2}{2}\right) \\ K_4 &= \Delta t f(t_n + \Delta t, x_n + K_3) \\ K &= \frac{1}{6}(K_1 + 2K_2 + 2K_3 + K_4) \quad ; \quad x_{n+1} = x_n + K \end{aligned}$$

### Controllers

The mode of control is the manner in which a control system makes corrections relative to an error that exists between the desired value (set point) of a controlled variable and its actual value. The mode of control used for a specific application depends on the characteristics of the process being controlled. For example, some processes can be operated over a wide band, while others must be maintained very close to the set point. Also, some processes change relatively slowly, while others change almost immediately. The following four types of controllers are widely used in chemical process control applications.

### Proportional Integral Derivative controller

The PID controller, which consists of proportional, integral and derivative elements, is widely used in feedback control of industrial processes. In applying PID controllers, engineers must design the control system: that is, they must first decide which action mode to choose and then adjust the parameters of the

controller so that their control problems are solved appropriately. To that end, they need to know the characteristics of the process. As the basis for the design procedure, they must have certain criteria to evaluate the performance of the control system.

Algorithm of PID controller

$$x(t) = Bias + K \left( e(t) + \frac{1}{\tau_i} \int_0^t e(t) dt + \tau_D \frac{de(t)}{dt} \right)$$

When used in this way, the three elements of the PID controller produce outputs with the following nature:

- P element: proportional to the error at the instant  $t$ , which is the “present” error.
- I element: proportional to the integral of the error up to the instant  $t$ , which can be interpreted as the accumulation of the “past” error.
- D element: proportional to the derivative of the error at the instant  $t$ , which can be interpreted as the prediction of the “future” error.

### Problem

The binary distillation column problem is given below:

$$\begin{aligned} \frac{dx_1}{dt} &= \left(\frac{V}{H_1}\right) (y_2 - x_1) \\ \frac{dy_i}{dt} &= \left(\frac{1}{H_i}\right) [-V\phi(y_i^* - y_{i+1}) + L(x_{i-1} - x_i)] \\ &\text{for } i=2,3,\dots,f-1 \\ \frac{dx_f}{dt} &= \left(\frac{1}{H_f}\right) [-V\phi(y_f^* - y_{f+1}) + Lx_{f-1} - (L+F)x_f + Fz] \\ \frac{dy_j}{dt} &= \left(\frac{1}{H_j}\right) [-V\phi(y_j^* - y_{j+1}) + (L+F)(x_{j-1} - x_j)] \\ &\text{For } j=f+1,\dots,N-1 \\ \frac{dx_N}{dt} &= \left(\frac{1}{H_N}\right) [-V\phi y_N^* + (L+F)x_{N-1} - (L+F-V)x_N] \end{aligned}$$

Where,

$$\begin{aligned} y_i^* &= \frac{\alpha y_i}{1 + (\alpha - 1)y_i} \quad \text{For } i=2,3,\dots,N \\ y_i &= y_{i+1} + \phi(y_i^* - y_{i+1}) \quad \text{For } i=2,3,\dots,N-1 \\ y_N &= \phi y_N^* \end{aligned}$$

The stage are numbered from the top with the condenser as 1 and the reboiler as stage N. Here  $H$ ,  $\alpha$ ,  $\phi$ ,  $z$  and  $F$  are the hold-up, relative volatility, Murphree stage efficiency, feed composition and feed-flow rate respectively.

### Operating conditions

Table 1: Operating conditions

H1	100mol	$\alpha$	3
H2	25mol	$\phi$	1
H3	25mol	$z$	0.5
H4	25mol	$F$	10 mol/h
H5	25mol	$D$	5 mol/h
H6	25mol	$V$	36.5 mol/h
H7	25mol	$L$	31.5 mol/h
H8	25mol		
H9	25mol		
H10	200mol		

## Methodology

### Simulation of open loop response

#### Finding of mole fraction values

In this problem the first step is to find the mole fraction values in steady state condition. To find these values we first assumed some rough values for the mole fraction from  $x_1$  to  $x_{10}$ . Then, we found out the mole fraction of vapour by using the below formulas. It is given by,

$$y_i^* = \frac{(x_{i+1})}{[1 + (\alpha - 1)x_i]} \text{ For } i=2,3,\dots,N$$

$$y_i = y_{i+1} + \theta(y_i^* - y_{i+1}) \text{ For } i=2,3,\dots,N-1$$

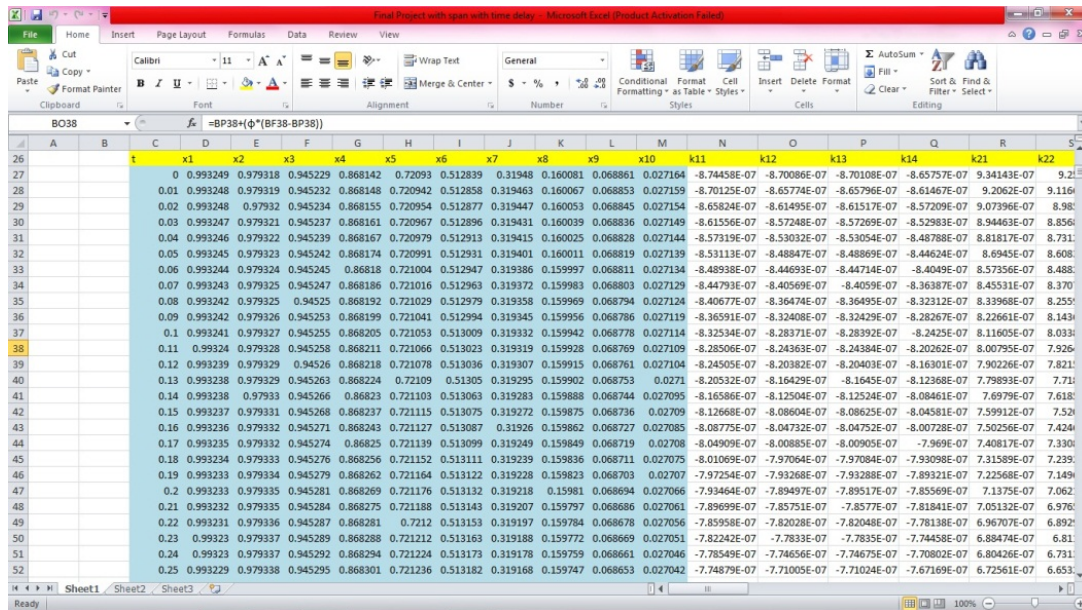
$$y_N = \theta y_N^*$$

By substituting these values in the differential equation which is given above in the problem we found out the mole fraction of

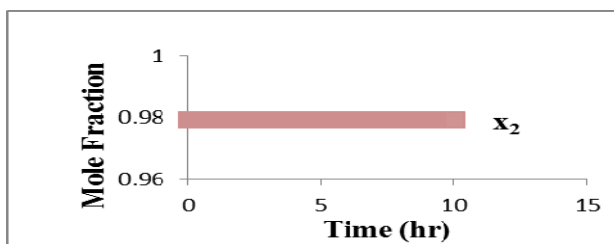
liquid in steady state conditions by solving these numerical equations in MS excel sheet.

**Table 2:** steady state mole fraction values of liquid

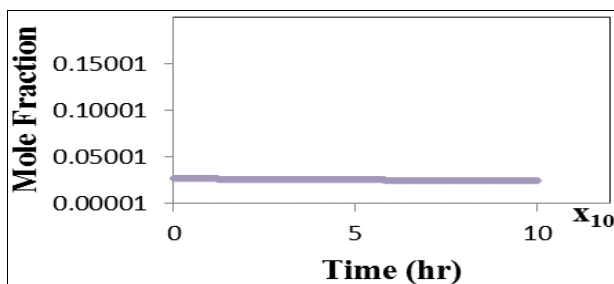
x1	0.993249
x2	0.979318
x3	0.945229
x4	0.868142
x5	0.720931
x6	0.512839
x7	0.319487
x8	0.160081
x9	0.068861
x10	0.027164



**Fig 1:** MS excel spread sheet for mole fraction values



**Fig 2:** Steady state top tray graph



**Fig 3:** Steady state bottom tray graph

#### Finding out 'k' values for different plates of tower

The k values is found out numerically for ten plates of the distillation column using fourth order Runge-Kutta method in MS excel.

The fourth order Runge-Kutta formula is given by

$$k_1 = hf(x_n, y_n)$$

$$k_2 = hf\left(x_n + \frac{h}{2}, y_n + \frac{k_1}{2}\right)$$

$$k_3 = hf\left(x_n + \frac{h}{2}, y_n + \frac{k_2}{2}\right)$$

$$k_4 = hf\left(x_n + h, y_n + k_3\right)$$

$$k = \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

The ten differential equations which is used to find out k values are,

$$\frac{dx_1}{dt} = \left(\frac{v}{V_1}\right) [y_2 - x_1]$$

$$\frac{dx_2}{dt} = \left(\frac{1}{H_2}\right) [-V\phi(y_2^* - y_2) + L(x_1 - x_2)]$$

$$\frac{dx_3}{dt} = \left(\frac{1}{H_3}\right) [-V\phi(y_3^* - y_4) + L(x_2 - x_3)]$$

$$\frac{dx_4}{dt} = \left(\frac{1}{H_4}\right) [-V\phi(y_4^* - y_5) + L(x_3 - x_4)]$$

$$\frac{dx_5}{dt} = \left(\frac{1}{H_5}\right) [-V\phi(y_5^* - y_6) + L(x_4 - x_5)]$$

$$\frac{dx_6}{dt} = \left(\frac{1}{H_6}\right) [-V\phi(y_6^* - y_7) + Lx_6 - (L + F)x_6 + Fz]$$

$$\frac{dx_7}{dt} = \left(\frac{1}{H_7}\right) [-V\phi(y_7^* - y_8) + (L + F)(x_6 - x_7)]$$

$$\frac{dx_8}{dt} = \left(\frac{1}{H_8}\right) [-V\phi(y_8^* - y_9) + (L + F)(x_7 - x_8)]$$

$$\frac{dx_9}{dt} = \left(\frac{1}{H_9}\right) [-V\phi(y_9^* - y_{10}) + (L + F)(x_8 - x_9)]$$

$$\frac{dx_{10}}{dt} = \left(\frac{1}{H_{10}}\right) [-V\phi(y_{10}^* - y_{10}) + (L + F)x_9 - (L + F - V)x_{10}]$$

By solving these differential equations we found out the k values for different plates of the tower.

Thus, we simulated the open loop response of binary distillation column in excel.

### 3.2 Control of top and bottom tray

Next, is the control of top and bottom tray of the tower by disturbing the feed composition from  $z = 0.7$  to  $0.3$  using proportional integral derivative controller in excel.

Here, we use L and V as the manipulated variable for top and bottom tray of the distillation column. The controller formula is given by,

$L = L_{max} CO$

$$CO = 0.5 + k_c(E + 1/\tau_i \int_0^t E dt + \tau_d dE/dt)$$

We also set the delay of two hours and span of control to both the trays of binary distillation column. The distillation column controller block diagram for top and bottom tray is given below.

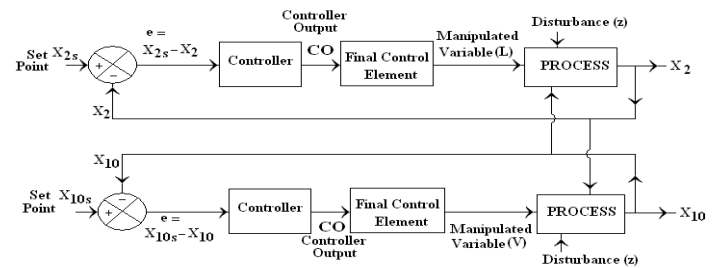


Fig 4: Block diagram of distillation column control

Fig 5: MS excel spreadsheet for control of top and bottom trays

### Disturbances and control of top and bottom tray

When the feed composition is disturbed to  $z=0.7$  the graph of top and bottom tray is given by,

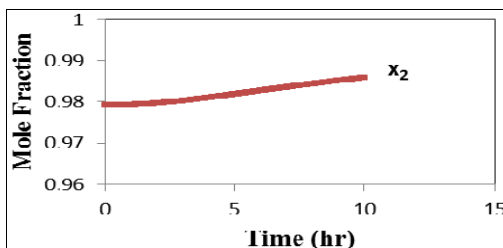


Fig 6: Feed disturbance graph for top tray when  $z = 0.7$

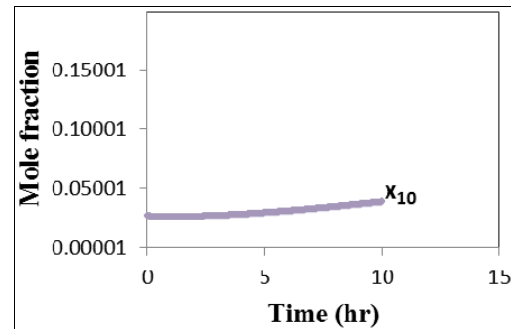
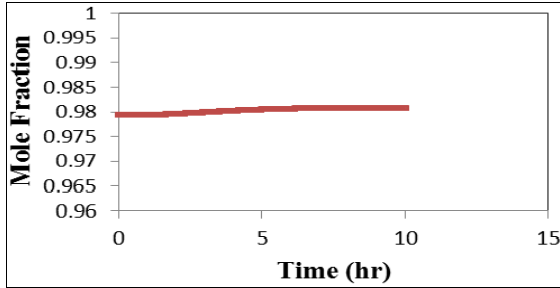


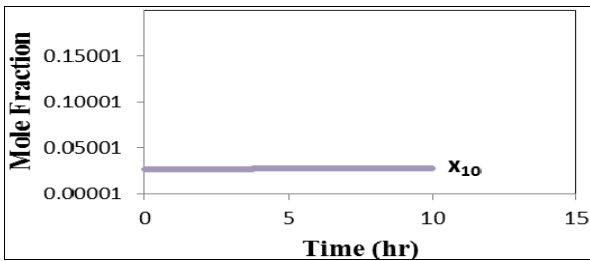
Fig 7: Feed disturbance graph for bottom tray when  $z = 0.7$

**Table 3:** Disturbances controlled by using PID controller for top and bottom tray

pc1	0.5	pc2	0.5
kc1	5.5	kc2	0.0001
ti1	0.001	ti2	0.01
td1	0.01	td2	0.01

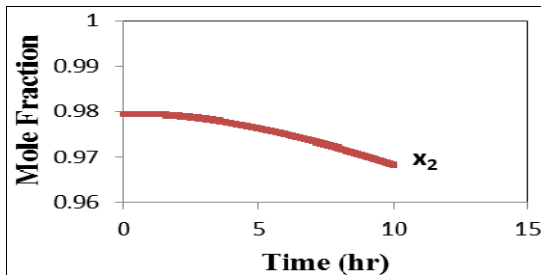


**Fig 8:** Control graph for top tray when  $z = 0.7$

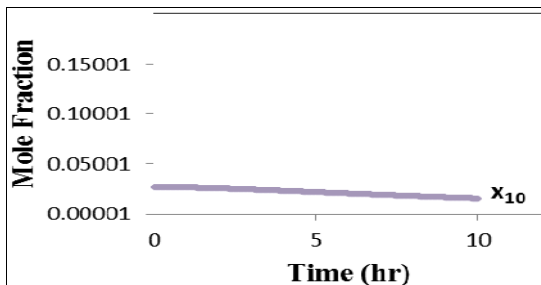


**Fig 9:** Control graph for bottom tray when  $z = 0.7$

When the feed composition is disturbed to  $z = 0.3$  the graphs are given by,



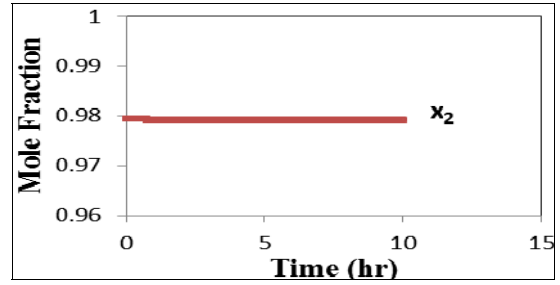
**Fig 10:** Feed disturbance graph for top tray when  $z = 0.3$



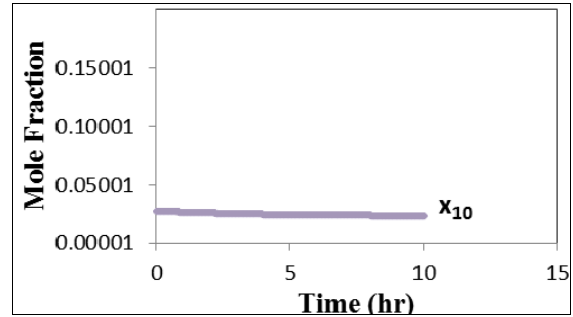
**Fig 11:** Feed disturbance graph for bottom tray when  $z = 0.3$

**Table 4:** control numerical values for both trays

pc1	0.5	pc2	0.5
kc1	20	kc2	0.00001
ti1	0.0001	ti2	0.0001
td1	0.001	td2	0.01



**Fig 12:** Control graph for top tray when  $z = 0.3$



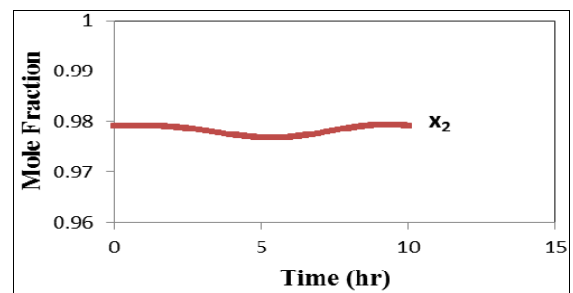
**Fig 13:** Control graph for bottom tray when  $z = 0.3$

#### Control of trays with span and time delay

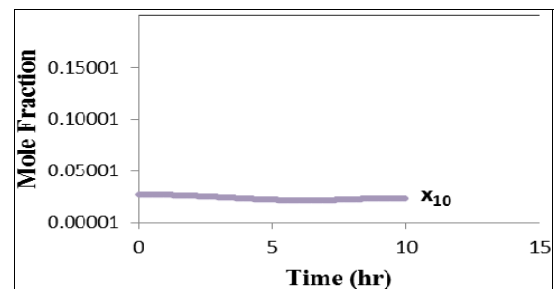
As we said before we have set the delay of two hours and span of control to the column, the numerical values and control graphs with span and time delay for both the trays is shown below,

**Table 5:** The numerical values when  $z = 0.7$

pc1	0.5	pc2	0.5
kc1	5	kc2	0.0001
ti1	0.001	ti2	0.01
td2	0.01	td2	0.01



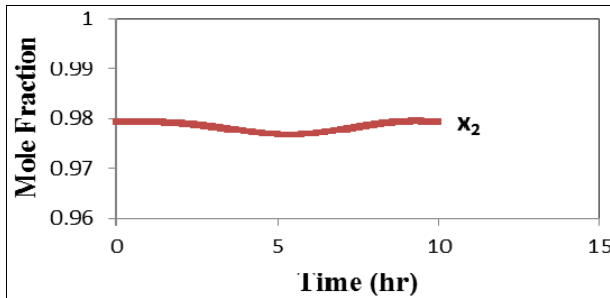
**Fig 14:** Control graph for top tray when  $z = 0.7$  with span and time delay



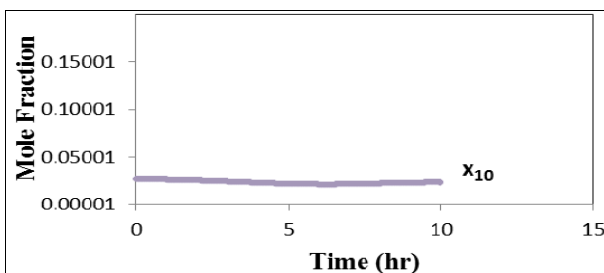
**Fig 15:** Control graph for bottom tray when  $z = 0.7$  with span and time delay

**Table 6:** The numerical values when  $z=0.3$

Pc1	0.5	pc2	0.5
Kc1	4.8	kc2	0.0001
Ti1	0.001	$\tau_i2$	0.001
$\tau_d1$	0.01	$\tau_d2$	0.01



**Fig 16:** Control graph for top tray hen  $z = 0.3$  with span and time delay



**Fig 17:** Control graph for bottom tray when  $z = 0.3$  with span and time delay

## Conclusion

So, the dynamics of binary distillation column was studied with open loop response and we controlled the top and bottom tray of the distillation column using proportional integral derivative controller in excel.

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