Dynamic Modeling and Control of Binary Distillation Column

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Abstract— Distillation column has always been and will continue to be one of the most important thermal separation equipment used in various types of industries for various applications, like in oil refineries, in water purification/ desalinization plants, in pharmaceutical industries etc. Modelling and simulation of distillation column are not new to the process and control engineer. The model used for distillation column varies from the simple to quite complex, depending on the assumption made in the material balance and energy balance equations to describe the distillation column behavior. This paper discuss about the dynamic modelling of continuous binary distillation column in Matlab tool and the response analysis while varying the assumptions made while developing the dynamic model. This paper also discuss about the tuning of PID controller using different tuning methods which is job of control engineer.

Key words: Binary, Distillation, Dynamic model, S-function

I. INTRODUCTION

Distillation is a thermal separation method for separating mixtures of two or more substances into its component fractions of desired concentration, based on differences in volatilities or the boiling point difference of these components by the application and removal of heat.

A simple distillation process is shown in the figure-1 below. The sequence of process is also mentioned clearly.

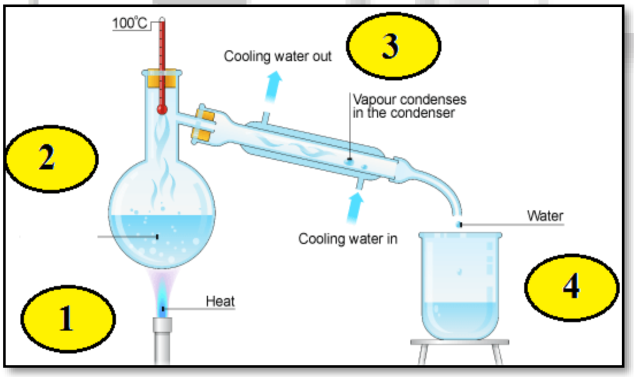

Fig. 1: Simple distillation process

A simple two-product continuous distillation column is shown in Fig. 2. The column has N stages on which the vapor-liquid equilibriums occur. The feed enters the column on the stage N_F. This stage divides the column into a rectifying section and a stripping section. At the bottom of the column there is a reboiler, which provides energy to the column in order to produce vapor.

The mixture is heated to form a flow of vapor rising up inside the column. In the stripping section, the less volatile component is enriched while in the rectifying section the more volatile component is enriched. The top product is condensed by the condenser from which there is a reflux flow back to the top of the column to enhance the purity of the product.

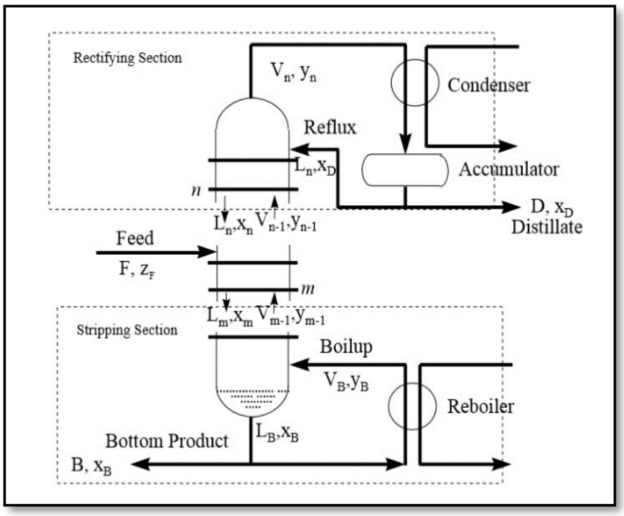

Fig. 1: Binary distillation column operation

In order to achieve the purest form of a component or to achieve the desired composition of a product depending according to the requirement, we need to manipulate & control various variables of the distillation column such as temperature of trays, reflux flow rate, distillate flow rate, vapor boil up rate and the pressure in the column. These variables may vary in practice due to different reasons.

This paper is organized as follows. Section-II gives some basic details about the modelling of binary distillation column by using the fundamental modelling approach. Section-III gives the details about how we can simulate a dynamic model of distillation column in Matlab tool. Section-IV will show the steps to be followed to derive a FOPDT model. Section-V will discuss about various PID tuning methods. Section-VI shows response comparison in terms of set-point tracking and disturbance rejection also provides statistical analysis. Finally, in Section-VII and Section-VIII, the conclusion is made and the work that can be extended in the future is mentioned respectively.

II. DYNAMIC MODELING OF DISTILLATION COLUMN

For the complex processes, it is not economically feasible to design the control system after installing the process plant. So, the first step in the design of a control system for any process should be the development of a process model. From the dynamic model we can understand the behavior of the system as well as we can predict how the system will behave if certain conditions arises. Depending on that we can design a control system prior to process system installation.

The model of binary distillation column can be obtained by using the differential equations which describe the relationship between the various variables of the process. Some of these variables act as disturbances, some as controlled variables, some as manipulated variables and some as uncontrolled variables. All these equations can be derived with the help of the laws of thermodynamics (energy balance equations) and mass-balance equations.

Modeling of the distillation column is often classified into three types as describe below:

A. Fundamental modeling method

In fundamental modelling method, the model is developed based on the physical properties of the system, such as the preservation of energy, mass and momentum. This method of modeling has an advantage of global validity, accuracy and it gives more detailed process understanding. However, this modeling method is quite complex for the controller design, because it requires a huge amount of computation and simplifications.

B. Empirical modeling method

The empirical modeling utilizes the input and output data from the operation of the column to build the relationship between the input and the output. This method is also known as "***Black box modeling***" because inner dynamics are not considered. With this type of modelling, the understanding of the inner dynamics of the column does not required. So, the computation can be reduced.

But by using this technique, we must carry out experiments on the real distillation column, and the results may not be applied for another distillation column, even the results from one distillation column can be different if the distillation column's conditions are different between the experiment and the real operation of the distillation column.

C. Hybrid modeling method

The hybrid modeling (or the '***grey-box' modeling***) combines the fundamental modeling and the empirical modeling. This method utilizes the advantages of both methods (fundamental modeling and empirical modeling), but the critical thing is that we must to decide for which part of the model do we need to use fundamental modelling and for which part to use empirical modelling.

Here, for this work I used fundamental modeling method for the development of dynamic model for the continuous binary distillation column. In order to develop this model we need to make some assumptions. So, next section will describe the assumption need to be made.

In the model of the distillation column the following assumptions are made:

1) The feed contains only two components (Binary mixture).
2) The column is perfectly insulated.
3) Constant relative volatility.
4) Constant molar flows.
5) No vapor holds up.
6) All the trays are ideal (100% efficient)
7) Linear liquid dynamics.
8) Equilibrium on all stages.
9) Pressure inside the column is fixed.
10) Total condenser and reboiler.

Here, for fundamental modeling, we will divide the distillation model in four envelopes, which are:

1) Condenser
2) Reboiler
3) Feed tray
4) All other trays (except feed tray)

D. Envelope – 1: Condenser

A condenser is used to cool and condense the vapor, which is leaving the top of the column. The condensed liquid is stored in a holding vessel known as the reflux drum. Some of this liquid is recycled back to the top of the column and this is called the reflux. The condensed liquid that is removed from the system is known as the distillate or top product.

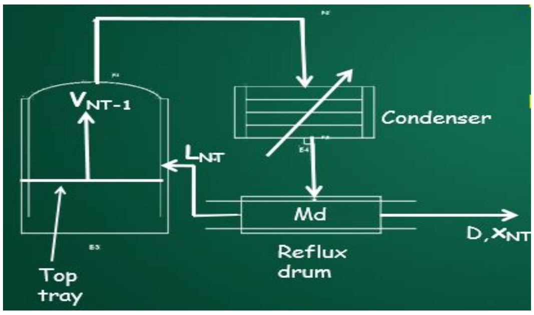

Fig. 2: Envelope-1 Condenser

The total material balance equation is:

$$\frac{d(M_{NT})}{dt} = V_{NT-1} - L_{NT} - D \qquad \text{….. (1)}$$

The component material balance equation is:

$$\frac{d(M_{NT}x_{NT})}{dt} = V_{NT-1}y_{NT-1} - L_{NT}x_{NT} - Dx_{NT} \qquad \text{….. (2)}$$

E. Envelope – 2: Reboiler

The heat is supplied to the reboiler to generate vapor. The vapor raised in the reboiler is re-introduced into the unit at the bottom of the column. The liquid removed from the reboiler is known as the bottom product or simply, bottom.

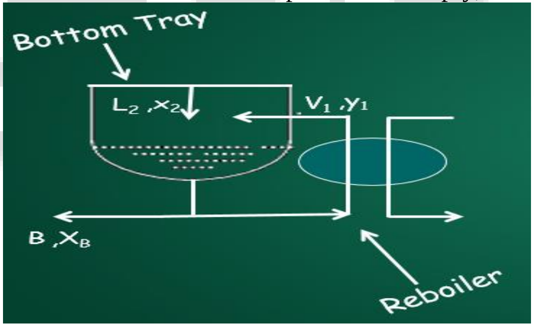

Fig. 3: Envelope-2 Reboiler

The total material balance equation is:

$$\frac{d(M_1)}{dt} = L_2 - V_1 - B \qquad \text{….. (3)}$$

The component material balance equation is:

$$\frac{d(M_1x_1)}{dt} = L_2x_2 - V_1y_1 - Bx_1 \qquad \text{….. (4)}$$

F. Envelope – 3: Feed tray

The liquid mixture that is to be processed is known as the feed and this is introduced usually somewhere near the middle of the column to a tray known as the feed tray.

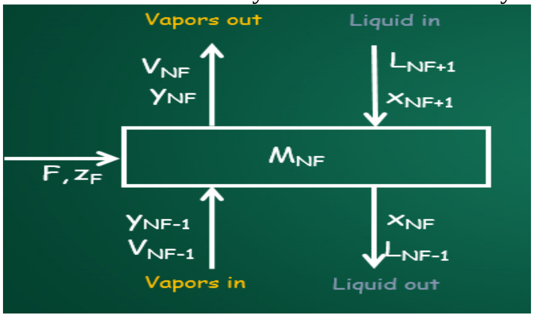

Fig. 4: Envelope-3 Feed tray

The total material balance equation at the feed stage (NF),

$$\frac{d(M_{NF})}{dt} = L_{NF+1} - L_{NF} + V_{NF-1} - V_{NF} + F \quad \text{….. (5)}$$

The total material balance equation at the feed stage (NF),

$$\frac{d(M_{NF}x_{NF})}{dt} = L_{NF+1}x_{NF+1} - L_{NF}x_{NF} + V_{NF-1}y_{NF-1} - V_{NF}y_{NF-1} + F_{z_F} \quad \text{….. (6)}$$

Where,

F is the feed flow rate,

z_F is the concentration of the light component in feed

G. Envelope – 4: Other trays (except feed tray)

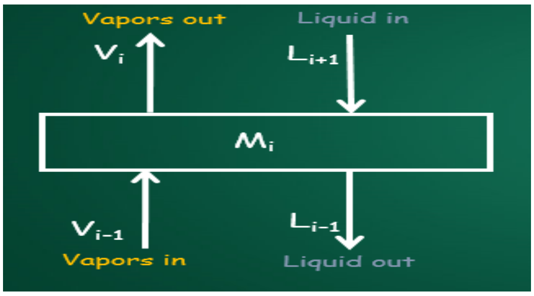

Fig. 5. Envelope-4 all other general trays (except feed tray)

The total material balance equations on stage i is given by,

$$\frac{dM_i}{dt} = L_{i+1} - L_i + V_{i-1} - V_i \quad \text{….. (7)}$$

Where,

M_i is liquid hold up on tray i ,

L_i is liquid flow rate,

V_i is vapor flow rate that comes toward tray i.

The material balance for the light component on tray (i) is given by,

$$\frac{d(M_i x_i)}{dt} = L_{i+1}x_{i+1} - L_i x_i + V_{i-1}y_{i-1} - V_i y_i \quad \text{….. (8)}$$

Where,

x_i & y_i is the composition of the light and heavy component on a tray (i) respectively.

The composition of the heavy component is related to the composition of the light component via the relative volatility, which is given by the equation,

$$y_i = \frac{\alpha_{x1}}{1+(\alpha-1)x_1} \quad \text{….. (9)}$$

The liquid flow dynamics is considered due to its important effect on the initial response of the distillation column. The liquid holdup given by the following equations,

$$L_i = L_{0b} + \frac{M_i - M_{0i}}{\tau} + (V_{i+1} - V_0)\lambda \quad \text{….. (10)}$$

For I from 2 to N_F and

$$L_i = L_0 + \frac{M_i - M_{0i}}{\tau} + (V_{i+1} - V_{0t})\lambda \quad \text{….. (11)}$$

For I from $N_F + 1$ to $N_T - 1$.

Where,

L_0 is the nominal reflux flow,

M_{0i} is the nominal re boiler hold up (kmol) on stage i.

τ is the time constant for liquid dynamics =0.063(min)

λ represents the effect of vapor flow on liquid flow.

III. Model Simulation in Matlab Tool

The basic idea of this simulation model is taken from the distillation model proposed by Skogested[4]. Here, for this work simulation is performed in Matlab tool with the help of S-function block. S-function block combines the advantages of both i.e. Matlab Simulink and m-script. In S-function block we need to provide initialization data and dynamic equations of mass and energy balances. An open loop model of binary distillation column is shown in the figure below.

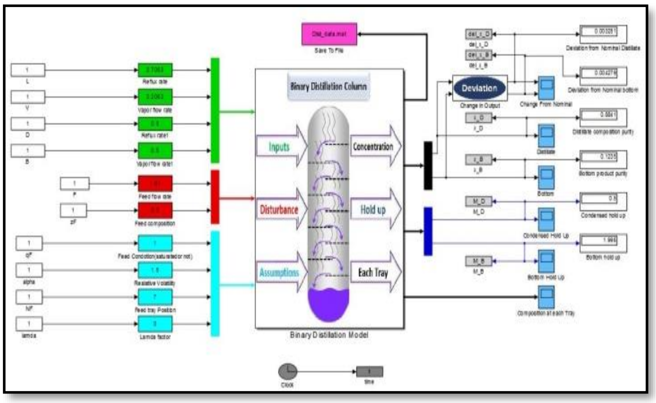

Fig. 7: Binary distillation column model in Matlab tool

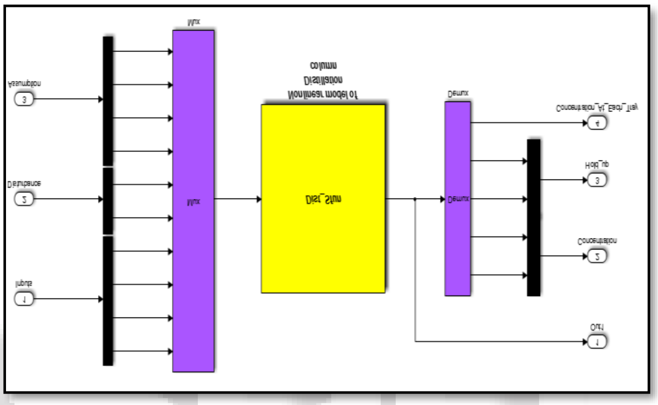

Fig. 8: Internal view of Binary distillation model block with S-function

The nominal values of distillation column dynamics are shown in the table 1.

Parameter	Value
Total number of trays ($\boldsymbol{N_T}$)	16
Feed tray location ($\boldsymbol{N_F}$)	7
Feed flow rate ($\boldsymbol{F}$)	1
Feed composition ($\boldsymbol{z_F}$)	0.5
Feed condition ($\boldsymbol{q_F}$)	1
Relative volatility ($\boldsymbol{\alpha}$)	1.5
Effect of vapour on liquid ($\boldsymbol{\lambda}$)	0
Reflux rate ($\boldsymbol{L}$)	2.70629
Vapor boil-up rate ($\boldsymbol{V}$)	3.20629
Distillate flow rate ($\boldsymbol{D}$)	0.5
Bottom flow rate ($\boldsymbol{B}$)	0.5

Table - 1. Steady-state data for distillation column dynamics

The steady-state values for the concentration of light component at all trays for bottom to top tray is listed in table-2 shown below that we can obtain by simulating the column for 20000 minutes in Matlab tool.

Tray number	x_D	M_D
1	0.1192	0.5
2	0.1621	0.5
3	0.2106	0.5
4	0.2634	0.5
5	0.3181	0.5
6	0.3722	0.5
7	0.4233	0.5

8	0.4581	0.5
9	0.4997	0.5
10	0.5478	0.5
11	0.6015	0.5
12	0.6590	0.5
13	0.7182	0.5
14	0.7764	0.5
15	0.8312	0.5
16	0.8807	0.5

Table - 2. Light component concentration values and hold-up on each tray at steady-state

The relative volatility is ultimately the difference of boiling points of MVC (More Volatile Component) and LVC (Less Volatile Component).

The table-3. Shows values of an optimal relative volatility (α) for different binary mixtures as listed. You need to specify that particular value of relative volatility for particular binary mixture in the simulation model.

MVC (boiling point in ℃)	LVC (boiling point in ℃)	Optimal relative volatility (α)
Benzene (80.1)	Toluene (110.6)	2.34
Toluene (110.6)	p-Xylene (138.3)	2.31
Benzene (80.6)	p-Xylene (138.3)	4.82
m-Xylene (139.1	p-Xylene (138.3)	1.02
Pentane (36.0)	Hexane (68.7)	2.59
Hexane (68.7)	Heptane (98.5)	2.45
Hexane (68.7)	p-Xylene (138.3)	7.0
Ethanol (78.4)	iso-Propanol (82.3)	1.17
iso-Propanol (82.3)	n-Propanol (97.3)	1.78
Ethanol (78.4)	n-Propanol (97.3)	2.10
Methanol (64.6)	Ethanol (78.4)	1.56
Methanol (64.6)	iso-Propanol (82.3)	2.26
Chloroform (61.2)	Acetic acid (118.1)	6.15

Table - 3. Some optimal relative volatilities that are used for distillation process design

The upcoming figures will show how the concentration of light component at condenser and reboiler varies when we vary variation in the different variables.

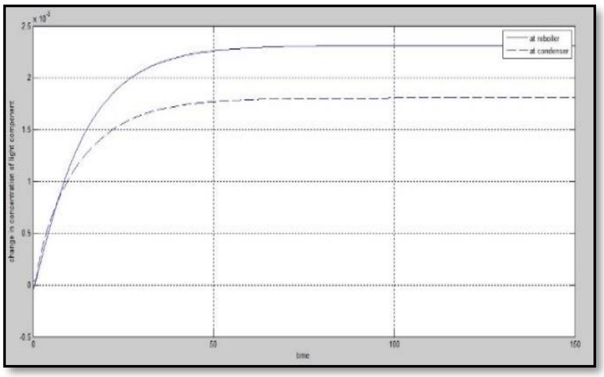

Fig. 9: Change in concentration due to 1% increase in reflux flow rate (L)

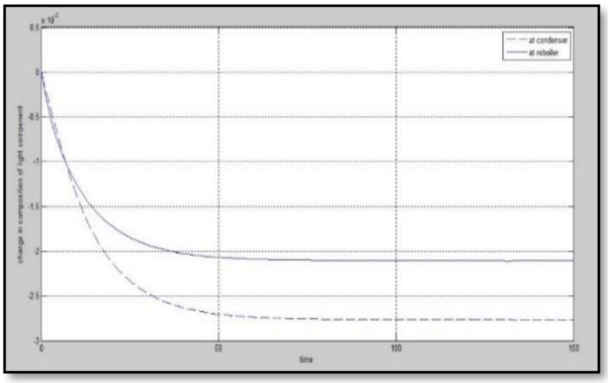

Figure. 10: Change in concentration due to 1% increase in vapor flow rate (V)

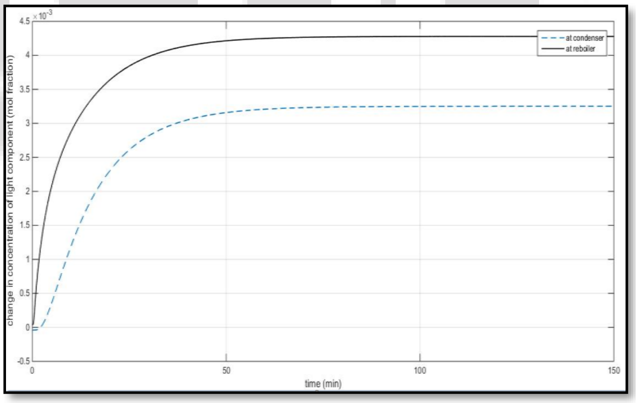

Fig. 11: Change in concentration due to 1% increase in feed flow rate (F)

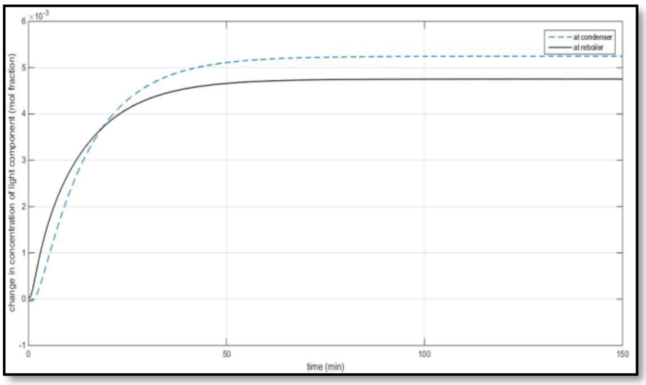

Fig. 12: Change in concentration due to 1% increase in feed composition (z_F)

From the above responses, it is clear that the change in the concentration of light component at condenser as well as at reboiler is significant due to the 1% variation in the feed composition (z_F) as compared to the same amount of variation in the feed flow rate (F).

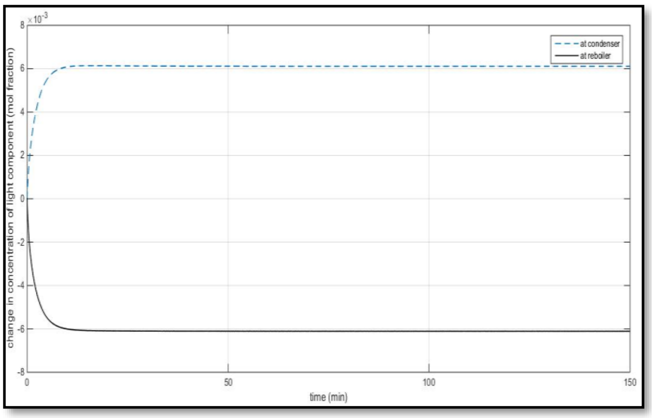

Fig. 13: Change in concentration due to 1% increase in relative volatility (alpha)

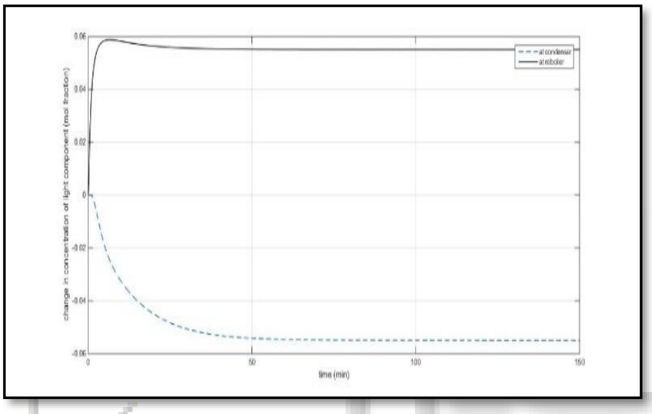

Fig. 14: Change in concentration due to feed tray location $(N_F)$is changed to 4 from 7

If the condition of feed gets changed then how the concentration of light component gets affected that is shown in the figure below.

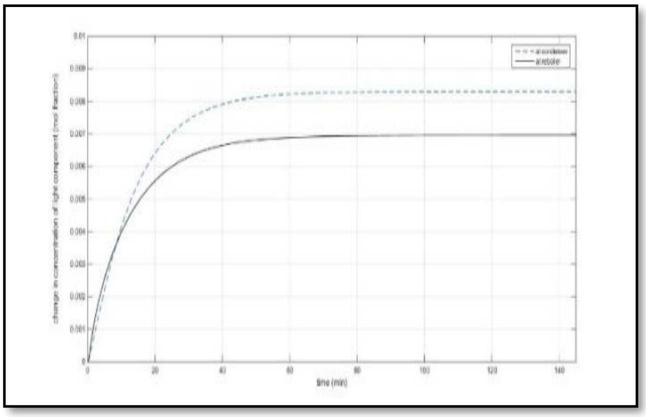

Fig. 15: Change in concentration due to 1% increase in q_F $(q_F = 1.01)$

Here, the value of q_F indicates whether the feed liquid is completely saturated or not. i.e. $q_F = 1$ for saturated feed.

IV. FOPDT MODEL DEVELOPMENT

The FOPDT model parameters can be determined from the actual process using a simple process reaction test. Several methods have been proposed to calculate the dead time, and time constant from the reaction curve. Here, for this work I have used Tangent Plus One Point method, which was proposed by C. Smith in order to find FOPDT model parameters.

The procedure to obtain values:

1) If the system is in closed loop, then we need to make it open to make it in manual mode of operation.
2) Give step change in input to process.
3) We will get S shaped response as shown in the figure below.

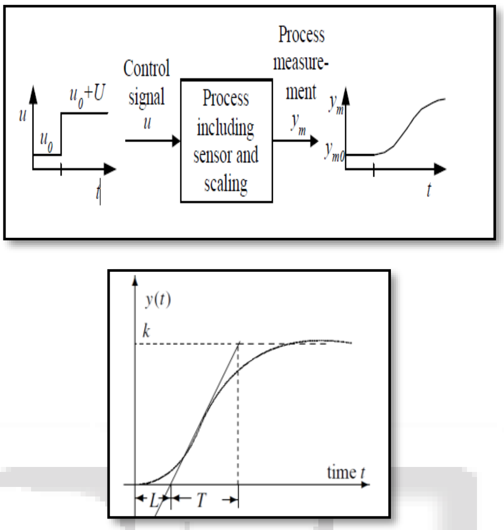

Fig. 16: FOPDT derivation

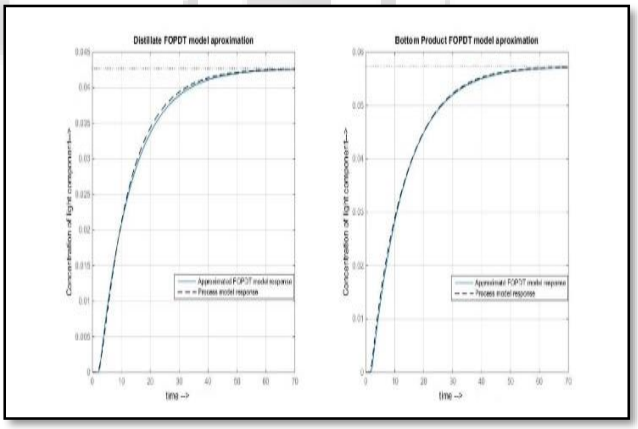

Fig. 17: FOPDT model response comparison

From this S shaped response we need to find values like, Dead time (L), Time Constant (T), Static gain (K), a=$T/(L * K)$ etc.

Here, for this work I used tangent plus one point method in order to derive a FOPDT model of binary distillation column. After getting the values of the variables mentioned above, we can get the approximated FOPDT model for distillate and bottom product compositions as listed in table-4.

FOPDT model equation	FOPDT model for distillate	FOPDT model for bottom

$G(s) = \frac{ke^{-Ls}}{Ts+1}$	$G(s) = \frac{0.0427e^{-(2.4115)s}}{(11.3423)s+1}$	$G(s) = \frac{0.0573e^{-(1.9776)s}}{([11.7761)s+1}$

Table. 4: FOPDT model equations

V. PID TUNING METHODS

The tuning of PID controller refers to the process of finding the value of the PID parameter (*namely* K_p, K_i, K_d), which can provide optimum performances.

The oldest method is trial and error method, which is simplest and easiest method but the problem is that it is very time consuming and not reliable. Instead of that, there are various methods available for PID tuning some of them are listed below [11].

1) Ziegler-Nichols open loop test tuning method
2) Cohen-Coon tuning method
3) Internal Model Control tuning method
4) ITAE tuning method
5) Lambda tuning method

Controller type	*Tuning parameters*		
	K_p	τ_i	τ_d
P	$\frac{1}{a}$	Very large	0
PI	$\frac{0.9}{a}$	3L	0
PID	$\frac{1.2}{a}$	2L	$\frac{L}{2}$

Table. 5:Ziegler-Nichols open loop test tuning method

Controller type	*Tuning parameters*		
	K_p	τ_i	τ_d
P	$\left(\frac{1}{a}\right)\left(1 + \frac{0.35\tau}{1-\tau}\right)$	Very large	0
PI	$\left(\frac{0.9}{a}\right)\left(1 + \frac{0.92\tau}{1-\tau}\right)$	$\frac{3.3-3\tau}{1+1.2\tau}L$	0
PD	$\left(\frac{1.24}{a}\right)\left(1 + \frac{0.13\tau}{1-\tau}\right)$	Very large	$\frac{0.27-0.36\tau}{1-0.87\tau}L$
PID	$\left(\frac{1.35}{a}\right)\left(1 + \frac{0.18\tau}{1-\tau}\right)$	$\frac{2.5-2\tau}{1-0.39\tau}L$	$\frac{0.37-0.37\tau}{1-0.81\tau}L$

Table 6. Cohen-Coon tuning method

Controller type	*Tuning parameters*		
	kk_c	τ_i	τ_d
PI	$\frac{2\tau+\theta}{2\lambda}$	$\tau + \frac{\theta}{2}$	0
PID	$\frac{2\tau+\theta}{2(\lambda+\theta)}$	$\tau + \frac{\theta}{2}$	$\frac{\tau\theta}{2\tau+\theta}$

Table 7. Internal Model Control (IMC) tuning method

Controller type	*Tuning parameters*		
	kk_c	$\frac{\tau}{\tau_i}$	$\frac{\tau_d}{\tau}$
PI setpoint	$0.586\left(\frac{\theta}{\tau}\right)^{-0.91}$	$1.030 - 0.165\left(\frac{\theta}{\tau}\right)$	–
PID setpoint	$0.965\left(\frac{\theta}{\tau}\right)^{-0.85}$	$0.796 - 0.1465\left(\frac{\theta}{\tau}\right)$	$0.308\left(\frac{\theta}{\tau}\right)^{-0.92}$
PIdisturbance	$0.859\left(\frac{\theta}{\tau}\right)^{-0.97}$	$0.674\left(\frac{\theta}{\tau}\right)^{-0.68}$	–
PID-disturbance	$1.357\left(\frac{\theta}{\tau}\right)^{-0.94}$	$0.842\left(\frac{\theta}{\tau}\right)^{-0.73}$	$0.381\left(\frac{\theta}{\tau}\right)^{-0.99}$

Table 8. ITAE tuning method

VI. RESPONSE ANALYSIS

In this section the response analysis is made for different PID tuning methods. The following figures will show the comparison of different PID tuning methods for set-point tracking as well as disturbance rejection.

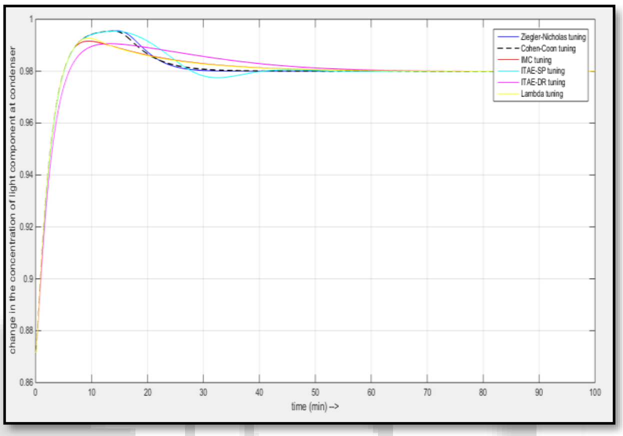

Fig. 18: Step-response comparison of different PID tuning methods

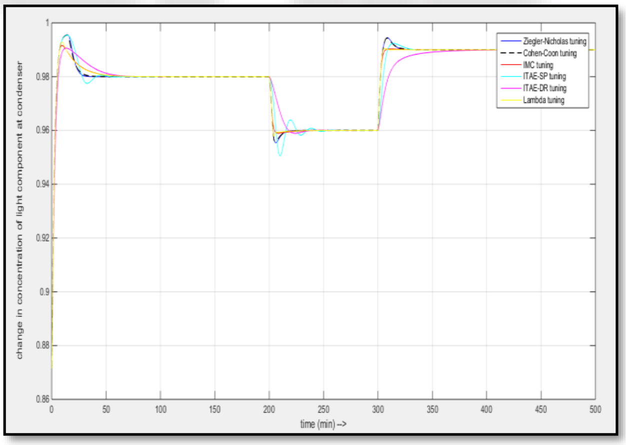

Fig. 19: Set-point tracking comparison (SP changed from 0.98 to 0.96 to 0.99)

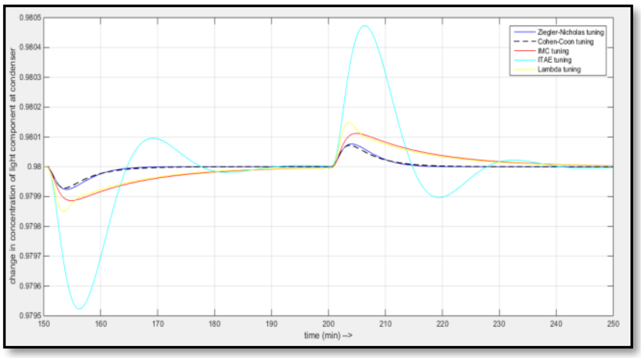

Fig. 20: Disturbance rejection comparison (first 10% decrease & then 10% increase in Feed flow rate)

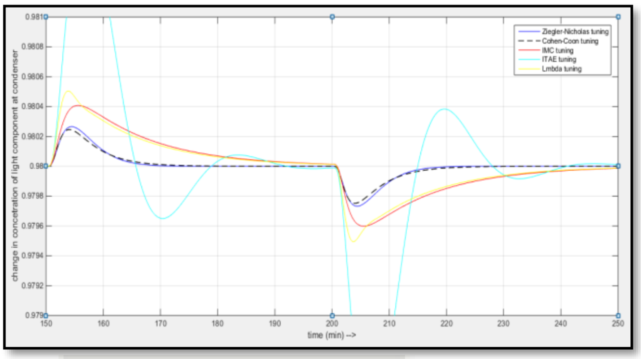

Fig. 21: Disturbance rejection comparison (first 10% decrease & then 10% increase in Feed composition)

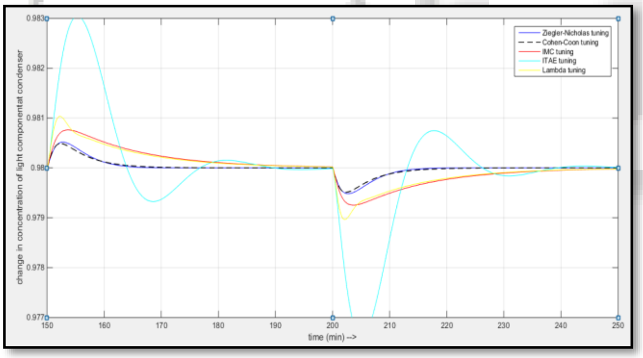

Fig. 22: Disturbance rejection comparison (first 10% decrease & then 10% increase in Feed condition)

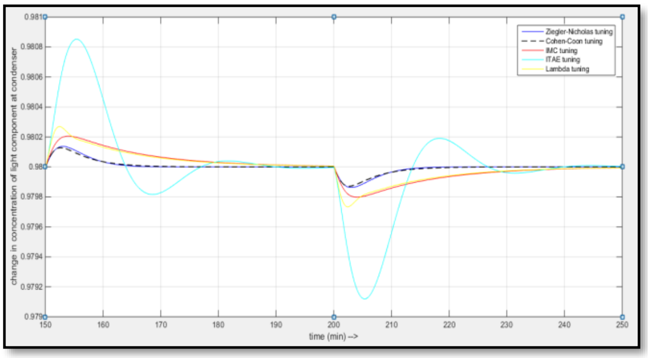

Fig. 23: Disturbance rejection comparison (first 10% decrease & then 10% increase in reflux rate)

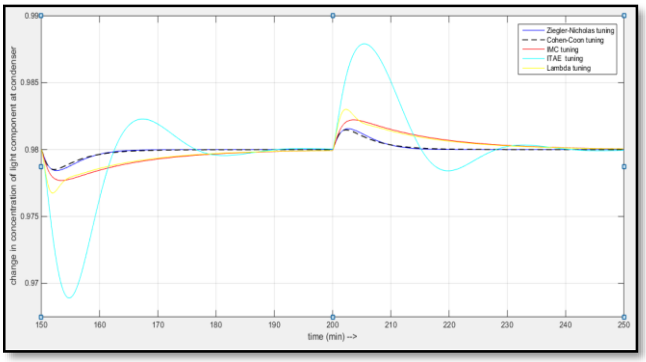

Figure 24. Disturbance rejection comparison (first 10% decrease & then 10% increase in vapor boil up rate)

The statistical analysis also made in terms of rise time, settling time, overshoot and steady-state error as shown in the table 8.

Tuning method	Rise tim (t_r)	Settling tim (t_s)	Overshoo (%)	e_{ss}
Z-N	3.4987	24.2660	1.5892	0
Cohen-Coon	3.4987	25.1904	1.5816	0
IMC	3.4987	33.8175	1.1829	0
ITAE (Set-point)	3.5115	34.4683	1.5791	0
ITAE(Disturbance)	4.0355	43.8031	1.0825	0
Lambda	3.5251	40.1757	1.0181	0

Table - 9. Response analysis for different tuning methods

Also the comparison is made for performance indexes i.e. RMS, MSE, IAE, ITAE, ISE, and ITSE etc. as shown in the table 9.

Tuning method	IAE	ITAE	ISE	ITSE
Z-N	0.4147	3.229	0.01634	0.04669
Cohen-Coon	0.4146	3.311	0.01621	0.04444
IMC	0.4196	4.585	0.0153	0.03442
ITAE (Set-point)	0.4725	4.766	0.01727	0.05799
ITAE (Disturbance)	0.5068	7.005	0.01726	0.05471
Lambda	0.4479	5.926	0.01539	0.04059

Table - 10. Performance index comparison

VII. Conclusion

The dynamics of distillation model, variation in the assumptions are made in order to develop models that can affect the response of process in a significant manner. So, we need to keep in mind these things while developing the model and controlling distillation column.

For this work, to control the distillate purity (concentration of light component at condenser), Cohen-Coon PID tuning proves to be more effective for set-point tracking as well as disturbance rejection.

VIII. Future Work

In this paper, it is shown that how we can develop the dynamic model of binary distillation column in Matlab tool and it is also shown that how the variation in different parameters of the model can affect the concentration of light component at the reboiler as well as at the condenser.

In order to control the composition of light component accurately at both ends we need to find optimal values of PID parameters so that exact amount of reflux or vapor rate to be updated in order to control the composition at particular end. So, the future work will be tuning of PID controller with advanced soft computing techniques like Ant Colony Optimization (ACO) and Particle Swarm Optimization (PSO) method.

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