

Dynamic Modelling and Model Predictive Control of a Binary Distillation Column

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A Final Year Project Report Submitted in
Partial Fulfilment of the Requirements for the
Degree of Bachelor of Science in Chemical Engineering
at
Bahá'í Institute for Higher Education (BIHE)

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September 2020

Abstract

Distillation columns are widely used in the industry as separation units. Maintaining the composition of the distillate and bottom products of a distillation column in a desired range with applying control techniques is a difficult issue due to the nonlinear characteristics of the process and existence of multiple inputs and multiple outputs of the column. In this project, a dynamic simulation of a binary water-ethanol distillation column is done with MATLAB and represented as a Simulink subsystem as well. An MPC controller is performed for controlling the column products compositions using Simulink MPC Toolbox. Also, PI and PID controllers are tuned for this model. The control simulation results are represented for evaluating the performance of MPC controller compared to PI and PID controllers.

Acknowledgment

I would like to express my very great appreciation to my supervisor, Dr. Sohrab Rohani. His guidance and support for this project are very much appreciated. I am also grateful for the technical support and advice given by Yuanyi Wu. My special thanks are extended to the Chemical Engineering Department of BIHE for their support. I would like to acknowledge the remarkable support provided by my parents during my education process and the preparation of my final year project.

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1. Introduction

Distillation columns are principal separation units widely used in the process industry. They are used to separate the liquid mixtures into their components. It is very important to maintain the composition of distillate and bottom products in a desired range to meet the demanded quality and purity of the products, and reduce the energy consumption. For a properly designed column, this can be achieved by an optimal control strategy. The control of the distillation columns is a complicated and challenging problem due to the existence of multiple inputs and multiple outputs (MIMO), constraints, significant interaction between the inputs and the outputs and nonlinear characteristics of the process. It makes the advanced Model Predictive Control (MPC) strategy a proper choice for controlling the composition of the top and bottom products in a distillation column.

1.1 Distillation Columns

Distillation is a process of mixtures separation based on the difference in the volatilities of components. The components separation process in the distillation columns works by the application and removal of heat as it provides a second phase with vaporization and condensation of the mixture. As the two vapor and liquid phases contact on the stages, mass transfer occurs due to the differences in concentrations, meaning that the more volatile components transfer from liquid phase to the vapor phase while the components with lower volatility transfer from vapor phase to liquid. Distillation columns can be designed as binary or multicomponent, also there are several different types of distillation columns for various applications. Packed column, tray column, vacuum, cryogenic, reactive and azeotropic are some examples of different types of the distillation columns.

Ethanol (C_2H_5OH) is an organic chemical component widely used in the industry. It is also used in medicine, as a solvent, and as a fuel. It can be manufactured by breakdown of sugar-based substances using yeasts (fermentation of sugars) or as a petroleum-derived product from petrochemical processes. Different processes for manufacturing ethanol, produce it as a mixture of ethanol and water. For industrial or other applications, it is required to purify ethanol.

In this project, the focus is on a tray distillation column, that is used to separate a binary mixture of water and ethanol. It consists of several parts that a typical distillation column is made of. This column contains N stages including a vertical vessel with $N-2$ trays, a condenser and reflux drum at the top of the column, and a reboiler at the bottom. The binary mixture enters the column from the feed tray that divides the column into rectifying (above feed tray) and stripping (below the feed tray) sections. The condenser cools and condenses the vapor from top of the column and provides the top product liquid stream that is rich with the more volatile component (ethanol) and the reflux stream that is recycled back to the column from top to increase the purity of the distillate product. The reboiler provides heat to form the required boil up vapor stream for the column that raises up from reboiler to the condenser in the column. It also provides the bottom product liquid stream that mostly contains the component with lower volatility (water) and contains only low amounts of ethanol. In this column, mass transfer occurs on the surface of trays as the two phases contact.

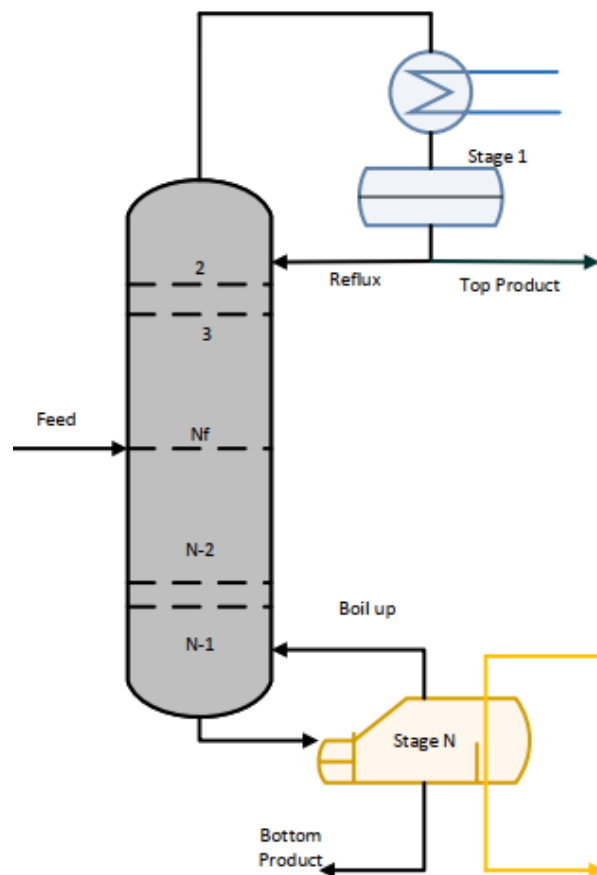


Figure 1. A two-product distillation column with condenser and reboiler

1.2 Model Predictive Control (MPC)

Model Predictive Control (MPC) is an advanced control approach which is a part of model-based control methods. Model predictive control has been widely used in the process industry since the 1980s due to the successful performance in complicated control problems, like systems with multiple inputs and outputs that have remarkable interactions, highly non-linear characteristics, constraints, and large time delays. As the optimization calculations in the MPC controllers can be complicated, a powerful computer might be required.

An MPC controller utilizes a dynamic model of the process to describe the relation between input and outputs to predict the future performance of the plant. The controller predicts the value of the controlled variables (output) over a finite horizon, and changes the manipulated variables (inputs) to minimize the difference between the predicted outputs and the desired target values. The MPC is a discrete time control method. At each sampling time instant, the controller simulates several future scenarios with the help of an optimizer to find the closest way to the desired values. It solves the optimization problems, so the determined optimal input can minimize the deviation of predicted outputs from the desired values. It also considers the constraints to avoid undesired consequences. At each time step, the control sequence is calculated over a finite number of future time steps. This value is called the prediction horizon, and shows how far the controller looks in the future. Also, the control horizon shows the number of control moves for optimization. A typical MPC controller implements only the first optimal input at each time step, and repeats the whole calculations for the next one, so that the predictions are updated based on the new measurements.

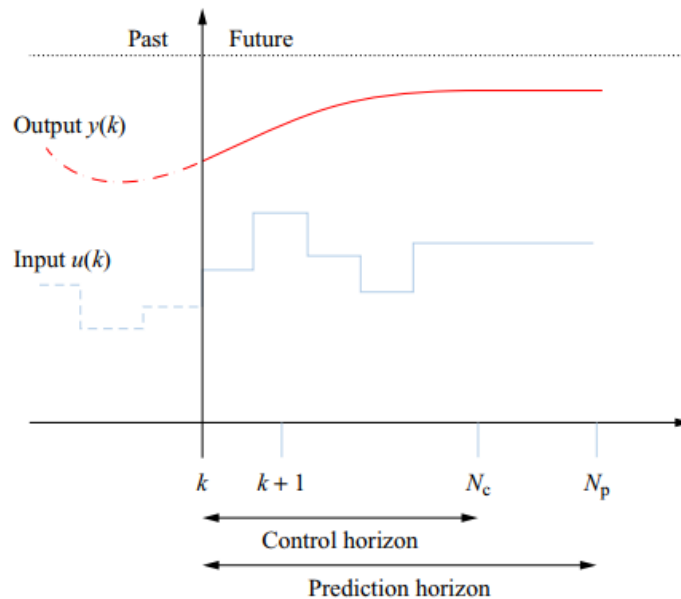


Figure 2. The control and prediction horizon principle in MPC with k sampling time instant

(credits: Coulson and Richardson's Chemical Engineering, volume 3B: Process Control, fourth edition)

Like any other model-based control system, the successful performance of an MPC controller significantly depends on the accuracy of the process model. An MPC controller can perform with nonlinear and linear plant models. A linear MPC works based on linearizing the model at an operating point. Frequently, the mismatch between the linearized model and the actual process does not expressively demote the performance of the controller. The optimal control problems are convex for a linear MPC. A nonlinear model predictive control known as NMPC utilizes a nonlinear plant model and the optimal control problems for it are not convex.

In this project the performance of a linear MPC controller is evaluated in maintaining the concentrations of the top and the bottom products of a binary water-ethanol distillation column at the desired values.

1.3 Scope of work

The distillation columns have several disturbances, multiple inputs, multiple outputs, and other characteristics that make them highly nonlinear and critical to control. The main objective of this project is to evaluate the performance of an MPC controller for controlling the purity and impurity of ethanol in the top and bottom products of a binary water-ethanol distillation column. The performance of this controller is compared with multiloops PI and PID controllers. One of the challenges in developing an optimal control system is construction of an accurate plant model. In this project a dynamic model of the plant is developed based on the mass and component mass balance equation on distillation column stages both in molar basis. A MATLAB code for this dynamic model is made to track the dynamic behavior of the distillation column. Once the dynamic model MATLAB code is developed and validated, it is used in making a distillation column subsystem in Simulink that can be linearized and used for tuning the controllers. The results will be used to evaluate the performance of an MPC controller compared to PI and PID controllers. Using MATLAB and Simulink makes it feasible to develop both dynamic model and control system simulation in one platform.

2. Review of the Previous Work

Distillation columns are widely used as separation units. Extensive research has been conducted on the design, operation and control of these units since the 20th. Control of top and bottom products composition in distillation columns is difficult because of the process nonlinear characteristics, and the interaction between the inputs and outputs. Obtaining a mathematical model of the distillation column is necessary for studying and evaluating the performance of different control techniques. A binary distillation model was proposed by Wood and Berry (1973) that has been used in many studies. Wood and Berry (1973) study applies the decoupling technique for controlling the composition of top and bottom products (x_D, x_B) of a binary water-methanol distillation column with reflux and boil up flow rates (R, S). This study represents the dynamic model of the distillation column as a transfer function:

$$\begin{bmatrix} x_D \\ x_B \end{bmatrix} = \begin{bmatrix} \frac{12.8e^{-s}}{16.7s + 1} & \frac{-18.9e^{-3s}}{21s + 1} \\ \frac{6.6e^{-7s}}{10.9s + 1} & \frac{-19.4e^{-3s}}{14.4s + 1} \end{bmatrix} \begin{bmatrix} R \\ S \end{bmatrix} + \begin{bmatrix} \frac{3.8e^{-8s}}{14.9s + 1} \\ \frac{4.9e^{-3.4s}}{13.2s + 1} \end{bmatrix} d$$

Here d is unmeasured feed flow rate.

Wood and Berry (1973) model is used as the distillation column model in many studies in the case of the distillation columns control, and it is extended to different control strategies.

MPC controllers were initially introduced to the industry in the 1970s, and significantly improved in the next 30 years. Today, MPC controllers are widely used in the process industry, and they are extended to different applications due to their successful performance in controlling complex systems. Many studies have been reported on the performance of the MPC controllers in chemical processes. Hovd et al. (1999) is one of the studies on the topic of developing MPC controllers for distillation columns. It evaluates the performance of MPC control strategy of a crude oil distillation column, and represents the benefits of this method.

The majority of MPC control of distillation columns, have used Wood and Berry (1973) models. A few studies have developed the dynamic models of the process and the MPC controllers. One of the recent studies addressing both on dynamic modelling and Model Predictive Control of a binary distillation column is Al-Shammari et al. (2014). The dynamic simulation in this work has been done by the Mathematica software and the MATLAB MPC Toolbox is used for the control simulations. The focus of this project is on developing a dynamic model and MPC control of a binary distillation column with MATLAB and Simulink.

3. Methodology

3.1 Dynamic Modelling and Simulation

Dynamic models are comprehensible models of systems that represent the variation of process variables with time. A process model expression in terms of a dynamic model can be used as a plant model for a model-based control strategy like an MPC controller. A dynamic model can be developed using two approaches: empirical approach that uses input and output data of a system or the theoretical approach that is based on first principles and conservation of physical properties. In this work, the theoretical approach is used to develop a dynamic model of a binary distillation column. Also, a MATLAB code of this model is developed that is a dynamic simulation of it. As the resulting model is nonlinear, the numerical method is used to solve the ODE equations in MATLAB. This dynamic simulation provides the opportunity to study the dynamic behavior of the process, and it is used as a plant model for developing an MPC controller for controlling the purity and impurities of top and bottom products of the column. It is also used for tuning the PI and PID controllers.

3.1.1 Theoretical Dynamic Model

As distillation columns are complex process units, it is necessary to consider some assumptions in order to make the model simpler and manageable for further steps.

In this work the model is represented under the following assumptions:

1. The vapor holdup on each tray is negligible.
2. Liquid molar holdups of condenser and reboiler are assumed constant.
3. Constant liquid holdup on each tray is assumed.
4. The operation is isothermal. (no heat loss from column)
5. The heats of vaporization of the feed components are equal. For every mole of liquid vaporized, a mole of vapor is condensed, and the heat effects such as heat of solutions are negligible.
6. Vapor and liquid leaving each tray are in equilibrium (Vapor and liquid composition and physical equilibrium). Tray efficiency is 100%.
7. Each stage is perfectly mixed. Liquid composition is homogenous and its composition is equal to the composition of liquid leaving the stage.
8. Entrainment of liquid drops in vapor and occlusion of vapor bubbles in liquid are negligible.
9. The required time for fluid to pass through the plates is neglected.
10. Constant molar overflow is considered. The vapor and liquid flow rates are constant in the rectifying and stripping sections.
11. Condenser and reboiler are operating at steady state.
12. The condenser operates as a total condenser and there is no vapor holdup in the condenser.
13. Pressure drop along the column is negligible.
14. Relative volatility remains constant.

From the theoretical approach, the dynamic model can be derived from mole balance and component mole balance, under the mentioned assumptions. As the process operation is assumed to be isothermal, the energy balance equations are not required for dynamic modeling. The equations for the k^{th} stage based on the composition of more volatile component (ethanol) are as:

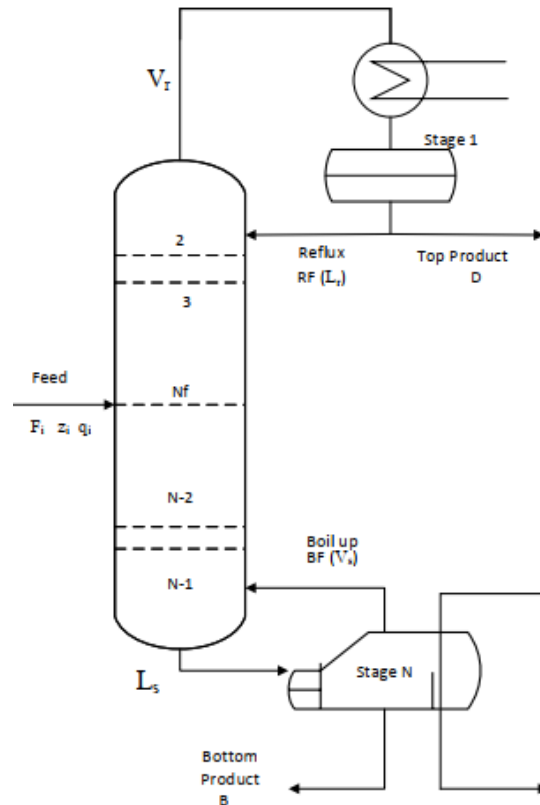


Figure 3. Binary water-ethanol distillation column condenser and reboiler

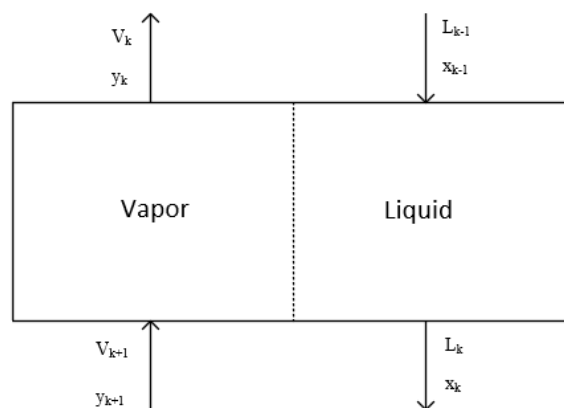


Figure 4. Model of phases flow on trays of distillation column

Table 1. Nomenclature

Nomenclature		
Symbol	Description	Unit
F_i	Inlet (feed) molar flow rate	$\frac{mol}{s}$
z_i	Inlet (feed) mole fraction of more volatile component	
q_i	Feed quality (liquid fraction)	
α	Relative volatility	
N	Number of stages (include condenser and reboiler)	
N_F	Feed tray stage (number of stage)	
D	Distillate molar flow rate	$\frac{mol}{s}$
B	Bottom product molar flow rate	$\frac{mol}{s}$
R_C	Reflux ratio	
R_B	Boil up ratio	
RF	Reflux molar flow rate	$\frac{mol}{s}$
BF	Boil up molar flow rate	$\frac{mol}{s}$
L_k	Molar flow rate of liquid leaving tray k	$\frac{mol}{s}$
L_r	Liquid molar flow rate in rectifying section	$\frac{mol}{s}$
L_s	Liquid molar flow rate in stripping section	$\frac{mol}{s}$
V_k	Molar flow rate of vapor leaving tray k	$\frac{mol}{s}$
V_r	Vapor molar flow rate in rectifying section	$\frac{mol}{s}$
V_s	Vapor molar flow rate in stripping section	$\frac{mol}{s}$
n_k	Liquid molar holdup on tray k	<i>mole</i>
x_k	Mole fraction of more volatile component in liquid leaving tray k	
y_k	Mole fraction of more volatile component in vapor leaving tray k	
n_1	Condenser holdup	<i>mole</i>
n_N	Reboiler holdup	<i>mole</i>

Liquid and vapor molar flow rate

Rectifying Section (above the feed stage):

$$L_r = L_1 = L_2 = \dots = L_{f-1} = RF \quad (1)$$

$$V_r = V_s + F_i(1 - q_i) = V_{f-1} = \dots = V_2 \quad (2)$$

Stripping Section (below the feed stage):

$$L_s = L_r + F_i q_i = L_{f+1} = \dots = L_{N-1} \quad (3)$$

$$V_s = V_N = \dots = V_{f+1} = BF \quad (4)$$

Feed tray (k=f)

Mole Balance:

$$\frac{dn_f}{dt} = F_i + L_{f-1} + V_{f+1} - L_f - V_f \quad (5)$$

$$\frac{dn_f}{dt} = F_i + L_r + V_s - L_s - V_r \quad (6)$$

$$\frac{dn_f}{dt} = F_i + L_r + V_s - L_r - F_i q_i - V_s - F_i(1 - q_i) \quad (7)$$

$$\frac{dn_f}{dt} = 0 \quad (8)$$

Component Mole Balance:

$$\frac{dn_f x_f}{dt} = F_i z_i + L_{f-1} x_{f-1} + V_{f+1} y_{f+1} - L_f x_f - V_f y_f \quad (9)$$

$$x_f \frac{dn_f}{dt} + n_f \frac{dx_f}{dt} = F_i z_i + L_{f-1} x_{f-1} + V_{f+1} y_{f+1} - L_f x_f - V_f y_f$$

$$\frac{dn_f}{dt} = 0$$

$$\frac{dx_f}{dt} = \frac{1}{n_f} (F_i z_i + L_{f-1} x_{f-1} + V_{f+1} y_{f+1} - L_f x_f - V_f y_f) \quad (10)$$

$$n_f = n_k \quad (11)$$

$$\frac{dx_f}{dt} = \frac{1}{n_k} (F_i z_i + L_r x_{f-1} + V_s y_{f+1} - L_s x_f - V_r y_f) \quad (12)$$

kth tray ($k \neq f$, $1 < f < N$)

Mole Balance:

$$\frac{dn_k}{dt} = L_{k-1} + V_{k+1} - L_k - V_k \quad (13)$$

Rectifying section($2 < k < f-1$):

$$\frac{dn_k}{dt} = L_r + V_r - L_r - V_r \quad (14)$$

$$\frac{dn_k}{dt} = 0 \quad (15)$$

Stripping section($f+1 < k < N-1$):

$$\frac{dn_k}{dt} = L_s + V_s - L_s - V_s \quad (16)$$

$$\frac{dn_k}{dt} = 0 \quad (17)$$

Component Mole Balance:

$$\frac{dn_k x_k}{dt} = L_{k-1} x_{k-1} + V_{k+1} y_{k+1} - L_k x_k - V_k y_k \quad (18)$$

$$x_k \frac{dn_k}{dt} + n_k \frac{dx_k}{dt} = L_{k-1} x_{k-1} + V_{k+1} y_{k+1} - L_k x_k - V_k y_k$$

$$\frac{dn_k}{dt} = 0$$

$$\frac{dx_k}{dt} = \frac{1}{n_k} (L_{k-1}x_{k-1} + V_{k+1}y_{k+1} - L_kx_k - V_ky_k) \quad (19)$$

Rectifying section($2 < k < f-1$):

$$\frac{dx_k}{dt} = \frac{1}{n_k} (L_r x_{k-1} + V_r y_{k+1} - L_r x_k - V_r y_k) \quad (20)$$

Stripping section($f+1 < k < N-1$):

$$\frac{dx_k}{dt} = \frac{1}{n_k} (L_s x_{k-1} + V_s y_{k+1} - L_s x_k - V_s y_k) \quad (21)$$

Condenser ($k = 1$)

Mole Balance:

$$\frac{dn_1}{dt} = V_2 - (L_1 + D) \quad (22)$$

$$\frac{dn_1}{dt} = 0 \quad (23)$$

$$D = V_2 - L_1 \quad (24)$$

$$D = V_r - L_r \quad (25)$$

Component Mole Balance:

$$\frac{dn_1 x_1}{dt} = V_2 y_2 - (L_1 + D)x_1 \quad (26)$$

$$n_1 \frac{dx_1}{dt} + x_1 \frac{dn_1}{dt} = V_2 y_2 - (L_1 + D)x_1$$

$$\frac{dn_1}{dt} = 0$$

$$\frac{dx_1}{dt} = \frac{1}{n_1} (V_2 y_2 - (L_1 + D)x_1) \quad (27)$$

$$(28)$$

$$\frac{dx_1}{dt} = \frac{1}{n_1} (V_r y_2 - (L_r + D)x_1)$$

Reboiler ($k = N$)

Mole Balance:

$$\frac{dn_N}{dt} = L_{N-1} - B - V_N \quad (29)$$

$$\frac{dn_N}{dt} = 0 \quad (30)$$

$$B = L_{N-1} - V_N \quad (31)$$

$$B = L_s - V_s \quad (32)$$

Component Mole Balance:

$$\frac{dn_N x_N}{dt} = L_{N-1} x_{N-1} - B x_N - V_N y_N \quad (33)$$

$$n_N \frac{dx_N}{dt} + x_N \frac{dn_N}{dt} = L_{N-1} x_{N-1} - B x_N - V_N y_N$$

$$\frac{dn_N}{dt} = 0$$

$$\frac{dx_N}{dt} = \frac{1}{n_N} (L_{N-1} x_{N-1} - B x_N - V_N y_N) \quad (34)$$

$$\frac{dx_N}{dt} = \frac{1}{n_N} (L_S x_{N-1} - B x_N - V_S y_N) \quad (35)$$

Auxiliary Equations

1. Equilibrium equation:

As the relative volatility is assumed to remain constant, the vapor-liquid equilibrium equation represents the relation of more volatile component composition in vapor and liquid phases as following for a binary system of A and B components (ethanol and water):

$$\alpha_{A,B} = \frac{\frac{y_A}{x_A}}{\frac{y_B}{x_B}} \quad (36)$$

$$y_{B,k} = 1 - y_{A,k} \quad (37)$$

$$x_{B,k} = 1 - x_{A,k} \quad (38)$$

$$y_{A,k} = \frac{\alpha_{A,B} x_{A,k}}{1 + x_{A,k}(\alpha_{A,B} - 1)} \quad (39)$$

2. Condenser:

$$R_c = \frac{L_1}{D} \quad (40)$$

$$L_1 = D R_c \quad (41)$$

$$D = V_2 - L_1 \quad (42)$$

$$L_1 = R_c V_2 - R_c L_1 \quad (43)$$

$$L_1 = \frac{V_2 R_c}{R_c + 1} \quad (44)$$

$$L_r = \frac{V_r R_c}{R_c + 1} \quad (45)$$

3. Reboiler:

$$R_B = \frac{V_N}{B} \quad (46)$$

$$V_N = B R_B \quad (47)$$

$$V_N + B = L_{N-1} \quad (48)$$

$$V_N = R_B L_{N-1} - R_B V_N \quad (49)$$

$$V_N = \frac{L_{N-1} R_B}{R_B + 1} \quad (50)$$

$$V_s = \frac{L_s R_B}{R_B + 1} \quad (51)$$

4. Francis weir equation:

This equation represents relation of liquid hold up on k^{th} tray (n_k) and liquid flow rate (L_k). In this equation, h_w and l_w are weir height and length. Also, g is gravitational acceleration, A_t is active area of tray, and ρ_k and $\overline{MW}_k$ are the average density and average molar weight on tray k .

$$n_k = \frac{\bar{\rho}_k}{\overline{MW}_k} \cdot A_t \cdot \left[h_w + 1.41 \left(\frac{L_k \overline{MW}_k}{\sqrt{g \cdot \bar{\rho}_k} \cdot l_w} \right)^{\frac{2}{3}} \right] \quad (52)$$

5. Modified Raoult's Law:

Raoult's law states that in an ideal mixture of liquids, the partial pressure of each component is equal to the mole fraction of that component in the mixture multiplied by the vapor pressure of the pure component. The deviation from this ideal situation is modified by the activity coefficient (γ_i). Modified Raoult's law is represented as:

$$y_i P = x_i \gamma_i P_i^{sat} \quad (53)$$

6. Wilson Model:

The activity coefficient can be predicted by Wilson model from the equation:

$$\ln(\gamma_k) = -\ln\left(\sum_{j=1}^{N_c} x_j A_{kj}\right) + 1 - \sum_{i=1}^{N_c} \frac{x_i A_{ik}}{\sum_{j=1}^{N_c} x_j A_{ij}} \quad (54)$$

$$A_{ij} = \frac{v_j}{v_i} \exp\left(-\frac{\lambda_{ij} - \lambda_{ii}}{RT}\right) \quad (55)$$

Degrees of Freedom

The degrees of freedom for a system can be shown by:

$$\text{Degrees of freedom} =$$

$$\text{Number of variables} - \text{Number of equations} - \text{Number of disturbances}$$

In a typical system, the degree of freedom should be zero if the model is supposed to have a unique solution. As there are two degrees of freedom here, two controller equations are required for this system. Overall degree of freedom analysis for the distillation column is:

Table 2. Degree of freedom analysis

Degree of freedom		
Number of variables	• Condenser: ○ D ○ R_c ○ x_1 ○ n_1 • Reboiler: ○ B ○ R_B ○ x_N ○ y_N ○ n_N • Feed tray: ○ F_i ○ q_i ○ z_i • All trays including feed tray ($\times N-2$): ○ x_k ○ y_k • n_k • L_k ○ L_r ○ L_s • V_k ○ V_r ○ V_s	$17 + 2(N - 2)$
State equations	• Condenser: ○ Equation 25 ○ Equation 28 • Reboiler: ○ Equation 32 ○ Equation 35 • All trays including feed tray ($\times N-2$): ○ Component Balance: Equation 12 or 20 or 21 • Molar Balance: ○ Equation 6 ○ Equation 14 ○ Equation 16	$7 + (N - 2)$
Auxiliary equations	• Reflux flow rate: ○ Equation 45 • Boil up flow rate ○ Equation 51 • Vapor flow rate ○ Equation 2 • Liquid flow rate ○ Equation 3 • All trays including feed tray ($\times N-2$): ○ Equilibrium Equation: Equation 39 • Equilibrium Equation for reboiler: ○ Equation 39	$5 + (N - 2)$
Disturbances	• F_i • x_i • q_i	3
Degree of freedom	$[17 + 2(N - 2)] - [15 + 2(N - 2)] = 2$	

3.1.2 Dynamic Simulation

In order to study the dynamic behavior of the distillation column a MATLAB code is developed based on the equations from the theoretical dynamic model with MATLAB software version 2019b. The code is presented in [Appendix](#). The molar basis mass and component mass balance equations and the vapor-liquid equilibrium equations from dynamic modelling are used for writing the code. The model parameters were defined as global variables. Due to the nonlinearity and complexity of the developed mathematical model, a numerical approach should be used to solve the model. In order to solve the Ordinary Differential Equations (ODEs) of the model, the ode45 solver of MATLAB is employed. This is a versatile solver for non-stiff problems with medium accuracy. The numerical values of model parameters are estimated from routine operating data and estimation from McCabe Thiele method. The numerical values of parameters, the ode45 solver, and required time span are represented in an individual MATLAB m file.

It is important to validate the results from the dynamic model as the accuracy of the dynamic model has a significant impact on the controller performance. One of the methods for validating the data from a computer simulation model is to compare its results with an accurate simulation model. Aspen HYSYS is a powerful process simulation software that is widely used in the industry. This software is extensively used for reliable and accurate modeling of chemical plants and unit operations. For verifying the validity of the MATLAB model, a simulation of a binary water-ethanol distillation column has been done with the Aspen HYSYS V10 software with the same values for the model parameters. The Wilson property package has been selected as it is an appropriate package for multi-component systems and considers the activity coefficient from Wilson equation. In order to validate the MATLAB code simulation results, different values of reflux and boil up flow rates have been applied to both MATLAB and HYSYS simulations. The composition of ethanol in the distillate and bottom products resulted from the MATLAB simulation are compared with the results from HYSYS simulation.

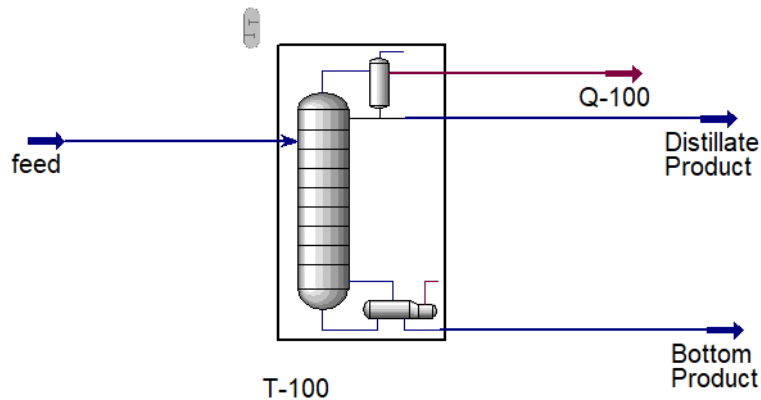


Figure 5. Distillation column HYSYS simulation

Some differences between the two models are expected as the assumptions and column characteristics are different. However, if the dynamic model simulation is expected to be valid, the rate of changes and the range of numbers are supposed to be close. Once the model is validated successfully, it can be used as the plant model for developing the control systems.

3.2 Control of Distillation Column

Developing an optimal control strategy for a distillation column is an important task in the industry, as controlling the purity and impurity of top and bottom outlet streams provides products with desired qualities, and influences the energy consumption. Multiple inputs and multiple outputs, interaction between inputs and outputs, and nonlinearity of distillation columns make their control a complex problem. Model Predictive Control (MPC) has a successful performance in controlling intricate systems due to its model-based strategy.

3.2.1 Model Predictive Control Toolbox™

The Model Predictive Control Toolbox of MATLAB that is presented as a block in the Simulink environment as well, is a collection of software that provides the ability to design and analyze the MPC strategy. This toolbox employs a plant model to supply prediction for the MPC control strategy. MPC Toolbox works as single-input single-output (SISO) or multi-input multi-output (MIMO) system. Disturbances can be added to the toolbox as unmeasured disturbances for feedback compensation or as measured disturbances for feedforward compensation. It can also involve plant's constraints and weights on variables. The toolbox is employed in this project in order to develop a linear MPC controller and track its performance.

3.2.2 Plant Model

Developing an optimal model-based control strategy like an MPC controller requires an accurate process model. For designing a linear MPC controller by MPC Toolbox, a linear plant model should be used. MPC Toolbox accepts plant models as linear time-invariant system (LTI) described by the equations or as input-output data models from the System Identification Toolbox. One of the ways for creating a LTI linear plant model is to linearize a nonlinear Simulink model to approximate the system around an operating point. In this work, the required model is provided as a subsystem of the binary water-ethanol distillation column. The MATLAB code generated for dynamic model simulation is used to make this subsystem in Simulink. This code is modified in order to be used in MATLAB function blocks of Simulink. The MATLAB code is first divided into five different functions, each representing one of the sections of the distillation column: condenser, rectifying, feed tray, stripping, and reboiler. Also, the global variables are removed, and any parameter that the code requires are added to the function blocks from constant blocks, as input signals, or connected from the blocks of the other sections. Integrators have been used for solving the ODEs that perform as ode45 in MATLAB. This subsystem model can be linearized around an operating point using linearizing app. Linearization can represent a state-space. State-space is a mathematical description of a system in terms of system state variables, inputs, and outputs related by a set of first order differential equations that is a proper description of the plant dynamics.

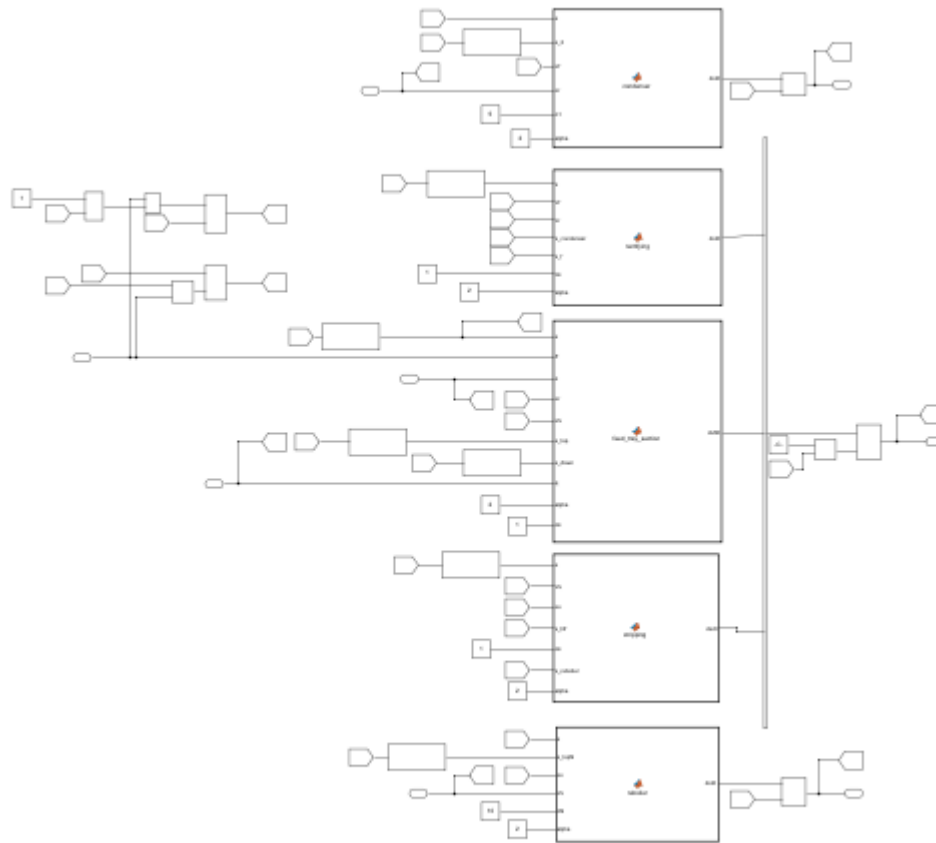


Figure 6. Distillation column subsystem in Simulink

3.2.3 MPC Control of Distillation Column

In this study, the Simulink MPC Toolbox is employed for evaluating the performance of an MPC controller for controlling the composition of ethanol in the top and bottom products. The required plant model for this toolbox is the distillation column subsystem in Simulink that is generated from modifying the dynamic modelling simulation in MATLAB. The toolbox linearizes the model around an operating point. Once the MPC structure is defined and linearized, the controller can be tuned. There are several guidelines for choosing the control parameters (sampling time, prediction horizon, and control horizon), adjusting constraints, weights, and scale factors on input and output variables. Generally, decreasing the sampling time improves the controller performance, but increases the

computational effort. So, it is important to test simulations with different sampling time to find a balance between these two factors. The value of the sampling time can be more or less than 1 second based on the application. The prediction horizon is related to the sampling time, but typically increasing the value of the prediction horizon improves the controller performance. However, a prediction horizon of more than 50 is rarely required. The control horizon should be smaller than the prediction horizon. It is usually between 2 to 20. Systems with smaller control horizons have faster computations. In this study, all these parameters are tuned based on guidelines and several tests on control performance.

3.2.4 PI and PID Control of Distillation Column

In order to evaluate the performance of the MPC controller the results can be compared with results from developing PI and PID controllers. These controllers use feedback control loop to continuously calculate the difference of the system output and the desired setpoint as an error signal. It will be employed to define the controller action getting the system outputs to desired setpoints. A PID controller applies correction in terms of proportional, integral, and derivative of the error while a PI controller applies only proportional and integral. In this work, one PI or PID controller is employed to control the composition of the top product of the distillation column and one is used for controlling the bottom product. The state space generated from linearizing the distillation column subsystem in Simulink is used for tuning the PI and PID controllers. As the distillation column is a MIMO system, controlling it with these controllers is challenging due to the significant interaction between the inputs and outputs of the system known as coupling. One of the methods for controlling a MIMO system with PI or PID controllers is by using the decoupling strategies that removes the interactions between inputs and outputs. In this project, the performance of PI and PID controllers are tested both with a decoupling matrix in series with controllers and without it. In order to tune the controller parameters, the looptune command in MATLAB is used that provides the ability to tune a MIMO feedback loop. The tuned parameters from looptune are then applied to the control system developed in Simulink for testing the performance.

4. Results and Discussion

4.1 Dynamic Modelling Results

As previously explained, a MATLAB code has been developed for dynamic modelling of the distillation column based on the theoretical dynamic model equations. Numerical values are considered for model parameters to run the code. The considered distillation column has $N=19$ stages consisting of 17 trays, a condenser at top of the column, and a reboiler at the bottom. The feed stream is entering the column from 9th tray (10th stage) with a molar flow rate of 50 mol/s. This stream is considered to be a binary mixture of water and ethanol with the quality of 0.9 and molar composition of 60% ethanol and 40% of water. Liquid holdups on the condenser and the reboiler are considered to be 5 and 10 moles. Liquid molar holdup on the trays is 1 mole. The relative volatility is considered to be 2, and the initial values of reflux and boil up flow rates are 52 mol/s and 78 mol/s. The initial value considered for composition of the stages is 0.6 of ethanol which is the composition of feed stream.

Table 3. Nomenclature table with model parameters values

Nomenclature			
Symbol	Description	Unit	Quantity
F_i	Inlet (feed) molar flow rate	$\frac{mol}{s}$	50
z_i	Inlet (feed) mole composition of more volatile component		0.6
q_i	Feed quality (liquid fraction)		0.9
α	Relative volatility		2
N	Number of stages (include condenser and reboiler)		19
N_F	Feed tray stage (number of stage)		10
RF	Reflux molar flow rate	$\frac{mol}{s}$	52
BF	Boil up molar flow rate	$\frac{mol}{s}$	78
n_k	Liquid molar holdup on tray k	<i>mole</i>	1
n_1	Condenser holdup	<i>mole</i>	5
n_N	Reboiler holdup	<i>mole</i>	10

Running the code for 10 seconds time span with the mentioned values for parameters result in the composition of ethanol for each stage:

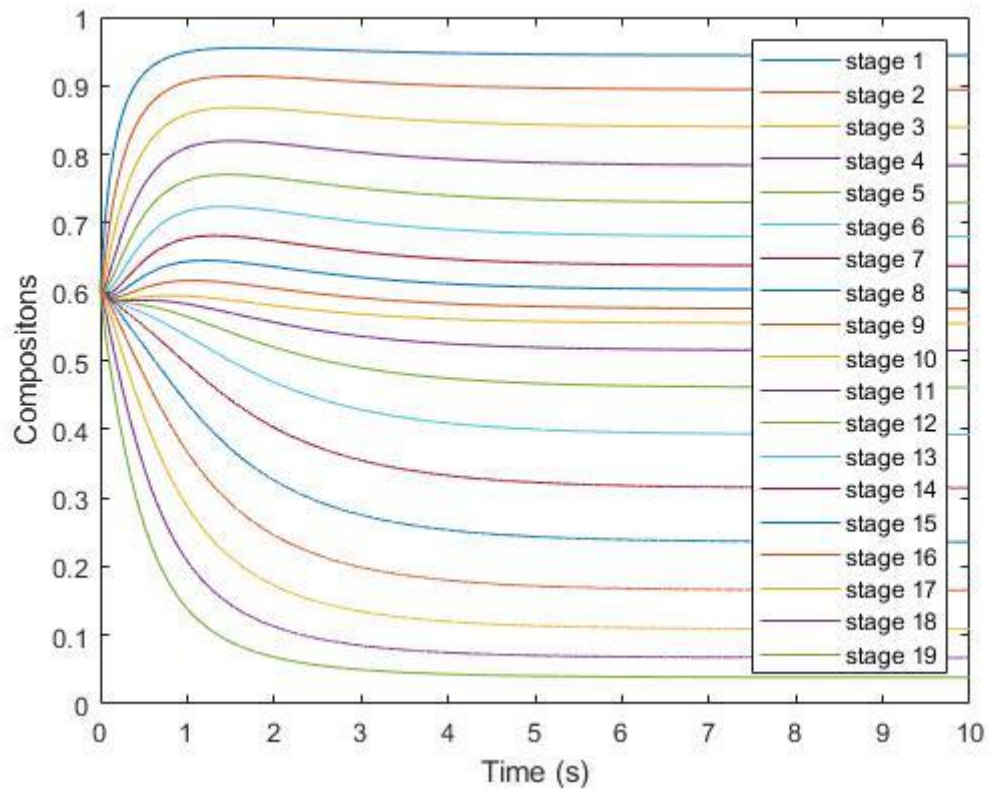


Figure 7. Ethanol composition for distillation column stages from MATLAB simulation

Table 4. Ethanol composition for distillation column stages from MATLAB

Stage	Symbol	Composition
1	x_1	0.944
2	x_2	0.894
3	x_3	0.840
4	x_4	0.784
5	x_5	0.730
6	x_6	0.680
7	x_7	0.638
8	x_8	0.603
9	x_9	0.575
10	x_{10}	0.554
11	x_{11}	0.515
12	x_{12}	0.461
13	x_{13}	0.392
14	x_{14}	0.314
15	x_{15}	0.236
16	x_{16}	0.165
17	x_{17}	0.109
18	x_{18}	0.067
19	x_{19}	0.039

4.2 Dynamic Model Validation

Due to the importance of dynamic model accuracy, the outcome data from MATLAB code model simulation should be validated. In this work, the model validation is based on a simulation of a binary water-ethanol distillation column on Aspen HYSYS V10 software with the same values for the model parameters. The Wilson property package is chosen, also ethanol and water are the only selected components for this simulation. A distillation column equipped with condenser and reboiler has been chosen for this simulation. The feed stream enters the column with the same condition considered for MATLAB simulation. The pressure of the stream is considered to be 1 atm. As pressure drop along the column is neglected for dynamic modeling, the pressure of condenser and reboiler are also considered as 1 atm. The column has 17 trays and the feed enters the column from the 9th tray. The

condenser operates as a total condenser, and the efficiency of all stages is 100%. Liquid flow rate of condenser stage and vapor flow rate from reboiler stage are applied as specs to the model. In order to validate the MATLAB code simulation results, different values of reflux and boil up flow rates with step changes of 5 mol/s have been applied to both MATLAB and HYSYS simulations. The value of boil up flow rate remained 78 mol/s while applying changes on reflux flow rate, also the reflux flow rate has the constant value of 52 mol/s during the step changes for boil up flow rate. The composition of ethanol in the distillate and bottom products resulted from the MATLAB simulation are compared with the results from HYSYS simulation.

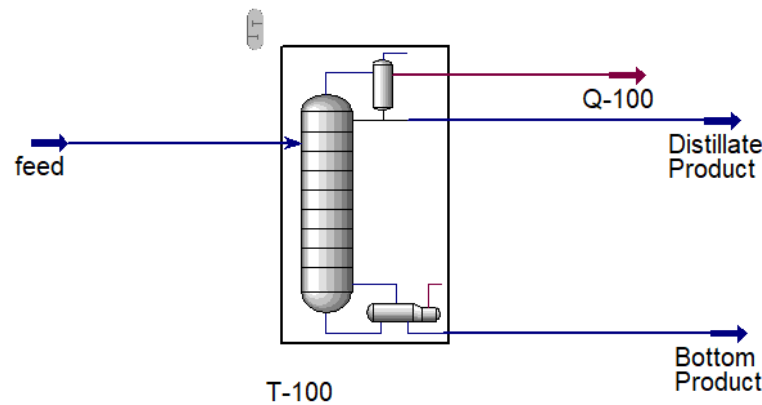


Figure 8. Aspen HYSYS simulation of binary distillation column

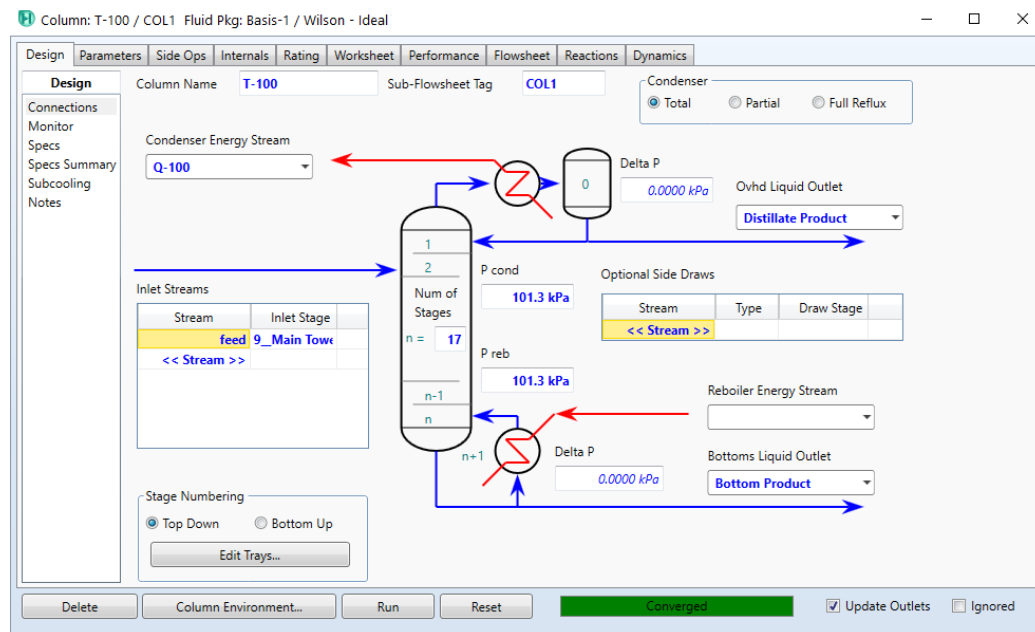


Figure 9. Aspen HYSYS simulation in details

The results for fixed values of 52 mol/s and 78 mol/s for reflux and boil up flow rates from both simulations are as:

Table 5. Ethanol composition for distillation column stages from MATLAB and HYSYS

Stage	Symbol	Composition of Ethanol	
		MATALB	HYSYS
1	x_1	0.944	0.819
2	x_2	0.894	0.798
3	x_3	0.834	0.779
4	x_4	0.784	0.760
5	x_5	0.730	0.742
6	x_6	0.680	0.723
7	x_7	0.638	0.703
8	x_8	0.603	0.681
9	x_9	0.575	0.655
10	x_{10}	0.554	0.623
11	x_{11}	0.515	0.623
12	x_{12}	0.461	0.622
13	x_{13}	0.392	0.621
14	x_{14}	0.314	0.619
15	x_{15}	0.236	0.613
16	x_{16}	0.165	0.599
17	x_{17}	0.109	0.560
18	x_{18}	0.067	0.447
19	x_{19}	0.039	0.167

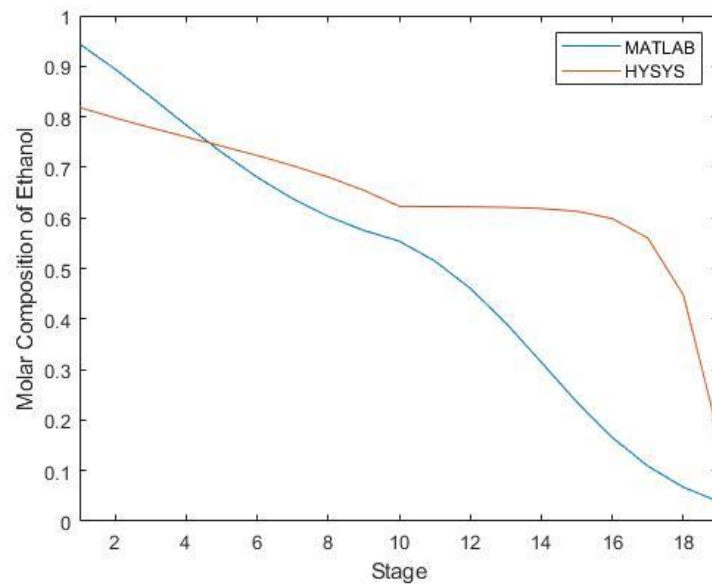


Figure 10. Ethanol composition for distillation column stages from MATLAB and HYSYS

The results from model validation with step changes on reflux and boil up flow rates are presented in the following graphs and tables:

Table 6. Results from changing reflux flow rate in MATLAB and HYSYS

Boil up flow rate (mol/s)	Reflux flow rate (mol/s)	Distillate composition from MATLAB	Distillate composition from HYSYS	Bottom composition from MATLAB	Bottom Composition from HYSYS
78	40	0.697	0.668	0.002	0
	45	0.788	0.744	0.006	0
	52	0.944	0.819	0.039	0.166
	55	0.974	0.825	0.125	0.267
	60	0.989	0.835	0.269	0.374
	65	0.995	0.844	0.378	0.446
	70	0.997	0.851	0.460	0.500
	75	0.999	0.857	0.524	0.542
	80	0.999	0.861	0.575	0.577

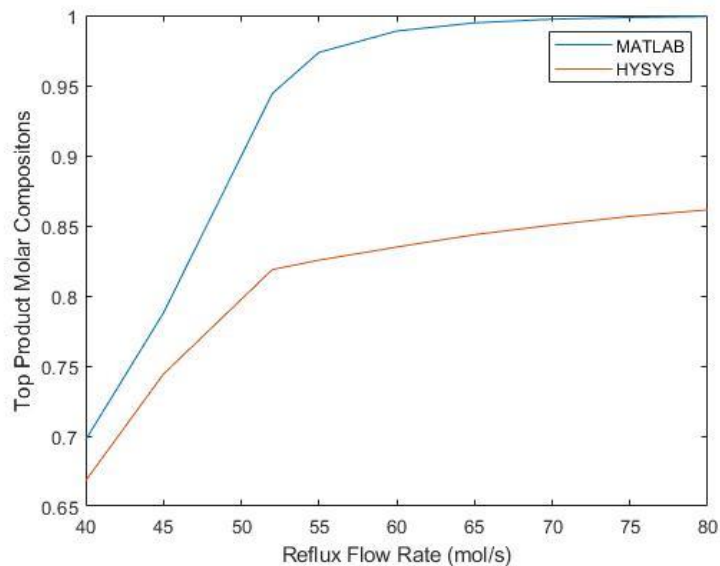


Figure 11. Composition change from changing reflux flow rate in MATLAB and HYSYS (top Product)

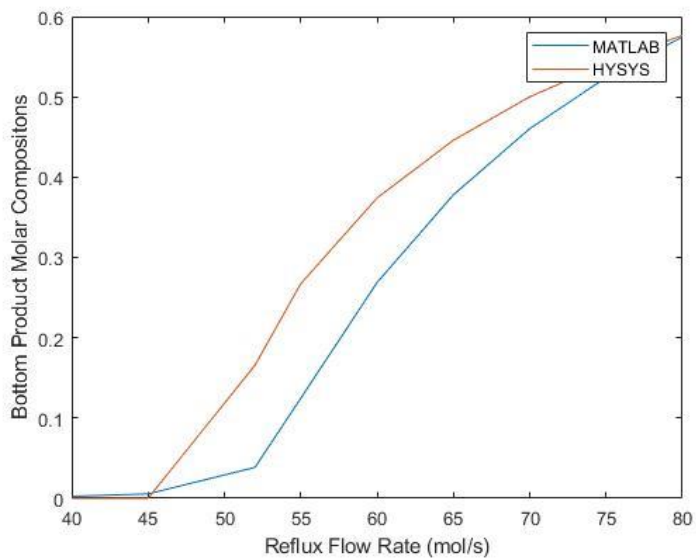


Figure 12. Composition change from changing reflux flow rate in MATLAB and HYSYS (bottom product)

Table 7. Results from changing boil up flow rate in MATLAB and HYSYS

Reflux flow rate (mol/s)	Boil up flow rate (mol/s)	Distillate composition from MATLAB	Distillate composition from HYSYS	Bottom composition from MATLAB	Bottom Composition from HYSYS
52	50	0.999	0.860	0.575	0.579
	55	0.997	0.853	0.524	0.546
	60	0.995	0.844	0.461	0.506
	65	0.991	0.838	0.380	0.453
	70	0.983	0.830	0.274	0.382
	75	0.969	0.823	0.131	0.274
	78	0.944	0.819	0.039	0.166
	85	0.788	0.740	0.004	0
	90	0.697	0.664	0.002	0

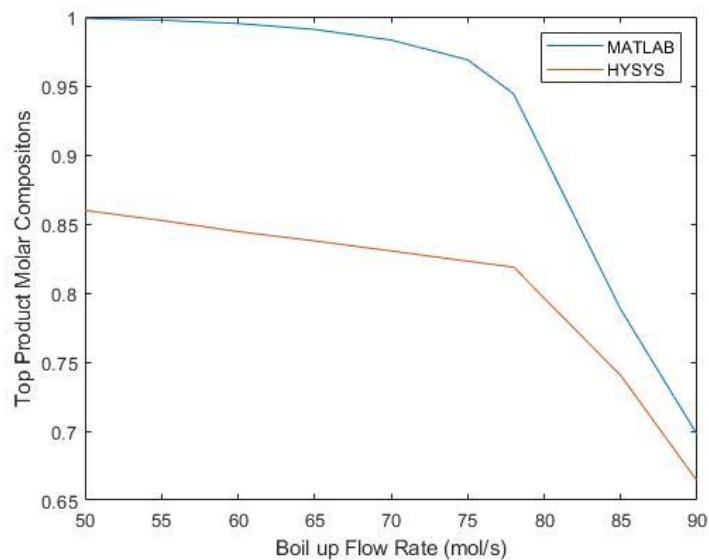


Figure 13. Composition change from changing boil up flow rate in MATLAB and HYSYS (top product)

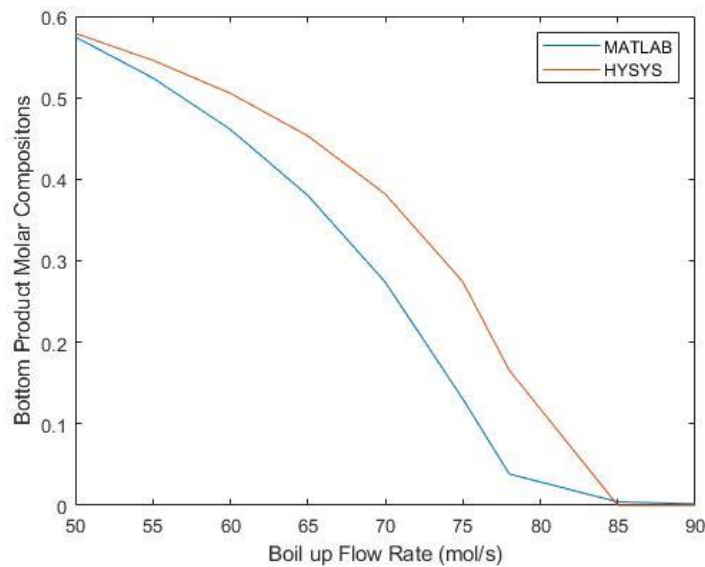


Figure 14. Composition change from changing boil up flow rate in MATLAB and HYSYS (bottom product)

The results from simulations are different, especially on the composition of top products, but the trends are mainly the same. The default assumptions of HYSYS software are different from the assumptions considered for dynamic modeling in this work model, and some other values like liquid holdup on trays, condenser and reboiler, and even heat energy fundamentals in the HYSYS model may vary from the developed model with MATLAB. These discrepancies of models justify the differences between the results from two simulations. Considering the total range and the rate of changes, the performance of the dynamic model simulation can be generally considered acceptable and valid.

4.3 Distillation Column Subsystem

The MATLAB code developed for dynamic modeling is modified for making a distillation column subsystem in Simulink with employing the MATLAB function blocks and integrators. For testing the performance, the subsystem is runned with the same numerical values used for running the MATLAB.

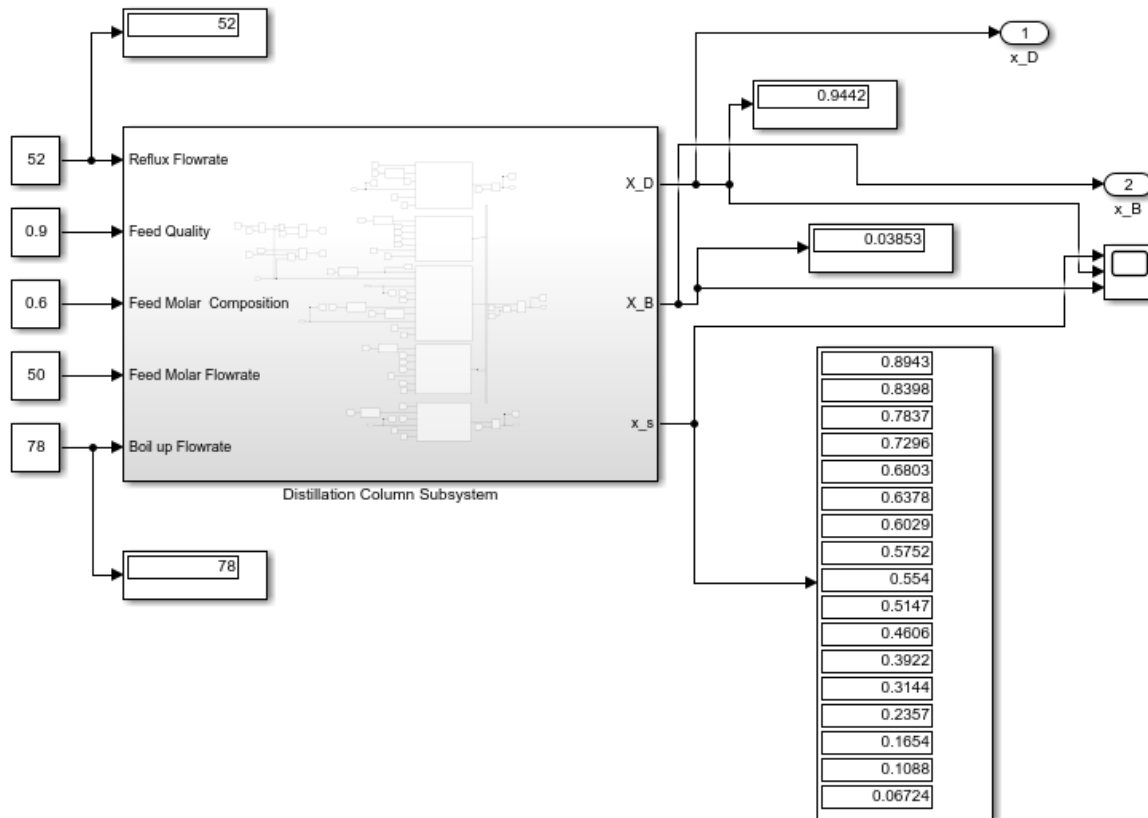


Figure 15. Distillation column subsystem in Simulink run for 10 seconds

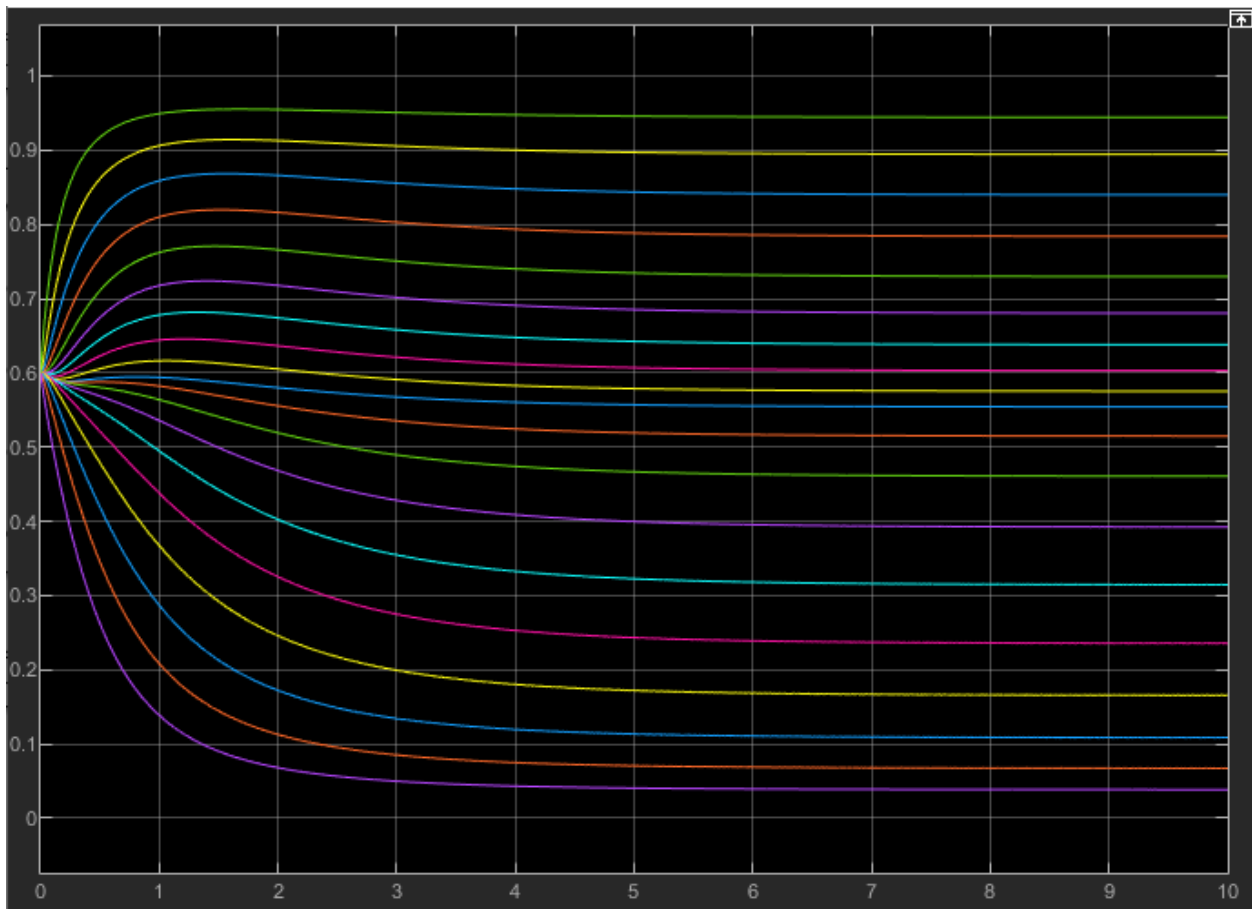


Figure 16. Scope of composition of ethanol for distillation column stages from Simulink

It is clear that the results from running the Simulink subsystem are identical to the validated values from the MATLAB model.

For linearizing the subsystem, the values of reflux and boil up flow rates are replaced by inlet signal blocks. In order to do the linearization, an operating point should be defined. For defining the operating point, the desired values for top and bottom product compositions (resulted from integrator) are set as 0.9 and 0.1. The details of the created operating point show that the values of actual derivatives are very small and close to zero, that means the operating point is at steady state.

State	Desired Value	Actual Value	Desired dx	Actual dx
BDistillationColumnraw/Distillation Column Subsystem/Integrator				
State - 1	0.9	0.9	0	-1.4211e-15
BDistillationColumnraw/Distillation Column Subsystem/Integrator1				
State - 1	[-Inf , Inf]	0.81818	0	1.1546e-14
State - 2	[-Inf , Inf]	0.74885	0	-1.9984e-14
State - 3	[-Inf , Inf]	0.69411	0	1.4433e-14
State - 4	[-Inf , Inf]	0.65325	0	-1.4433e-14
State - 5	[-Inf , Inf]	0.62402	0	1.3767e-14
State - 6	[-Inf , Inf]	0.60372	0	1.9984e-15
State - 7	[-Inf , Inf]	0.58994	0	2.1094e-15
State - 8	[-Inf , Inf]	0.5807	0	-1.2268e-14
State - 9	[-Inf , Inf]	0.57457	0	0
State - 10	[-Inf , Inf]	0.56042	0	-1.9984e-15
State - 11	[-Inf , Inf]	0.53828	0	1.7764e-14
State - 12	[-Inf , Inf]	0.5049	0	2.6645e-15
State - 13	[-Inf , Inf]	0.45721	0	4.4409e-16
State - 14	[-Inf , Inf]	0.3941	0	-1.1546e-14
State - 15	[-Inf , Inf]	0.31854	0	7.9936e-15
State - 16	[-Inf , Inf]	0.23817	0	-3.5527e-15
State - 17	[-Inf , Inf]	0.1628	0	1.7764e-15
BDistillationColumnraw/Distillation Column Subsystem/Integrator2				
State - 1	0.1	0.1	0	-1.7764e-16

Figure 17. Details of the operating point

By linearizing the distillation column around the created operating point, Simulink represents a two input and two output state space model with 19 stages. The state space continuous time is in the form of:

$$\dot{x} = Ax + Bu$$

$$y = Cx + Du$$

Where x is the state vector and y is the output vector. A , B , C , and D are state space matrixes. A is the state matrix, B is input, and C is output matrix. Also, D is the feedforward matrix. The state space matrixes from linearization are represented as following:

Matrix A

A =

Columns 1 through 15

-13.3831	8.0968	0	0	0	0	0	0	0	0	0	0	0	0	0
35.6653	-76.1491	43.7573	0	0	0	0	0	0	0	0	0	0	0	0
0	35.6653	-79.4226	46.6308	0	0	0	0	0	0	0	0	0	0	0
0	0	35.6653	-82.2962	48.9642	0	0	0	0	0	0	0	0	0	0
0	0	0	35.6653	-84.6295	50.7429	0	0	0	0	0	0	0	0	0
0	0	0	0	35.6653	-86.4083	52.0351	0	0	0	0	0	0	0	0
0	0	0	0	0	35.6653	-87.7005	52.9416	0	0	0	0	0	0	0
0	0	0	0	0	0	35.6653	-88.6069	53.5620	0	0	0	0	0	0
0	0	0	0	0	0	0	35.6653	-89.2273	53.9795	0	0	0	0	0
0	0	0	0	0	0	0	0	35.6653	-134.6449	50.8565	0	0	0	0
0	0	0	0	0	0	0	0	0	80.6653	-131.5219	52.3308	0	0	0
0	0	0	0	0	0	0	0	0	0	80.6653	-132.9961	54.6782	0	0
0	0	0	0	0	0	0	0	0	0	0	80.6653	-135.3436	58.3155	0
0	0	0	0	0	0	0	0	0	0	0	0	80.6653	-138.9809	63.7147
0	0	0	0	0	0	0	0	0	0	0	0	0	80.6653	-144.3800
0	0	0	0	0	0	0	0	0	0	0	0	0	0	80.6653
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Figure 18. State space matrix A

Columns 16 through 19

0	0	0	0
0	0	0	0
0	0	0	0
0	0	0	0
0	0	0	0
0	0	0	0
0	0	0	0
0	0	0	0
0	0	0	0
0	0	0	0
0	0	0	0
0	0	0	0
0	0	0	0
0	0	0	0
0	0	0	0
0	0	0	0
71.2270	0	0	0
-151.8924	80.7731	0	0
80.6653	-161.4385	91.5837	0
0	80.6653	-172.2490	102.3394
0	0	8.0665	-12.1089

Figure 19. State space matrix A (continued)

Matrix B

$$B = \begin{bmatrix} 0 & 0 \\ 0.0818 & -0.0436 \\ 0.0693 & -0.0370 \\ 0.0547 & -0.0292 \\ 0.0409 & -0.0218 \\ 0.0292 & -0.0156 \\ 0.0203 & -0.0108 \\ 0.0138 & -0.0073 \\ 0.0092 & -0.0049 \\ 0.0061 & -0.0115 \\ 0.0142 & -0.0184 \\ 0.0221 & -0.0288 \\ 0.0334 & -0.0435 \\ 0.0477 & -0.0621 \\ 0.0631 & -0.0822 \\ 0.0756 & -0.0985 \\ 0.0804 & -0.1047 \\ 0.0754 & -0.0982 \\ 0.0063 & -0.0082 \end{bmatrix}$$

Figure 20. State space matrix B

Matrix C

$$C = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Figure 21. State space matrix C

Matrix D

$$D = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$

Figure 22. State space matrix D

4.4 MPC Controller Performance

In order to evaluate the performance of an MPC controller for controlling the composition of ethanol in the top and bottom products, the distillation column Simulink subsystem is connected to the MPC Toolbox. The reflux and boil up flow rates are manipulated variables (inputs), and the compositions of ethanol in top and bottom products are controlled variables (outputs). Also, the disturbances (feed flow rate, composition, and quality) are considered to be constant. The desired setpoint values for compositions of top and bottom products are 0.95 and 0.05. As the MPC Toolbox linearizes the connected plant, there is no need to linearize the block separately, and only the operating point should be created. For defining the operating point, the desired values for top and bottom product compositions are set as 0.9 and 0.1. The values of the actual derivatives are very small and close to zero, that shows the operating point is at steady state.

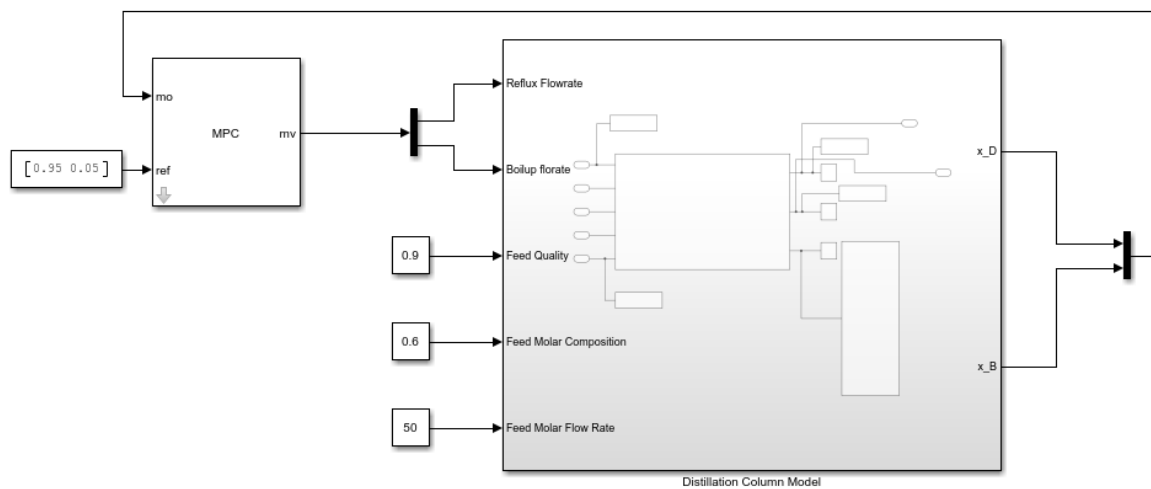


Figure 23. MPC control system on Simulink

State	Desired Value	Actual Value	Desired dx	Actual dx
BDistillationColumnM/Distillation Column Model/Distillation Column Subsystem/Integrator				
State - 1	0.9	0.9	0	-1.4211e-15
BDistillationColumnM/Distillation Column Model/Distillation Column Subsystem/Integrator1				
State - 1	[-Inf , Inf]	0.81818	0	1.1546e-14
State - 2	[-Inf , Inf]	0.74885	0	-1.9984e-14
State - 3	[-Inf , Inf]	0.69411	0	1.4433e-14
State - 4	[-Inf , Inf]	0.65325	0	-1.4433e-14
State - 5	[-Inf , Inf]	0.62402	0	1.3767e-14
State - 6	[-Inf , Inf]	0.60372	0	1.9984e-15
State - 7	[-Inf , Inf]	0.58994	0	2.1094e-15
State - 8	[-Inf , Inf]	0.5807	0	-1.2268e-14
State - 9	[-Inf , Inf]	0.57457	0	0
State - 10	[-Inf , Inf]	0.56042	0	-1.9984e-15
State - 11	[-Inf , Inf]	0.53828	0	1.7764e-14
State - 12	[-Inf , Inf]	0.5049	0	2.6645e-15
State - 13	[-Inf , Inf]	0.45721	0	4.4409e-16
State - 14	[-Inf , Inf]	0.3941	0	-1.1546e-14
State - 15	[-Inf , Inf]	0.31854	0	7.9936e-15
State - 16	[-Inf , Inf]	0.23817	0	-3.5527e-15
State - 17	[-Inf , Inf]	0.1628	0	1.7764e-15
BDistillationColumnM/Distillation Column Model/Distillation Column Subsystem/Integrator2				
State - 1	0.1	0.1	0	-1.7764e-16
BDistillationColumnM/MPC Controller/MPC/last_mv				
State - 1	[-Inf , Inf]	35.6653	0	0
State - 2	[-Inf , Inf]	61.9153	0	0

Figure 24. Details of the operating point

After the MPC structure is defined by linearization, the controller can be tuned. After testing several values for these parameters, the sampling time of 0.1 is defined as MPC is a discrete time control strategy. The performance is mentioned with both prediction horizons of 10 and 20. The control horizon is chosen to be 5 as it is supposed to be smaller than the prediction horizon. Due to the performance of the controller on tracking the setpoints and the rate of inputs changes, no constraints and weights were specified and the values were kept as the designer defaults. The results from running the simulation for 100 seconds are:

Prediction horizon of 10:

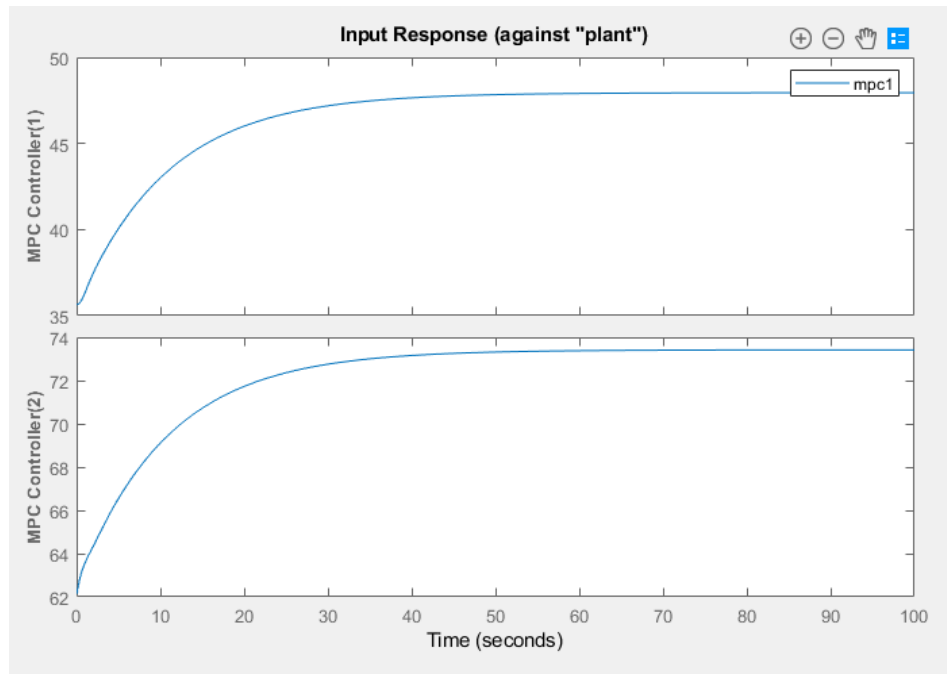


Figure 25. MPC control input responses

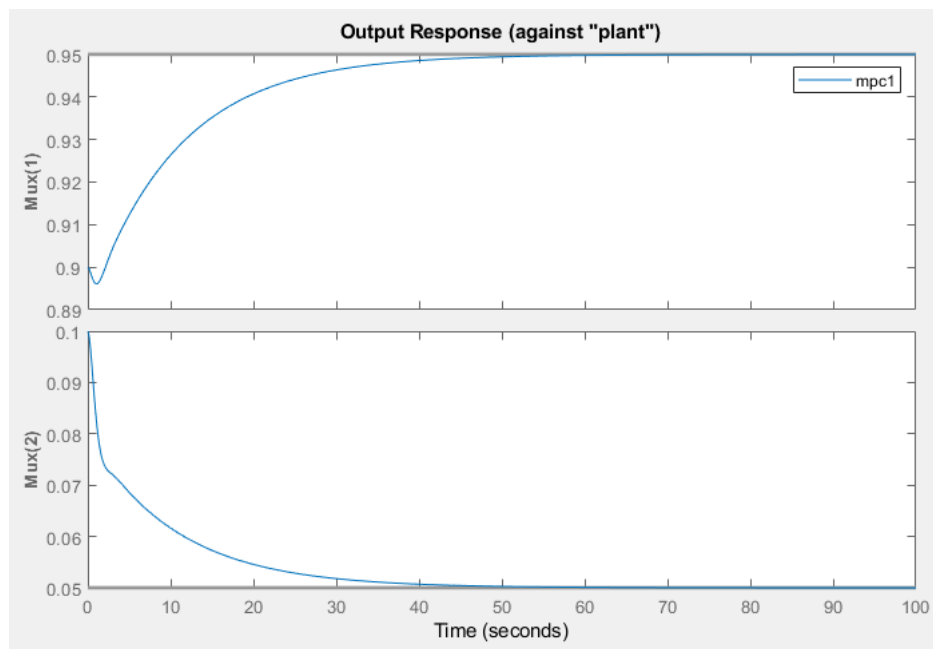


Figure 26. MPC control output responses

Prediction horizon of 20:

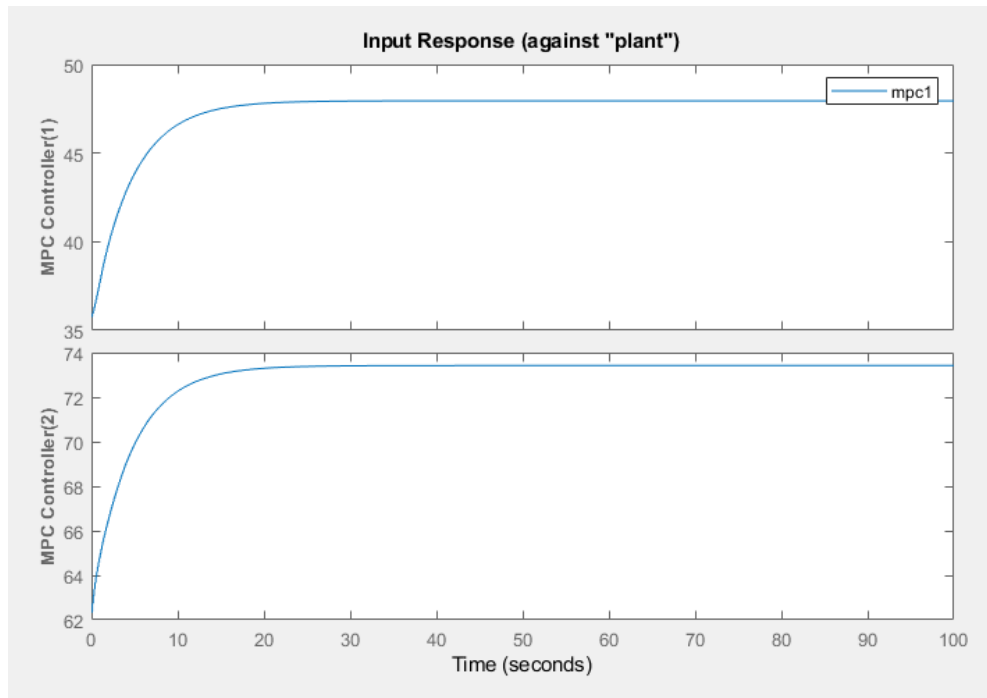


Figure 27. MPC control input responses

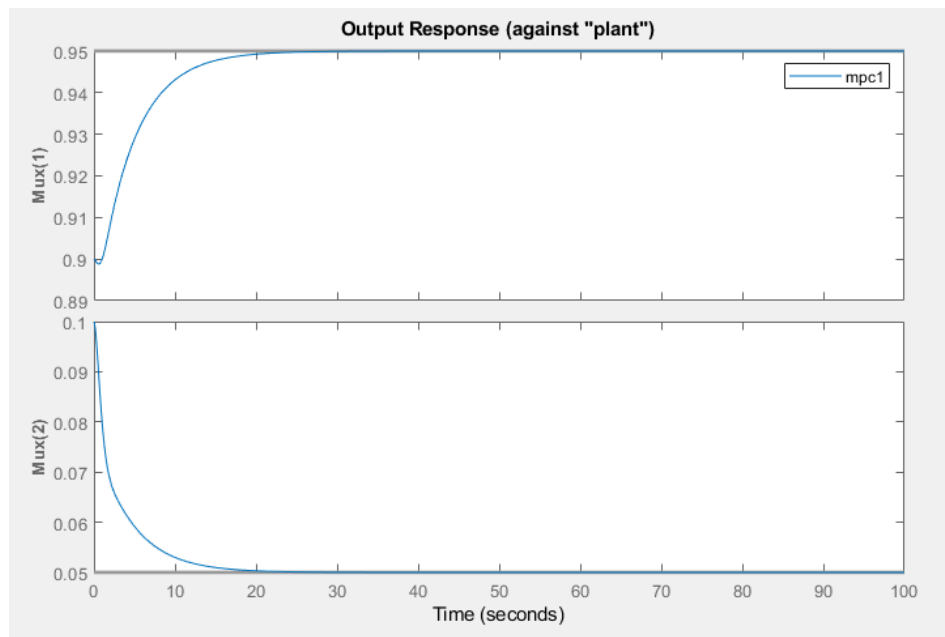


Figure 28. MPC control output responses

Design review for MPC Toolbox that represents summaries of performed tests, detected no problem in different parts except the scale factor. Scaling converts the relationship between output and input variables to dimensionless form, also the scale factor specification improves quadratic programming (QP) numerical accuracy. The warning affirms that at least one output variable response indicates poor scaling and recommends adjusting scale factors. A scale factor should equal or approximate the variables span that is the difference between the upper and lower limits of variables. For specifying the scale factor on output variables, it is obvious that the compositions can vary from 0 to 1. However, considering that the composition of the top product shouldn't be less than feed composition (0.6), and the composition of the bottom product shouldn't exceed this value, we can specify a scale factor of 0.5 on each output variable and the results are:

Prediction horizon of 10:

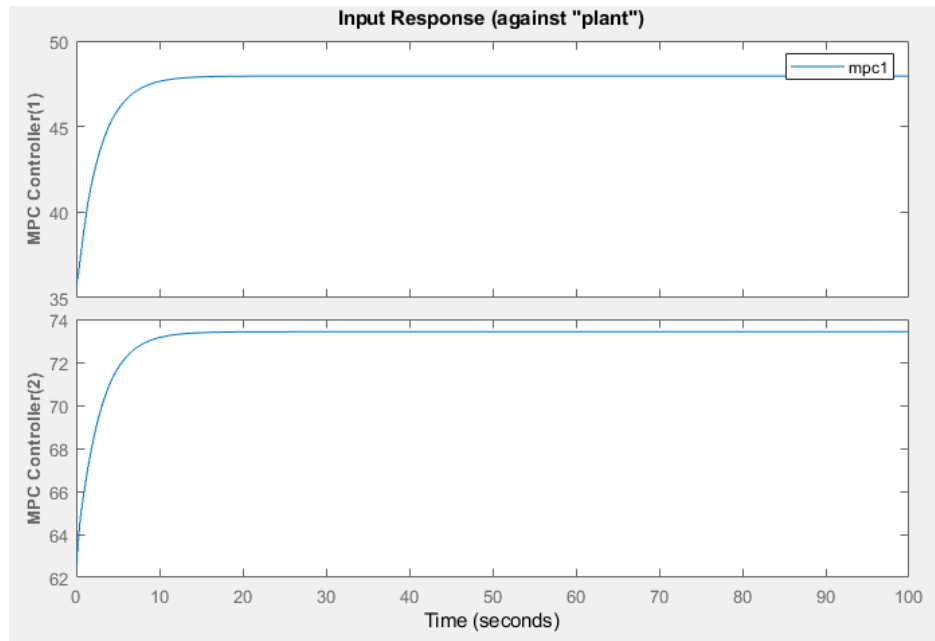


Figure 29. MPC control input responses

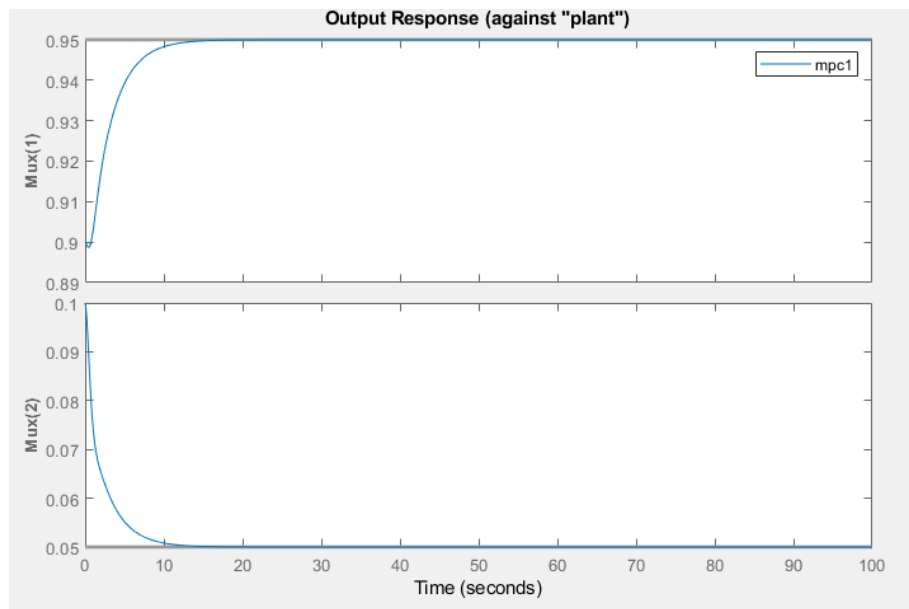


Figure 30. MPC control output responses

Prediction horizon of 20:

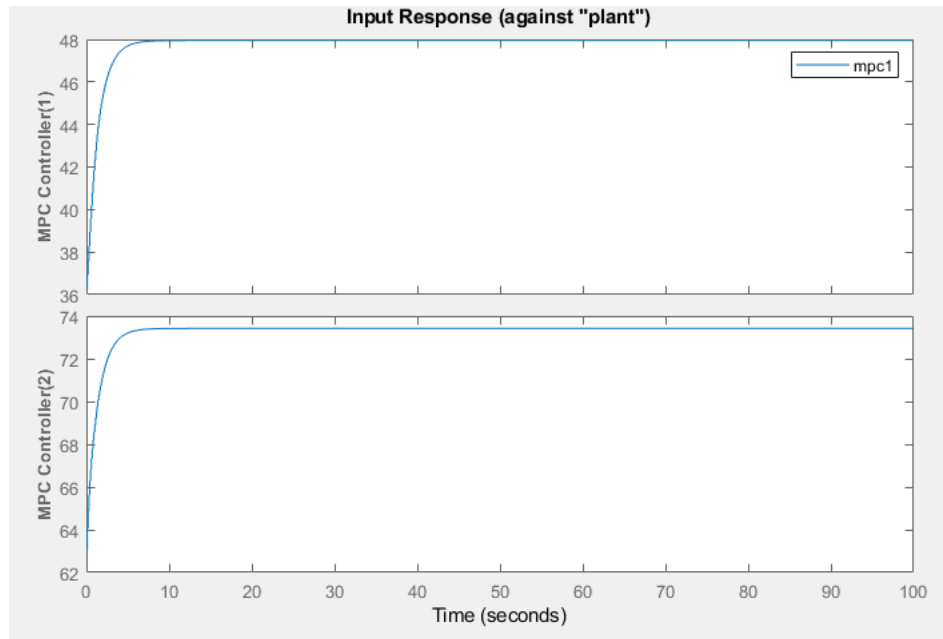


Figure 31. MPC control input responses

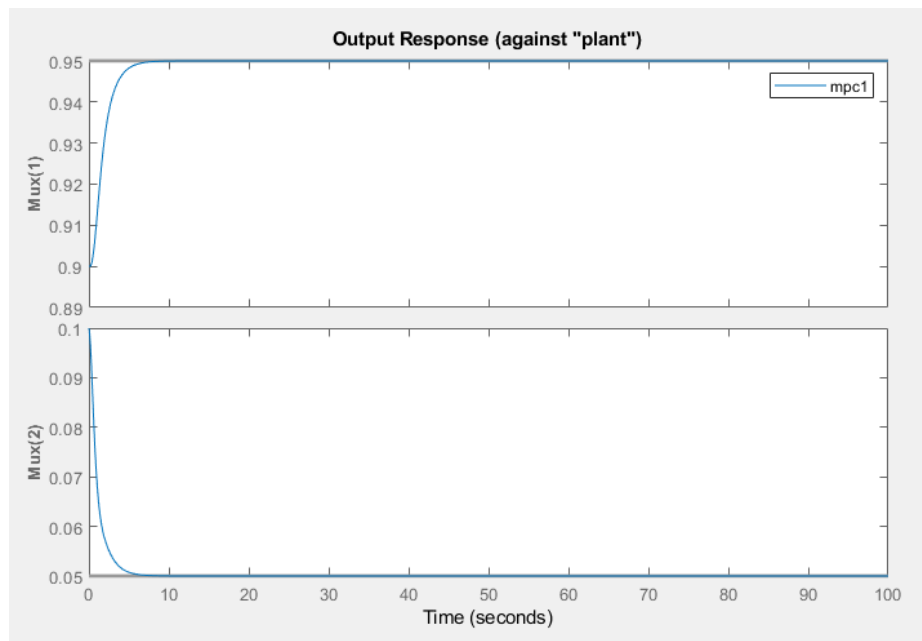


Figure 32. MPC control output responses

The impact of adjusting the scale factors on better performance of controller is evident.

4.5 PI and PID Controllers Performance

In order to compare performance of the MPC controller, the performance of PI and PID are evaluated. The state space model generated from linearizing the distillation column subsystem in Simulink is used for tuning the PI and PID controllers. The matrixes from this state space model are saved in the workspace of MATLAB and reloaded in the state space block of Simulink. Because of the coupling characteristics of the distillation column, the control performance of tracking the desired setpoints is tested with and without a decoupling matrix. Same as the control system for the MPC controller, the desired setpoints for composition of ethanol in the top and bottom products of the column are 0.95 and 0.05. The looptune command in MATLAB is used for feedback tuning of the parameters for PI and PID controllers and the decoupling matrix (DM). The tuning parameters from looptune command are entered to the control systems modeled in Simulink for running the simulation. As previously described, the reflux and boil up flow rates are manipulated variables (inputs), and the compositions of ethanol in top and bottom products are controlled variables (outputs). No change is considered for the value of disturbances (feed flow rate, composition, and quality). The crossover frequency is considered as 0.5 rad/min for tuning parameters.

4.5.1 PI Control Results

Results from tuning PI controllers are as following:

PI controller tuning parameters with a decoupling matrix (DM):

Table 8. PI controller control parameters with decoupling

	K_p	K_i
PI_1	1.15	2.47
PI_2	-5.22	-8.05
DM	$\begin{bmatrix} 35.65 & -11.54 \\ -8 & 4.938 \end{bmatrix}$	

The PI controller performance with these parameters for 100 seconds is:

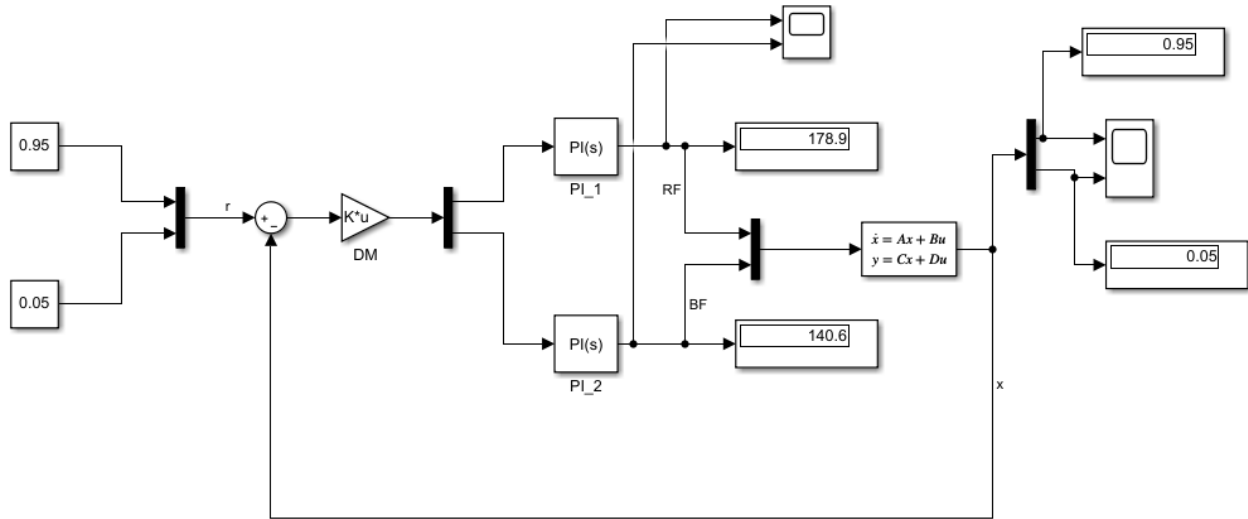


Figure 33. Simulink PI control system performance with decoupling

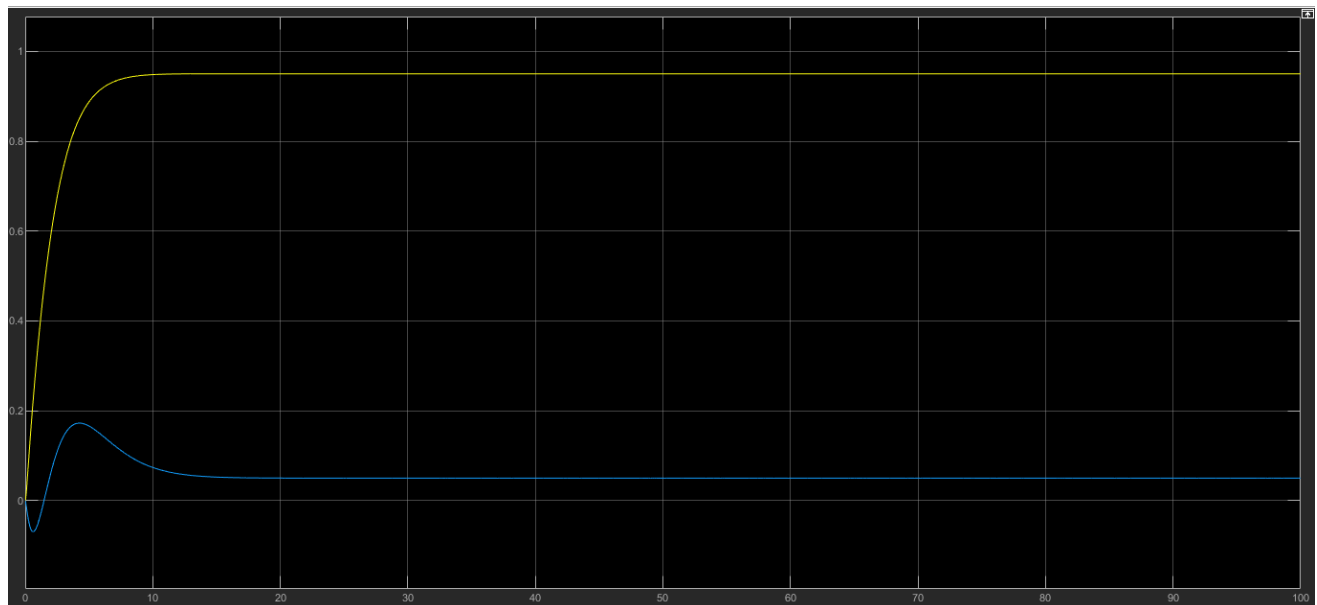


Figure 34. PI controller performance with decoupling

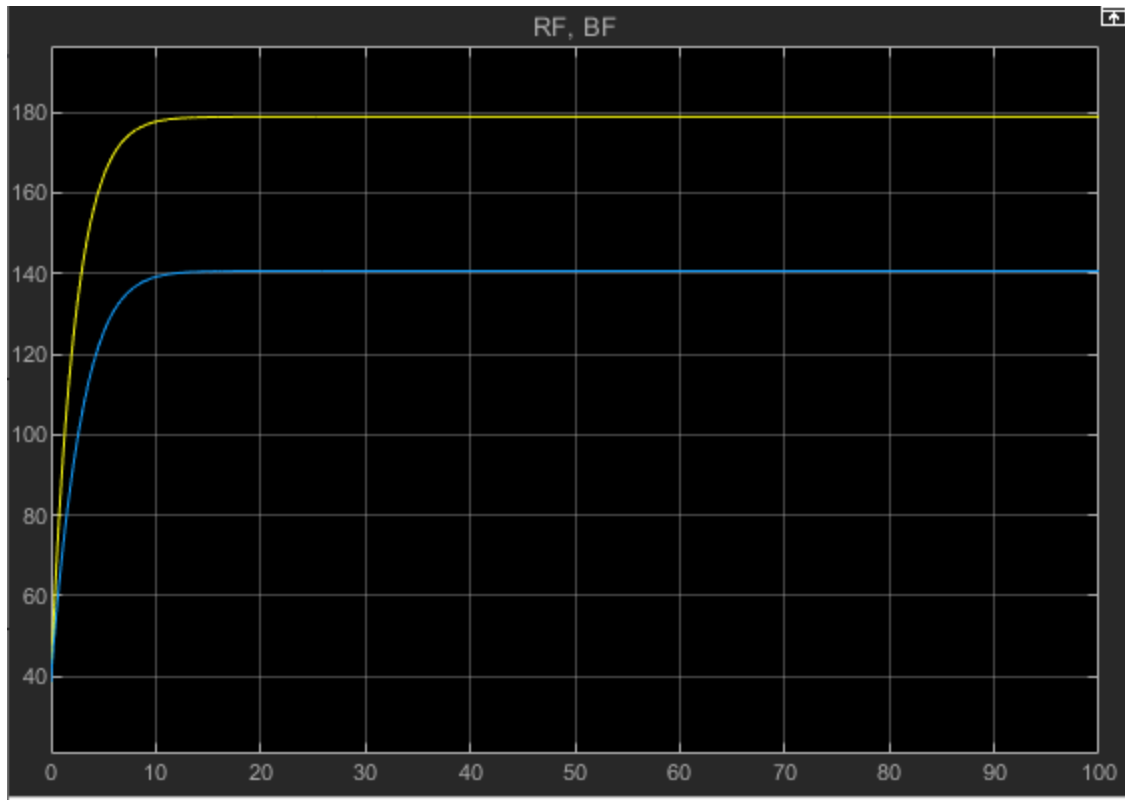


Figure 35. Rate of change of reflux and boil up flow rates, PI controller with decoupling

For addressing the issues of negative gains and over-parametrized tunable elements, constraints are added to decoupling matrix (DM) by fixing the (1,1) and (2,2) entries of it to 1 and -1. Without these constraints the second PI controller had negative gains, but here both controllers have positive gain values. The results for 100 seconds run are:

Table 9. PI controller control parameters with decoupling and constraints

	K_p	K_i
PI_1	36.3	52.8
PI_2	31.5	34.2
DM	$\begin{bmatrix} 1 & -0.455 \\ 0.7644 & -1 \end{bmatrix}$	

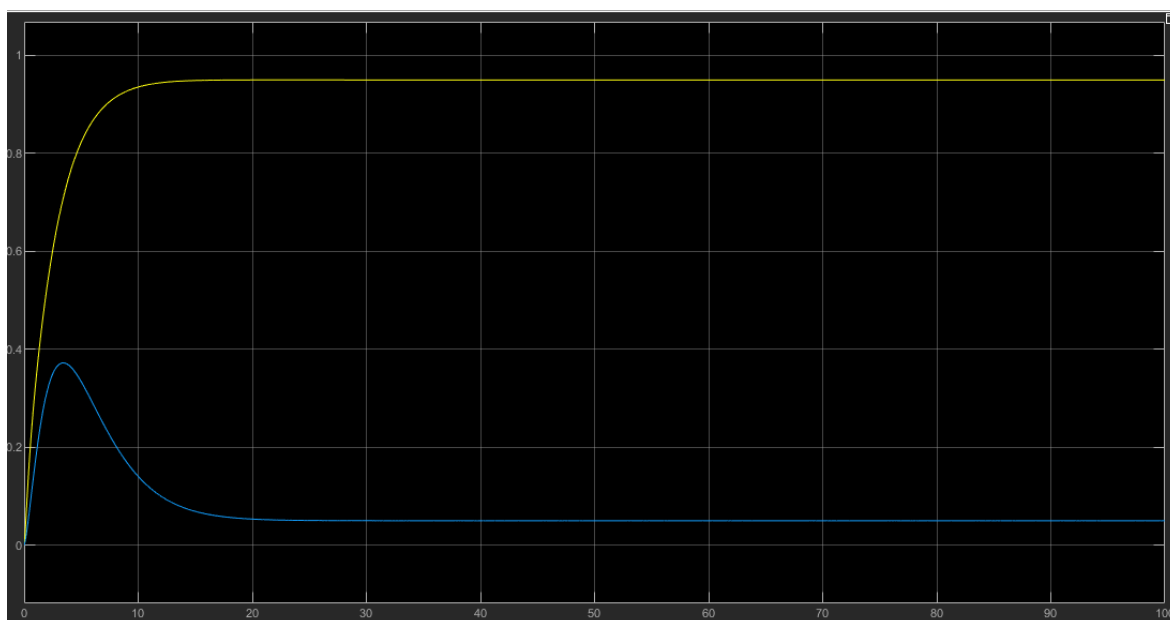


Figure 36. PI controller performance with decoupling and constraints

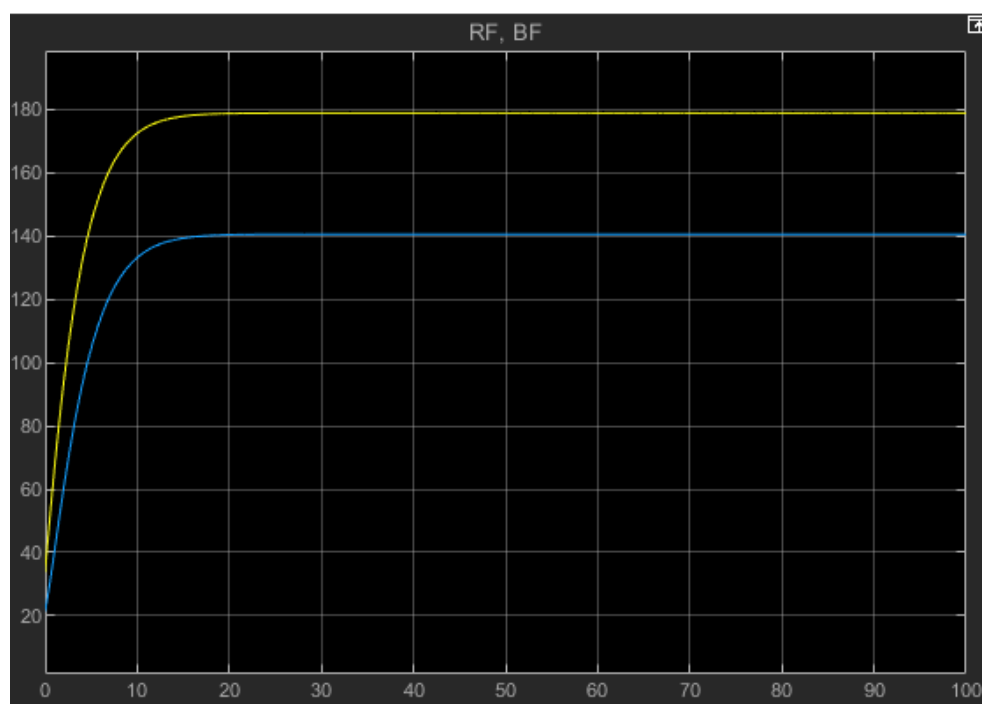


Figure 37. Rate of change of reflux and boil up flow rates, PI controller with decoupling and constraints

PI controller tuning parameters without a decoupling matrix, and results for 100 seconds run:

Table 10. PI controller control parameters without decoupling

	K_p	K_i
PI_1	35	72.9
PI_2	-11.4	-30.4

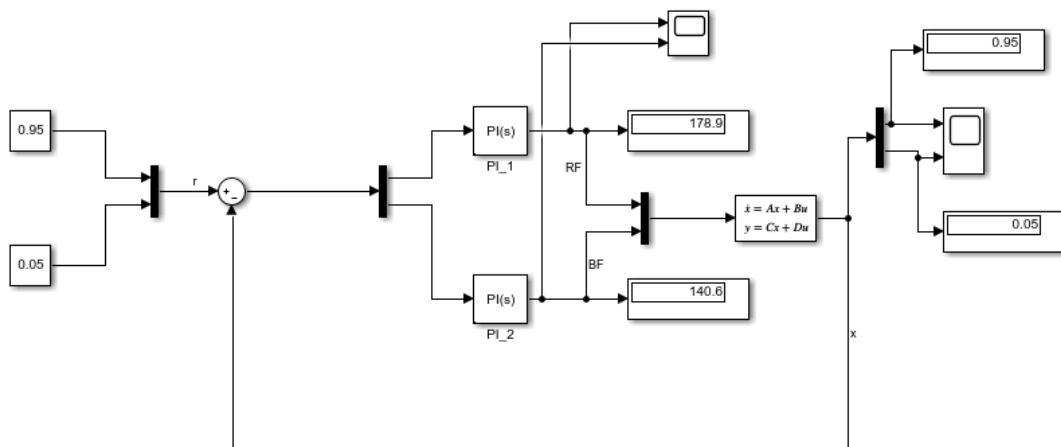


Figure 38. Simulink PI control system performance without decoupling

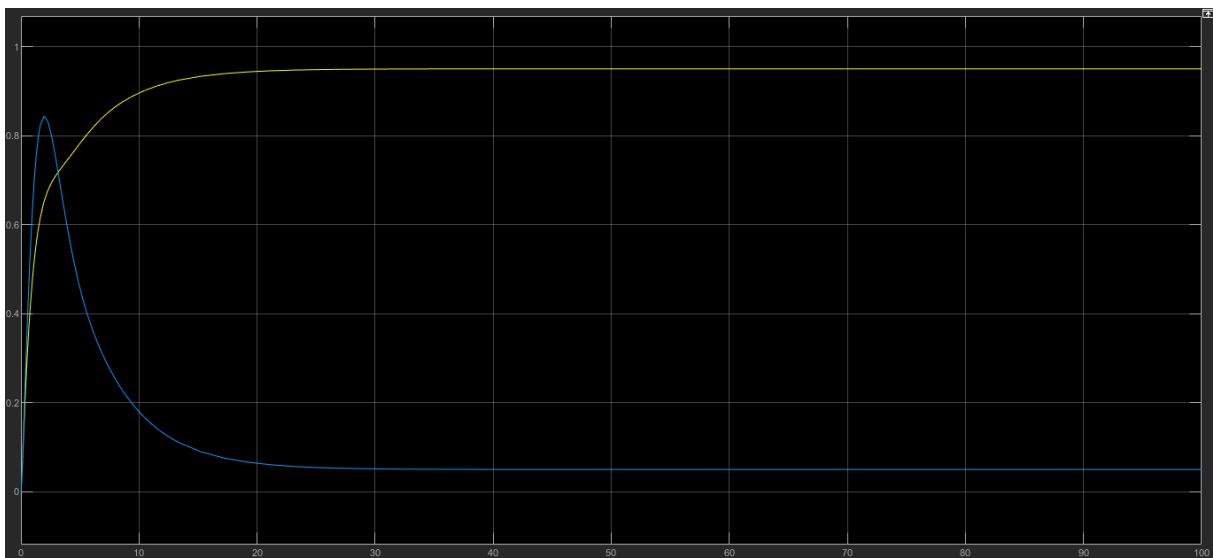


Figure 39. PI controller performance without decoupling

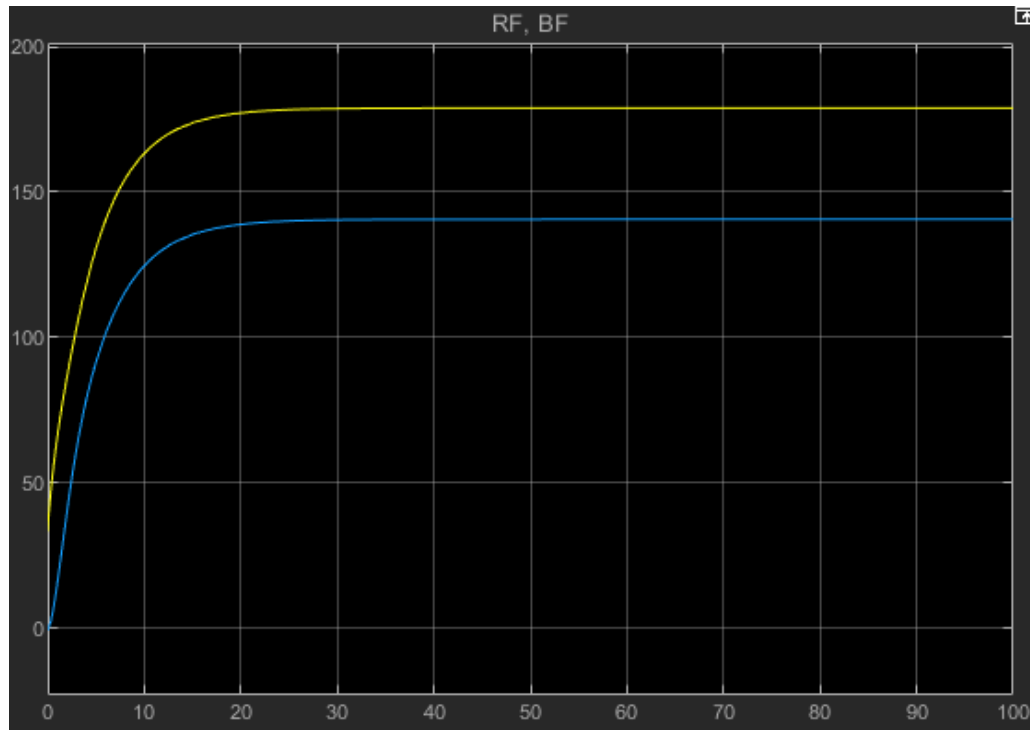


Figure 40. Rate of change of reflux and boil up flow rates, PI controller without decoupling

4.5.2 PID Control Results

Results from tuning PID controllers are as following:

PID controller tuning parameters with a decoupling matrix (DM):

Table 11. PID controller control parameters with decoupling

	K_p	K_i	K_D	Tf
PID_1	0.732	2.42	0.0523	0.00992
PID_2	-3.52	-8	-0.222	0.0104
DM	$\begin{bmatrix} 37.44 & -9.674 \\ -7.468 & 4.384 \end{bmatrix}$			

The PID controller performance with these parameters for 100 seconds is:

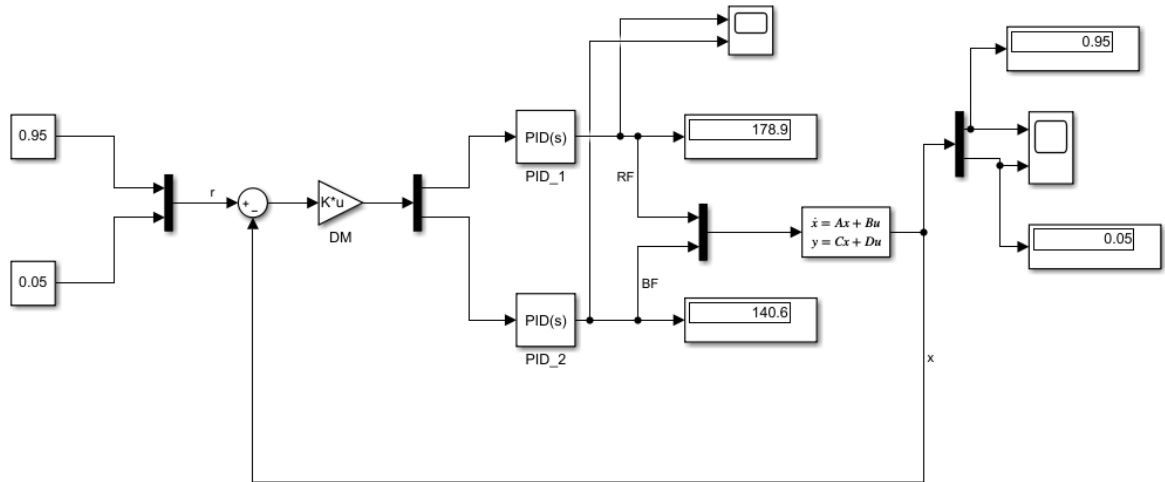


Figure 41. Simulink PID control system performance with decoupling

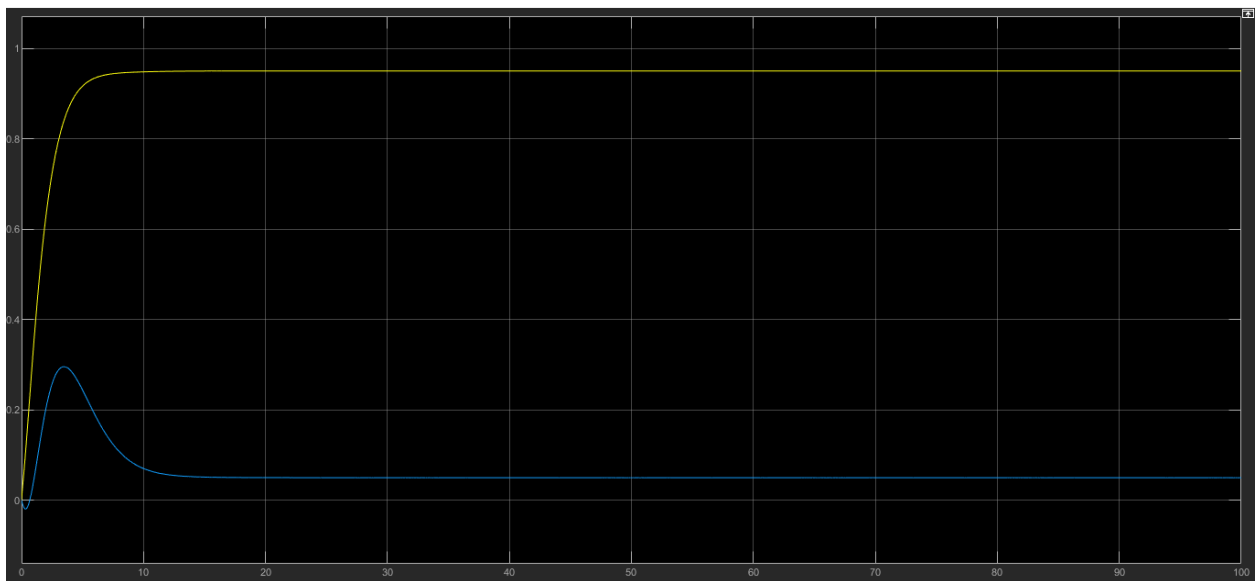


Figure 42. PID controller performance with decoupling

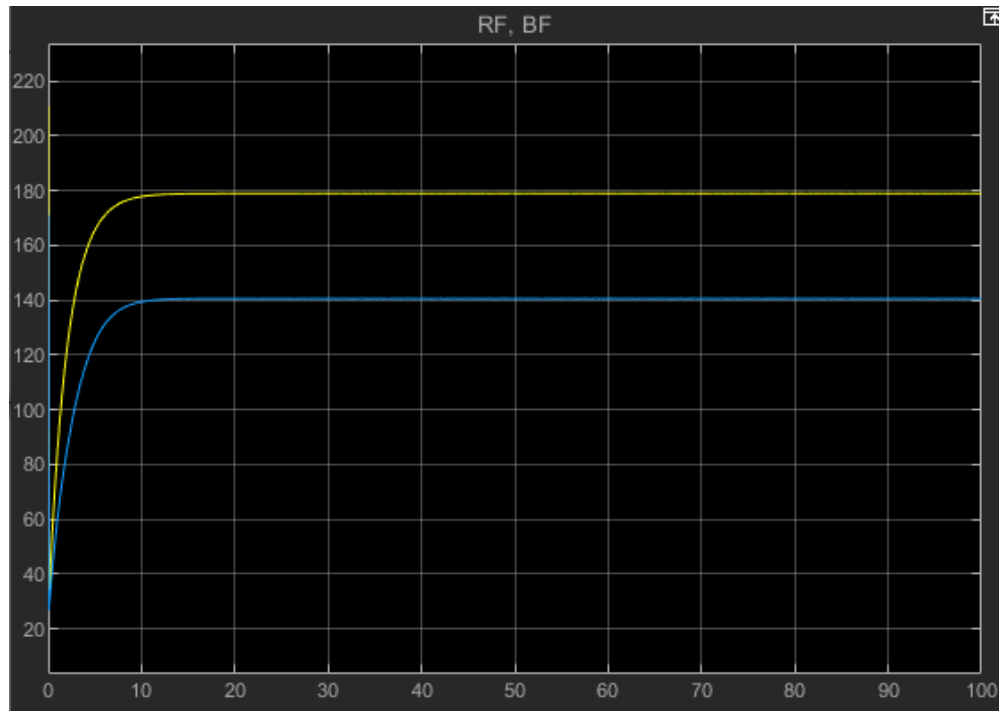


Figure 43. Rate of change of reflux and boil up flow rates, PID controller with decoupling

Same as the PI control system, constraints are applied to decoupling matrix (DM) by fixing the (1,1) and (2,2) entries of it to 1 and -1. Here, the proportional and integral gains of second controller have positive values while their values were negative without the constraints. However, the sign of derivative gain of first controller changed from positive to negative. The results for 100 seconds run are:

Table 12. PID controller control parameters with decoupling and constraints

	K_p	K_i	K_D	Tf
<i>PID_1</i>	56	48	-42.4	1.61
<i>PID_2</i>	51.9	35.6	-91.6	4.16
<i>DM</i>	$\begin{bmatrix} 1 & -0.5347 \\ 0.5413 & -1 \end{bmatrix}$			

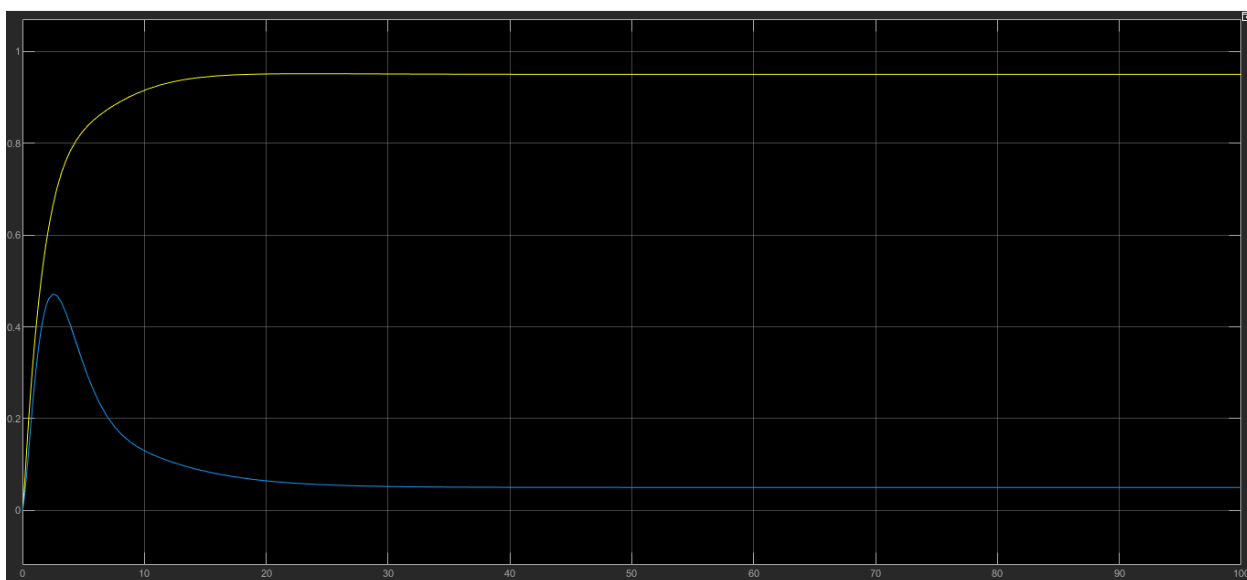


Figure 44. PID controller performance with decoupling and constraints

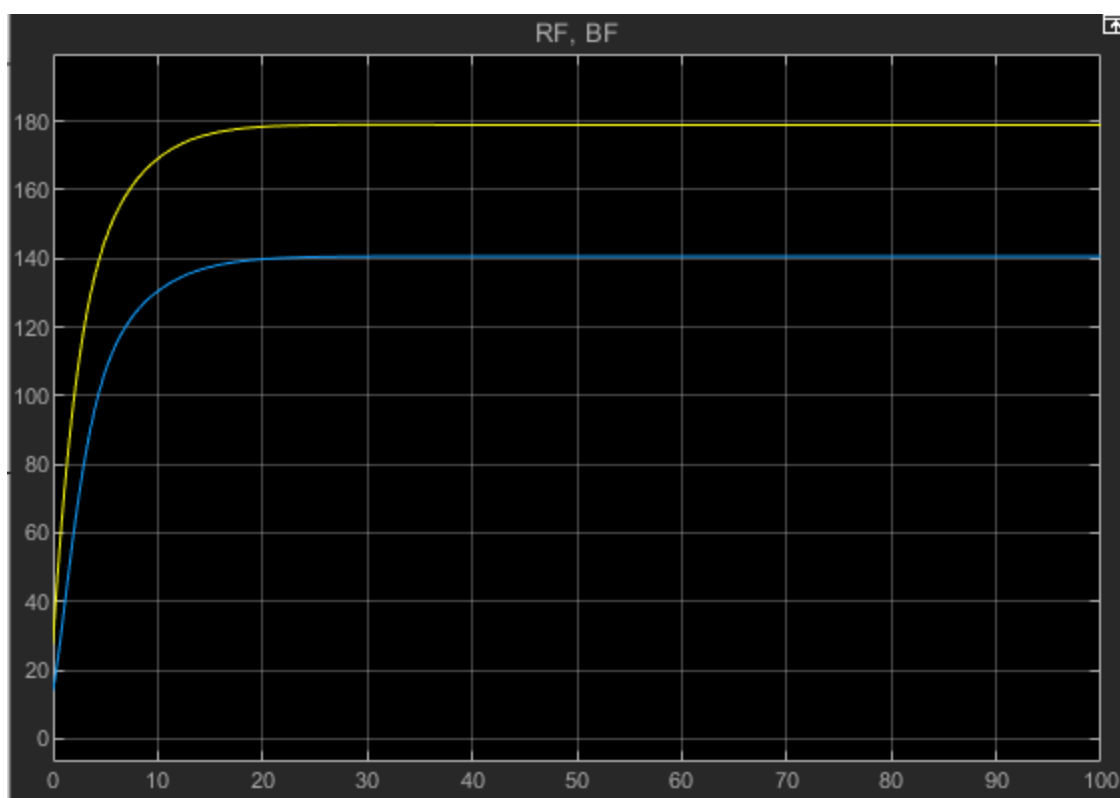


Figure 45. Rate of change of reflux and boil up flow rates, PID controller with decoupling and constraints

PID controller tuning parameters without a decoupling matrix, and results for 100 seconds run are:

Table 13. PID controller control parameters without decoupling

	K_p	K_i	K_D	Tf
PID_1	21.5	66.6	1.86	0.0197
PID_2	-2.03	-43.7	-21.8	0.901

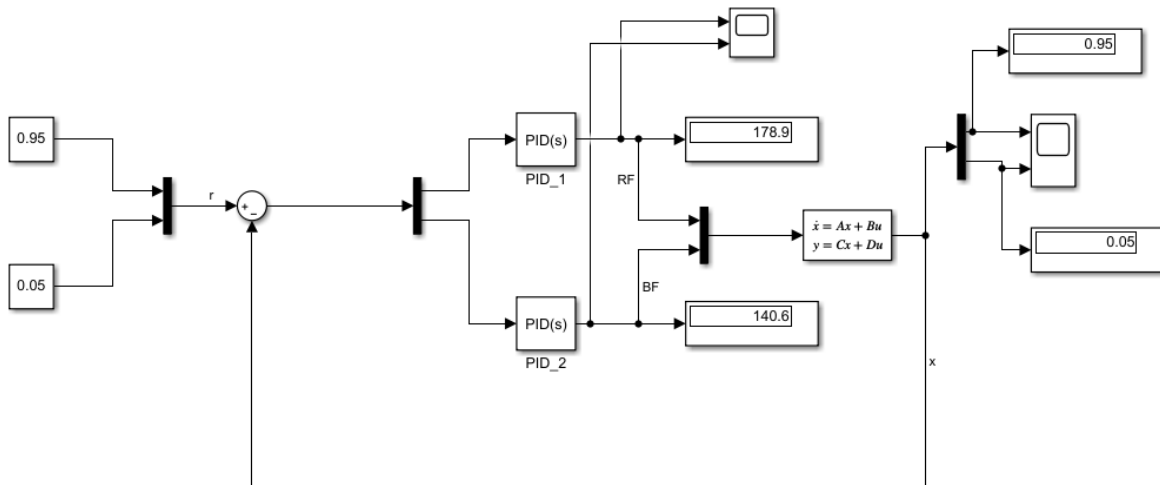


Figure 46. Simulink PID control system performance without decoupling

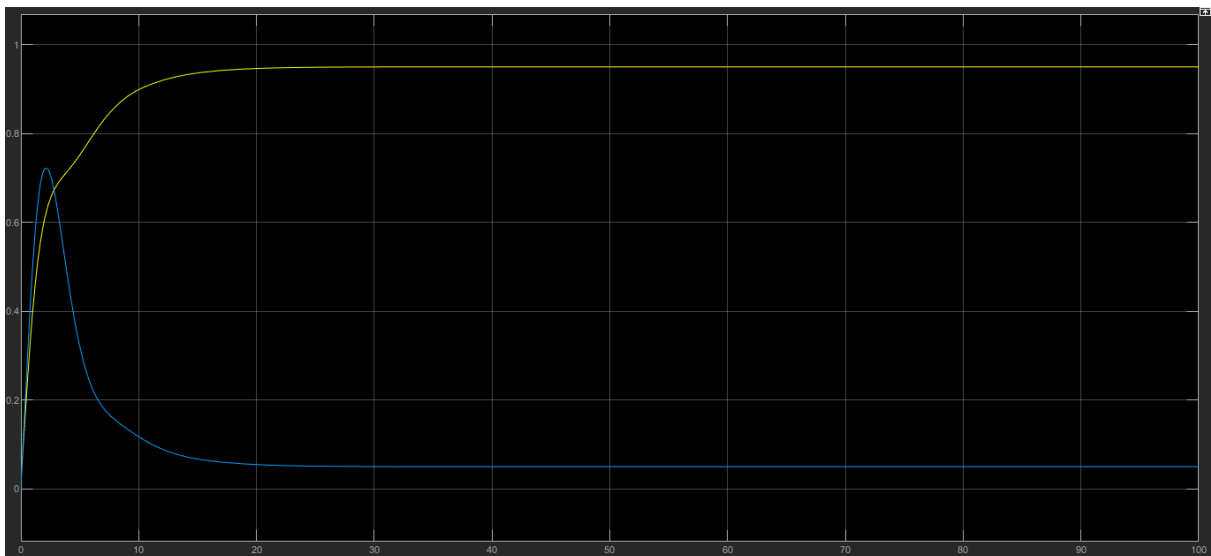


Figure 47. PID controller performance without decoupling

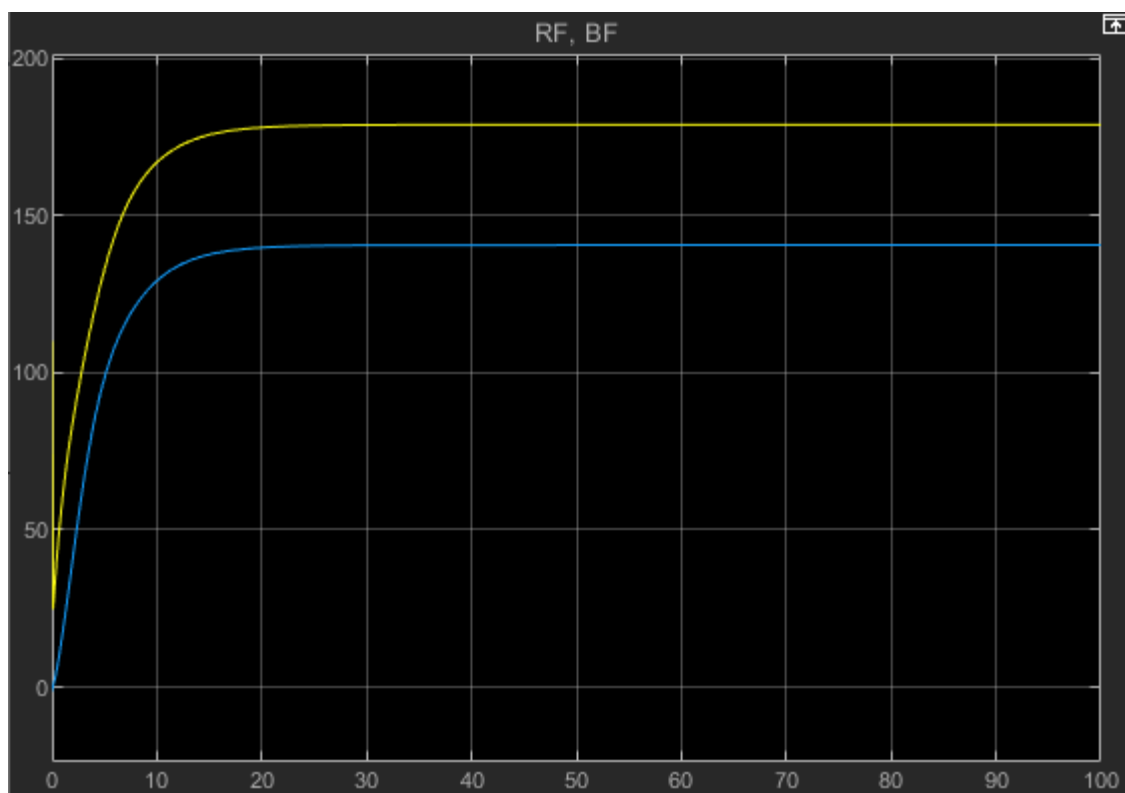


Figure 48. Rate of change of reflux and boil up flow rates, PID controller without decoupling

4.6 Summary of Findings

In this project, a dynamic model of a distillation column has been derived as a MATLAB code and modified to a Simulink subsystem. The distillation column subsystem was used to study the performance of the MPC controller. The results from tuning the controller with different parameters, shows that the MPC controller has good performance in tracking the setpoints. Responses from MPC were fast, and without over shoots. A scale factor of 0.5 has been applied to both outputs of the plant. The results show that adding scale factors has improved the controller performance. Although the control simulation results are represented with prediction horizons of 10 and 20, the faster response of the controller with a bigger prediction horizon is evident. PI and PID controllers have been tuned based on the state space model from linearizing the distillation column Simulink subsystem. The performance of PI and PID controllers was tested with and without the presence of a decoupling matrix that removed the interactions between inputs and outputs of the plant. Based on the results, eliminating the interactions by tuning a decoupling matrix can significantly improve the performance of PI and PID controllers, as it decreases the overshoots on the bottom compositions. Also, applying constraints on the decoupling matrix removed undesired negative overshoots, but it slowed down the performance and caused bigger overshoots. Comparing the results, in general, shows that although all controllers tracked the desired setpoints successfully, the MPC controller had the best performance as it was faster, with no overshoots and represented smaller values for manipulated variables.

5. Conclusion

Controlling the composition of top and bottom products of the distillation columns is very important in the industry, but it is a challenging problem due to the high nonlinearity of the MIMO systems. In this study a theoretical dynamic model of a water-ethanol binary distillation column has been developed using the molar basis total and component mass balance equations. The dynamic simulation of this model has been implemented in MATLAB environment and validated using data from HYSYS simulation of a binary distillation column. This model has been modified and represented as a Simulink subsystem of the distillation column. This dynamic simulation has been employed as a plant model for developing an MPC controller with MATLAB MPC Toolbox. It was also used for tuning PI and PID controllers for the distillation column in order to control the top and bottom products compositions. The control simulations have been performed with different scenarios, and the represented results demonstrate the better performance of MPC compared to PI and PID controllers.

6. Recommendation and Suggestions for Future Work

In case someone is interested to work on this topic or any related topic to this work, here are some recommendations:

1. This project is done under several assumptions in dynamic modelling including assuming an isothermal column. Including the energy balance equations, evaluating the impacts of temperature on products compositions, and the temperature change along the column, would be a good choice.
2. In this work, the performance of MPC controller is compared to PI and PID controllers. Developing other advanced control strategies like fuzzy logic control, model-based control strategies like Model Reference Adaptive Control (MRAC), and Nonlinear Model Predictive Control (NMPC), and comparing their performance with MPC provides a great opportunity for evaluating the performance of advanced control strategies in the case of a binary distillation column.
3. Tracking the disturbances effects on dynamic behavior of the system, testing the performance of the controllers disturbance rejection, and defining measured disturbances for evaluating feedforward performance of the MPC controller can be a great scope of work for this topic.

7. References

- [1] Abdullah, Zalizawati & Aziz, Norashid & Ahmad, Zainal. (2007). Nonlinear Modelling Application in Distillation Column. Chemical Product and Process Modeling. 2. 10.2202/1934-2659.1082.
- [2] Ahmed D. F. and Nawaf M. Y. "Simulation Study in Control System Configuration of a Distillation Column", Journal of Chemical Engineering & Process Technology; 2018, 9/4, 1- 12.
- [3] Ahmed, Duraid & Nawaf, Mohanad. (2018). Simulation Study in Control System Configuration of a Distillation Column. Journal of Chemical Engineering & Process Technology. 09. 10.4172/2157-7048.1000388.
- [4] Ahmed, Duraid & Nawaf, Mohanad. (2019). Design of Multivariable Control System of a Distillation Tower via Simulation Using MATLAB/Simulink. Tikrit Journal of Engineering Sciences. 26. 51-61. 10.25130/tjes.26.3.07.
- [5] Alama, William Ipanaqué, and Marco Lovera. 1997. "State Space Identification for a Pilot Distillation Column." *IFAC Proceedings Volumes* 30 (6). Elsevier BV: 553–57. doi:10.1016/s1474-6670(17)43422-7.
- [6] Al-Shammari, Abdallah & Faqir, Naim & Housam, Binous. (2014). Model predictive control of a binary distillation column.
- [7] Bemporad, Alberto, Manfred Morari, and N. Lawrence Ricker. "Model Predictive Control Toolbox User's Guide." *The mathworks* (2010).
- [8] Ciannella, Stefano & Cluett, W.R.. (2014). Applied Model Predictive Control - a brief guide do MATLAB/Simulink MPC toolbox. 10.13140/RG.2.1.2334.7369.
- [9] Forbes, Michael & Patwardhan, Rohit & Hamadah, Hamza & Gopaluni, Bhushan. (2015). Model Predictive Control in Industry: Challenges and Opportunities. IFAC-PapersOnLine. 48. 531-538. 10.1016/j.ifacol.2015.09.022.
- [10] Hovd, Morten & Michaelsen, Rune & Montin, Tomas. (1999). Model predictive control of a crude oil distillation column. Modeling, Identification and Control. 20. 10.4173/mic.1999.2.2.

- [11] Lone, Sohail & Ahmad, Syed Akhlaq. (2013). MODELING AND SIMULATION OF A DISTILLATION COLUMN USING MATLAB. International Journal of Engineering Research and Science and Technology. 02. 198-209.
- [12] Minh, Vu & Abdul-Rani, Ahmad-Majdi. (2009). Modeling and Control of Distillation Column in a Petroleum Process. Mathematical Problems in Engineering. 2009. 10.1155/2009/404702.
- [13] Perry, Robert H., Don W. Green, and James O. Maloney. 1997. *Perry's chemical engineers' handbook*. New York: McGraw-Hill.
- [14] Rajendran, Sivakumar & Mathew, Shennes. (2013). Design and Development of Model Predictive Controller for Binary Distillation Column. International Journal of Science Education. 2. 445-451.
- [15] Rohani, Sohrab. 2017. *Coulson and Richardson's chemical engineering. Volume 3B, Volume 3B*. Oxford, United Kingdom: Elsevier/Butterworth-Heinemann.
- [16] Ruchika, Neha Raghu."Model Predictive Control: History and Development". International Journal of Engineering Trends and Technology (IJETT). V4(6):2600-2602 Jun 2013. ISSN:2231-5381.
- [17] Shukla, Gaurav. (2017). Study the Dynamic Behaviour of Distillation Column with Fundamental Modelling and Simulation by MATLAB. International Journal of Engineering Research and. V6. 10.17577/IJERTV6IS040665.
- [18] Skogestad, Sigurd, and Manfred Morari. 1988. "Understanding the Dynamic Behavior of Distillation Columns." Industrial and Engineering Chemistry Research 27 (10): 1848–62. doi:10.1021/ie00082a018.
- [19] Treybal, Robert Ewald. 1980. *Mass-transfer operations*. New York: McGraw-Hill.
- [20] Truong, H.S. & Ismail, Idris & Razali, Radzuan. (2010). Fundamental modeling and simulation of a binary continuous distillation column. 2010 International Conference on Intelligent and Advanced Systems, ICIAS 2010. 1 - 5. 10.1109/ICIAS.2010.5716218.
- [21] Wahid, Abdul & Ahmad, Arshad. (2016). Improved Multi-model Predictive Control to Reject Very Large Disturbances on a Distillation Column. International Journal of Technology. 7. 962-971. 10.14716/ijtech.v7i6.3524.

- [22] Wood, R. K., and M. W. Berry. 1973. "Terminal Composition Control of a Binary Distillation Column." *Chemical Engineering Science* 28 (9): 1707–17. doi:10.1016/0009-2509(73)80025-9.
- [23] XI, Yu-Geng & Li, Dewei & Lin, Shu. (2013). Model Predictive Control — Status and Challenges. *Acta Automatica Sinica*. 39. 222–236. 10.1016/S1874-1029(13)60024-5.

Appendix

MATLAB Code Distillation Column Dynamic Simulation

```
function dxdt=distillationC(t,x)
%
global distillp
%
if length(distillp) < 11
    disp('ERROR!: Please enter all parameters')
    return
end
%
alpha    = distillp(1); %Relative Volatility
N        = distillp(2); %Total number of stages
Nf       = distillp(3); %Feed stage
q        = distillp(4); %Feed quality
z        = distillp(5); %Feed molar composition of more volatile component
F        = distillp(6); %Feed molar flow rate
RF       = distillp(7); %Reflux molar flow rate
BF       = distillp(8); %Boil up molar flow rate
nk       = distillp(9); %Liquid holdup on trays
n1       = distillp(10); %Condenser holdup
nN       = distillp(11); %Reboiler holdup

% liquid flow rate in rectifying section (above feed tray)
Lr       = RF;
% liquid flow rate in stripping section (below feed tray)
Ls       = (Lr + (F*q));
% vapor flow rate in stripping section (below feed tray)
Vs       = BF;
% vapor flow rate in rectifying section (above feed tray)
Vr       = (Vs + (F*(1-q)));
%
% distillate product flowrate
D        = Vr-Lr;
% bottoms product flowrate
B        = Ls-Vs;
% Reflux and Boilup ratio
Rc=Lr*(D^(-1));
Rb=Vs*(B^(-1));

if D < 0
    disp('ERROR!: D < 0')
    return
end
if B < 0
    disp('ERROR!: B < 0')
    return
end
%
dxdt = zeros(N,1);
```

```
% Equilibrium equation
for k=1:N
    y(k)=(alpha*x(k))*(1.+(alpha-1.)*x(k)^(-1));
end
%
%% component molar balances on stages:
%
% Condenser
    dxdt(1)=(n1^(-1))*(Vr*y(2)-(D+Lr)*x(1));
%
% rectifying section (above feed tray)
for k=2:Nf-1
    dxdt(k)=(nk^(-1))*(Lr*x(k-1)+Vr*y(k+1)-Lr*x(k)-Vr*y(k));
end
%
% feed stage
    dxdt(Nf) = (nk^(-1))*(F*z+Lr*x(Nf-1)+Vs*y(Nf+1)-Ls*x(Nf)-Vr*y(Nf));
%
% stripping section (below feed tray)
for k=Nf+1:N-1
    dxdt(k)=(nk^(-1))*(Ls*x(k-1)+Vs*y(k+1)-Ls*x(k)-Vs*y(k));
end
%
% Reboiler
    dxdt(N)=(nN^(-1))*((Ls*x(N-1))-(B*x(N))-(Vs*y(N)));
```

Run Code

```
global distillp

title = 'Parameters';

ind1 = {'Relative volatility'
        'Total number of stages'
        'Feed stage'
        'Feed quality'
        'Feed molar composition'
        'Feed flow rate (mol/s)'
        'Reflux flow rate (mol/s)'
        'Boil up flow rate (mol/s)'
        'Tray holdup (mol)'
        'Condenser holdup (mol)'
        'Reboiler holdup (mol)'};

setpar = {'2','19','10','0.9','0.6','50','52','78','1','5','10'};

prompt = ind1;
def = setpar;
dlgTitle = title;
lineNo = 1;
```

```
Parameters_input = inputdlg(prompt,dlgTitle,lineNo,def);
distillp = str2num(char(Parameters_input));
x0=0.6*ones(distillp(2),1);
lengthx0 = length(x0);

if lengthx0 == distillp(2)

time_menu=menu('Time span:', '10 seconds', '50 seconds', '100 seconds', '200
seconds');

switch time_menu
    case 1
        t0=0;
        tfinal=10;
    case 2
        t0=0;
        tfinal=50;
    case 3
        t0=0;
        tfinal=100;
    case 4
        t0=0;
        tfinal=200;
end
[t,x] = ode45(@distillationC,[t0 tfinal],x0);
size_m=size(x);
rw=size_m(1);
comp=x(rw,:);
composition=comp';
%
plot_menu=menu('Select:', 'Plot and Results', 'Plot', 'Results', 'cancel');
switch plot_menu
    case 1
        plot(t,x);
        legend(plot(t,x));
        xlabel('Time (s)'); ylabel('Compositons');
        msgbox(num2str(composition), 'Molar Composition');

    case 2
        plot(t,x);
        legend(plot(t,x));
        xlabel('Time (s)'); ylabel('Compositons');

    case 3
        msgbox(num2str(composition), 'Molar Composition');
    case 4
        disp('canceled')
end
else
    disp('Not enough number of initial conditions!')
end
```