STUDY OF MATHEMATICAL MODELING OF CONTROL SYSTEM FOR CONTINUOUS STIRRED TANK REACTOR

by

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FINAL PROJECT REPORT

Submitted to the Electrical & Electronics Engineering Programme
in Partial Fulfillment of the Requirements
for the Degree
Bachelor of Engineering (Hons)
(Electrical & Electronics Engineering)

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CERTIFICATION OF APPROVAL

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Approved:

____

(AP Dr Radzuan Razali)
Project Supervisor

UNIVERSITI TEKNOLOGI PETRONAS
TRONOH, PERAK
DECEMBER 2010

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

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(Muhammad Hakimi b Abdullah Zamawi)

ABSTRACT

This simulation-based approach for this project is to provide better understanding of plant model design and enabling me to optimize the design to meet predefined performance criteria. By using these tools in the designing application, errors are detected early, test more thoroughly with multiple scenarios, carry out robustness and sensitivity analyses, and troubleshoot existing issues effectively. This leads to cost savings, shorter development cycles, fewer hardware prototypes, and high quality. In this project there are several input variables that can affect to optimize the output product of a certain plant. Among those inputs, not all of them can bring significant changes to the output, so this project also aims to identify only the significant inputs that contribute to the output changes.

ACKNOWLEDGEMENT

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CHAPTER 1

INTRODUCTION

1.1 Background of Study

Chemical reactors are the most influential and therefore important units that chemical engineer will encounter. To ensure the successful operation of a continuous stirred tank reactor (CSTR) it is necessary to understand their dynamic characteristics. A good understanding will ultimately enable effective control systems design. The aim of this project is to introduce some basic concepts of chemical reaction systems modeling and develop simulation models for CSTR's. Non-linear and linear systems descriptions are derived [1].

1.2 Problem Statement

For this progress report, the problems encountered are to find the inputs and outputs that are going to be used in the MATLAB. Since in the MATLAB, the design requires a plant model to define the relationship between the plant inputs and outputs, therefore the Model Predictive Control Toolbox is used and requires the model to be linear time invariant (LTI). Moreover, there are 3 types of model that can be defined [2]:

- Create a transfer function, state space, or zero/pole/gain model using methods provided by Control System Toolbox.
- Derive it from plant data using, e.g., methods provided by System Identification Toolbox.
- Derive it by linearizing a Simulink model.

1.3 Objectives

The objectives of this project are:

1. Study of mathematical modeling of control system for continuous stirred tank reactor
2. To manipulate input variables to achieve optimize output in plant process.

1.4 Scope of Study

The scope of this project is on the non-isothermal chemical reactor. The most important processes for the engineer are the chemical reactor because of its strong influence on product quality and profit. The dynamic behaviors of chemical reactors vary from quite straightforward to highly complex, and to evaluate the dynamic behavior, the engineer often must develop fundamental models. A simple model of a non-isothermal chemical reactor is introduced here with a sample dynamic response, and further details on modeling a continuous-flow stirred-tank reactor (CSTR) are presented further below along with the additional aspects of its dynamic behavior [3].

CHAPTER 2
LITERATURE REVIEW

2.1 Control System

A control system consists of subsystem and processes or plants assembled for the purpose of obtaining a desired output with desired performance, given a specified input.

With control system large equipment can be moved with precision which is impossible to be done by human. Huge antennas can be pointed toward the farthest reaches of the universe to pick up faint radio signals which is obviously impossible to be controlled by human hand. There are four primary purposes of control systems:

1. Power amplification
2. Remote control
3. Convenience of input form
4. Compensation for disturbances

As an example, a radar antenna is positioned by the low-power rotation of a knob at the input, requires a large amount of power for its output rotation. A control system can produce the needed power amplification, or power gain. [4]

2.1.1 Open-Loop System

A generic open-loop is shown in Figure 1 below. It starts with a subsystem called an input transducer, which converts the form of the input to that used by the controller. The controller drives a process or a plant. The input is also called the reference, while the output can be called the controlled variable. Other signals, such as disturbances, are shown added to the controller and process outputs via summing junctions, which yield the algebraic sum of their input signals using associated signs.[4]

A very simple example of open loop control is the remote controller of an RC toy car which the human have to constantly check the position and the velocity of the car to adapt to the situation and move the car to the desired place.

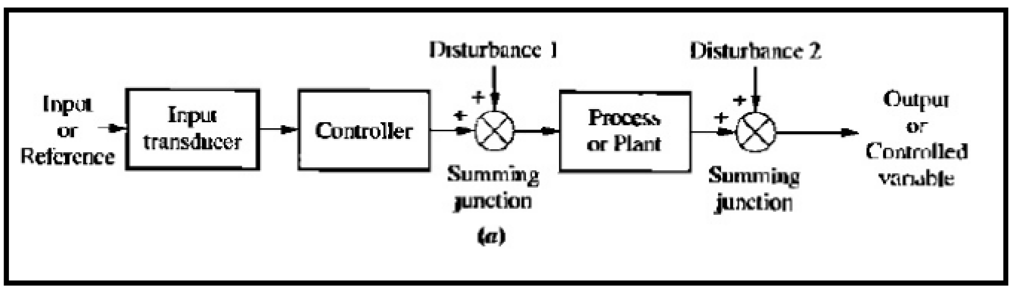

Figure 1: Open Loop System

The disadvantages of open loop systems are the systems do not correct for disturbances and are simply commanded by input. The open loop sensitivity to disturbances and inability to correct for these disturbances may be overcome in closed loop systems. In the closed loop systems, the electronics is left to handle a part and not all of the tasks performed by a human in an open loop controller while obtaining more accurate results with extremely short response time.

2.1.2 Closed-Loop System

The closed loop system compensates for disturbances by measuring the output response which the measurement is feeding back through a feedback path. The difference between of the response of the input at the summing junction will drives the plant via the actuating signal to make a correction. The system does not drive the plant if there is no difference in input and output since the plant's response is already the desired response.[4]

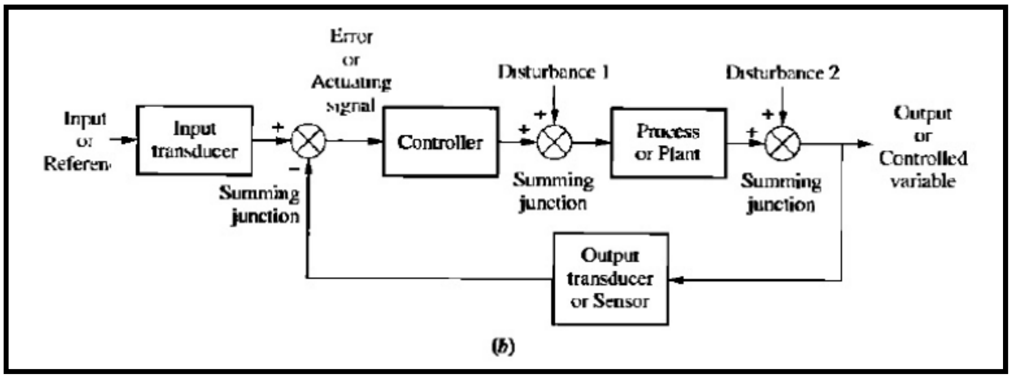

Figure 2: Closed Loop System

2.1.3 Other techniques

Some feedback systems will oscillate at just one frequency. By filtering out that frequency, one can use very "stiff" feedback and the system can be very responsive without shaking itself apart.

The most complex linear control systems developed to date are in oil refineries (model predictive control). The chemical reaction paths and control systems are normally designed together using specialized computer-aided-design software.

Feedback systems can be combined in many ways. One example is cascade control in which one control loop applies control algorithms to a measured variable against a setpoint, but then actually outputs a setpoint to another controller, rather than affecting power input directly.

Usually if a system has several measurements to be controlled, feedback systems will be present for each of them. [5]

2.2 Model Predictive Control

Model Predictive Control (MPC) originated from late seventies and continuously developed since then. The term Model Predictive Control does not designate a specific control strategy but a range o of control methods which make explicit use of a model of the process to obtain the control signal by minimizing an objective function. MPC has been use in process industries such as chemical plants and oil refineries. [6] The ideas of MPC are such as follows:

- Predict the future behavior of the process state/output over the finite time horizon.
- Compute the future input signals on line at each step by minimizing a cost function under inequality constraints on the manipulated (control) and/or controlled variables.
- Apply on the controlled plant only the first of vector control variable and repeat the previous step with new measured input/state/output variables.

2.3 Background of Mathematical Modeling

A mathematical model is the use of mathematics to describe a system. The system can be in the form of for example the real-world phenomena. The mathematical language is used to explain real-world phenomena, test ideas and make predictions about the real world. Here the real world refers to the area of engineering, physics, physiology, ecology, wildlife management, chemistry, economics and many more. The process of developing a mathematical model is termed mathematical modeling (also modeling). Eykhoff (1974) defined a mathematical model as 'a representation of the essential aspects of an existing system (or a system to be constructed) which presents knowledge of that system in usable form'[7].

When engineers analyze a system to be controlled or optimized, they use a mathematical model. In analysis, engineers can build a descriptive model of the system as a hypothesis of how the system could work, or try to estimate how an unforeseeable event could affect the system. Similarly, in control of a system, engineers try different control approaches in simulations.

A mathematical model usually describes a system by a set of variables and a set of equations that create relationships between the variables. The values of the variables can be anything such as real or integer numbers, boolean values or strings, and etc. The variables represent some properties of the system, for example, measured system outputs often in the form of signals, timing data, counters and event occurrence. The actual model is the set of functions that describe the relations between the different variables [8]. The process of mathematical modeling can be described as the diagram below.

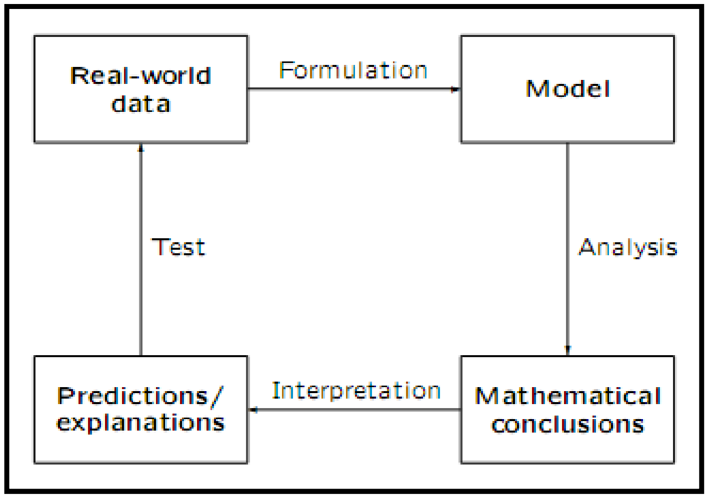

Figure 3: Mathematical Modeling Process

2.4 CSTR Background

The most important unit operation in a chemical process is basically a chemical reactor. Chemical reactions are either exothermic (release energy) or endothermic (require energy input) and therefore require that energy either be removed or added to the reactor for a constant temperature to be maintained.

Exothermic reactions are the most interesting systems to study due to the potential safety problems such as rapid increases in temperature, sometimes called "ignition" behavior and the possibility of exotic behavior such as multiple steady-states [9]. It means that for the same value of the input variable there may be several possible values of the output variable.

The design of a chemical reactor deals with multiple aspects of chemical engineering. Chemical engineers design reactors to maximize net present value for the given reaction. Designers make sure that the reaction proceeds with the highest efficiency towards the desired output product, producing the highest yield of product while requiring the least amount of money to purchase and operate. Normal operating expenses such as energy input, energy removal, raw material costs, labor, etc. Energy changes can come in the form of heating or cooling, pumping to increase pressure, frictional pressure loss, agitation and etc.

For this project, a perfectly mixed, continuously stirred tank reactor (CSTR), shown in Figure 4 is considered. The case of a single, first-order exothermic irreversible reaction, A --> B. Consider a stream of butene in cyclohexane that is converted to butene epoxide by reaction with peroxide in a CSTR. The ratio of butene epoxide to butene is governed by the temperature, catalyst concentration, effectiveness of the catalyst and the residence time in the reactor [9]. At steady-state, the flow rate in must equal the mass flow rate out, otherwise the tank will overflow or go empty

A master curve in terms of conversion at constant conditions as a function of reaction time can easily be made in the lab. Then a calculation of residence time distribution in the reactor can be directly mapped, using the lab results, to conversion ratio for the desired product. If the butene epoxide is to be used in a second CSTR to produce the final product then this conversion ratio becomes the input concentration for the second CSTR. Typically a synthetic chemical process will involve a number of CSTR's joined in this way [9].

2.5 Factors Affecting CSTR

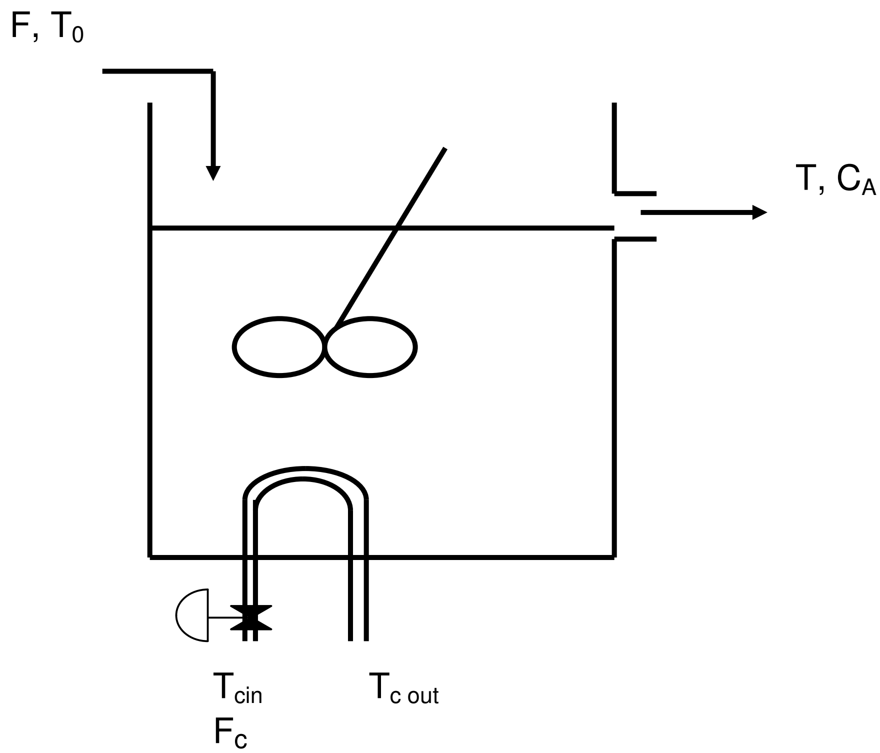

Figure 4: Non-isothermal CSTR

The parameters and variables that will appear in the modeling equations:

- F - Volumetric flowrate (volume/time)
- F_C - Heating liquid flowrate (volume/time)
- T - Reactor temperature
- T_0 - Feed temperature
- C_{A0} - Concentration of A in feed stream
- C_A - Concentration of A at output stream
- T_{cin} - Temperature of heating liquid coming in
- T_{cout} - Temperature of heating liquid coming out

2.5.1 Mass Balance

To setup the model, the mass and energy balances need to be considered across the reactor. From these energy balances, we will be able to develop relationships for the temperature of the reactor and the concentration of the limiting reactant inside of it. The general equation for a mass balance in any system is as follows:

$$(\,Rate\ Accumulation) = (Flow\ In) - (Flow\ Out) - (Rate\ Generation) \quad (1)$$

$$(Rate\ Accumulation) = V\frac{dC_A}{dt} \quad (2)$$

$$(Flow\ In) - (Flow\ Out) = F(C_{A0} - C_A) \quad (3)$$

$$(Rate\ Generation) = V(-r_a) = VC_Ak_0e^{-E/RT} \quad (4)$$

In the case of a CSTR, the rate of accumulation will be equal to $V\frac{dC_A}{dt}$. This comes from overall number of moles in the CSTR is VC_A , so the accumulation of moles will just be the differential of this.

The flow of moles in versus the flow of moles out is equal to $F(C_{A0} - C_A)$, which is the flow rate, multiplied by the difference in the concentration of moles in the feed stream and the product stream.

Finally, the rate of generation of moles in the system can determine by using the Arrhenius Equation. This will give the rate of generation equal to $VC_Ak_0e^{-E/RT}$.

Combining all of these equations and then solving for $V\frac{dC_A}{dt}$, the equation becomes:

$$\frac{dC_A}{dt} = F(C_{A0} - C_A) - k_0 e^{-E/RT} C_A \quad (5)$$

2.5.2 Energy Balance

From our thermodynamics coursework, we know that the general equation for an energy balance in any system is as follows:

$$(Rate\ Energy\ Accumulation) = (Heat\ In) - (Heat\ Out) + (Rate\ Heat\ Generation) + (Heat\ Transfer) \quad (6)$$

$$(Rate\ Energy\ Accumulation) = V_\rho C_\rho \frac{dT}{dt} \quad (7)$$

$$(Heat\ In) - (Heat\ Out) = \rho C_p F(T_0 - T) \quad (8)$$

$$(Rate\ Heat\ Generation) = -V\Delta H_{rxn}(-r_a) = (-\triangle H_{rxn}) V k_0 C_A e^{-E/RT} \quad (9)$$

$$(Heat\ Transfer) = UA_s^*(T - T_{Cin}) \quad (10)$$

$$UA_s^* = a(F_c)_s^{b+1}/[(F_c)_s + a(F_s^b)/2\rho_c C_{pc}] \quad (11)$$

In the case of a CSTR, the rate of energy accumulation within the reactor will be equal to $V_\rho C_\rho \frac{dT}{dt}$. This equation is basically the total number of moles (mass actually) in the reactor multiplied by the heat capacity and the change in temperature.

The heat generated by this reaction is $(-\Delta H_{rxn})Vk_0e^{-E/RT}C_A$, which is the rate of mass generation ($-Vr_a$) times the specific heat of reaction (ΔH_{rxn}).

The overall rate of heat transfer into and out of the system is given by $\rho C_pF(T_0-T)$. This equation is the flow rate multiplied by the heat capacity and the temperature difference, which gives us the total amount of heat flow for the system.

Finally, the amount of heat transferred into the system is given by $UA_s^*(T-T_{Cin})$. Combining all of these equations and solving the energy balance for $\frac{dT}{dt}$, the equation becomes:

$$\frac{dT}{dt}=\frac{\rho C_pF(T_0-T)-\dfrac{aF_c^{b+1}}{F_c+\dfrac{aF_c^b}{2\rho_cC_{pc}}}(T-T_{cin})+(-\Delta H_{rxn})Vk_0e^{-E/RT}C_A}{V\rho\Delta C_p}$$

(12)

In a realistic situation in which many chemical processed deal with multiple reactions and heat effects slight changes to the modeled equation must be done. The diagram below evaluates the heat exchanger under heat effects in which there is an inlet and outlet temperature that is accounted for in the enthalpy term in the newly modeled equation.

The reactor in Figure 4 is modeled where it is well mixed, constant-volume CSTR with a single first-order reaction, exothermic heat of reaction, and a cooling coil. In a CSTR, one or more fluid reagents are introduced into a tank reactor equipped with an impeller. The impeller stirs the reagents to ensure proper mixing. The system is the liquid in the reactor. Since the concentration changes, a component material balance is required, and since heat is transferred and the heat of reaction is significant, an energy balance is required. Thus we need to consider the following equations [10]:

$$\frac{dC_A}{dt} = F(C_{A0} - C_A) - k_0 e^{-E/RT} C_A \tag{13}$$

$$\frac{dT}{dt} = \frac{\rho C_p F(T_0 - T) - \dfrac{aF_c^{b+1}}{F_c + \dfrac{aF_c^b}{2\rho_c C_{pc}}}(T - T_{cin}) + (-\Delta H_{rxn}) V k_0 e^{-E/RT} C_A}{V\rho\Delta C_p} \tag{14}$$

The linearized equations in deviation variables are as follows [6]:

$$\frac{dC'_A}{dt} = a_{11}C'_A + a_{12}T' + a_{13}C'_{A0} + a_{14}F'_c + a_{15}T'_0 + a_{16}F' \tag{15}$$

$$\frac{dT'}{dt} = a_{21}C'_A + a_{22}T' + a_{23}C'_{A0} + a_{24}F'_c + a_{25}T'_0 + a_{26}F' \tag{16}$$

where

$$a_{11} = -\frac{F}{V} - k_0 e^{-\frac{E}{RT_S}} \tag{17}$$

$$a_{12} = -\frac{E}{RT_S^2} k_0 e^{-\frac{E}{RT_S}} C_{AS} \tag{18}$$

$$a_{13} = \frac{F}{V} \tag{19}$$

$$a_{14} = 0 \tag{20}$$

$$a_{15} = 0 \tag{21}$$

$$a_{16} = \frac{(C_{A0} - C_A)_S}{V} \tag{22}$$

$$a_{21} = \frac{-\Delta H_{rxn} k_0 e^{-\frac{E}{RT_S}}}{\rho C_p} \tag{23}$$

$$a_{22} = -\frac{F}{V} - \frac{UA_s^*}{V\rho C_p} + (-\Delta H_{rxn})\frac{\frac{E}{RT_s^2}}{\rho C_p} k_0 e^{-\frac{E}{RT_s}} C_{As} \quad (24)$$

$$a_{23} = 0 \quad (25)$$

$$a_{24} = \frac{-abF_{cs}^b\left(F_{cs} + \frac{a \quad F_{cs}^b}{b2\rho_c C_{pc}}\right)[T_s - (T_{cin})_s]}{(V\rho C_p)(F_{cs} + \frac{aF_{cs}^b}{2\rho_c C_{pc}})^2} \quad (26)$$

$$a_{25} = \frac{F}{V} \quad (27)$$

$$a_{26} = \frac{(T_0 - T)_s}{V} \quad (28)$$

$$UA_s^* = a(F_c)_s^{b+1}/[(F_c)_s + a(F_s^b)/2\rho_c C_{pc}] \quad (29)$$

2.6 Plant Model

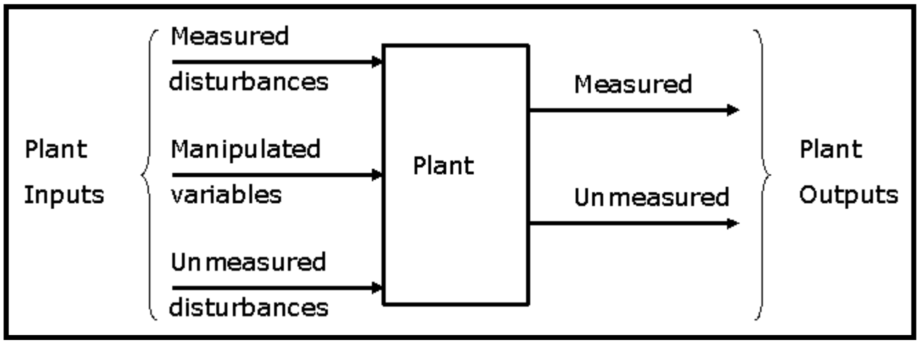

Figure 5: Plant with Input and Output Signals

Figure 5 above shows the plant system (process or device) that we intend to control. There are two sides of the plant which are the plant inputs and plant outputs.

<u>Inputs</u>

The plant inputs are the independent variables affecting the plant. As shown in Figure 5, there are three types:

Measured disturbances **-**The controller can't adjust them, but uses them for feedforward compensation.

Manipulated variables **-**The controller adjusts these in order to achieve its goals.

Unmeasured disturbances **-**These are independent inputs of which the controller has no direct knowledge, and for which it must compensate.

<u>Outputs</u>

The plant outputs are the dependent variables that need to be controlled or monitored. As shown in Figure 5, there are two types:

Measured outputs -The controller uses these to estimate unmeasured quantities and as feedback on the success of its adjustments.

Unmeasured outputs -The controller estimates these based on available measurements and the plant model. The controller also holds unmeasured outputs at setpoints or within constraint boundaries. [11]

CHAPTER 3

METHODOLOGY

3.1 Procedure Identification

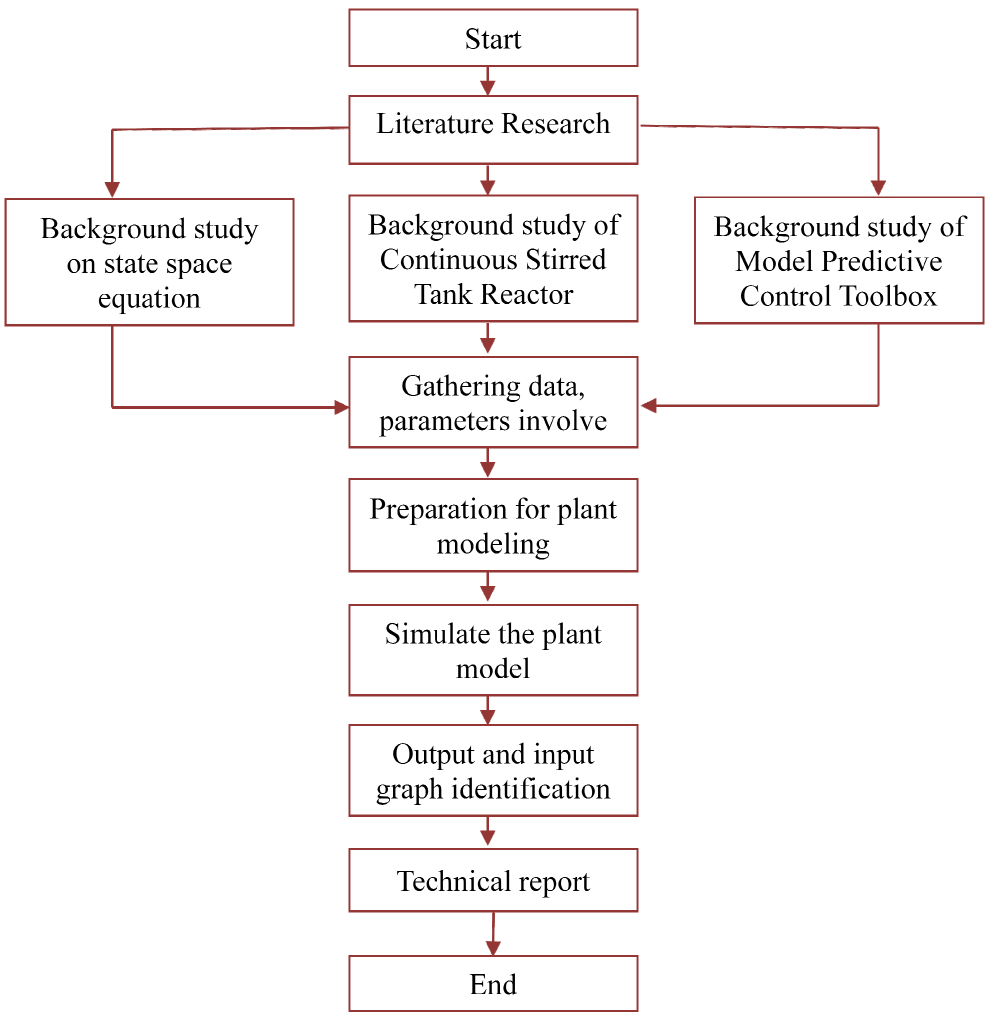

Figure 6: Flowchart of the project

1. Literature Research
    - Control System – Study the concept of control system such as open loop system, closed loop system, feedback control, and model predictive control. Learn using the MATLAB.

    - Mathematical Modeling – Study on the concept of mathematical modeling and how can it represent a system in real life situation.

    - Continuous Stirred Tank Reactor – Conduct some background research on how do CSTR works and the previous work about its modeling system.

    - Model Predictive Control – Learn using MATLAB by referring to the Model Predictive Control Toolbox user guide.

    - State Space – Study the basic state space equation and how to represent a plant model into a state space equation.

2. Gathering Data/Parameters
    - Find data on CSTR based on books.

    - Identify the inputs involved and how does it affect the outputs of CSTR.

    - Identify the inputs which are significant and also the assumptions that need to be considered in modeling the CSTR.

3. Preparation for Plant Model
    - Convert the state space into the plant model using MATLAB and load it into the Plant Model Importer.

4. Simulate the Plant Model

- Compile the program.

- Check for errors.

- By using the Model Predictive Control Toolbox, the CSTR model is simulated.

5. Output and Input Graph Identification

- Analyze the data.

- Compare the simulation to the books as references in order to verify the results.

6. Technical Report

- Results obtained are discussed and put into the report.

In order for the project timeframe, there are some procedures to be followed:

- **Data research and gathering**

Elements of projects involved in this stage include the study of mathematical modeling of control system for maximizing plant product and modeling regarding MATLAB software.

- **Development of mathematical modeling**

With the completion of data gathering, next is to develop a similar mathematical model using MATLAB. The significant input variables are known and excluding the insignificant ones.

- **Model implementation and testing**

In this stage, after the development of the mathematical modeling, next is to implement it with the data received.

3.2 Tools and Equipment Required

Software:

MATLAB/ Model Predictive Toolbox

The programming tool is for algorithm programming purposes.

CHAPTER 4
DISCUSSION AND RESULTS

4.1 Discussion

Equations below indicate the imported plant model and it is showing the number of inputs and outputs with the number in each subclass. The states for the equations are considered below:

$$\frac{dC'_A}{dt} = a_{11}C'_A + a_{12}T' + b_{11}T'_{Cin} + b_{12}C'_{Ai}$$

$$\frac{dT'}{dt} = a_{21}C'_A + a_{22}T' + b_{21}T'_{Cin} + b_{22}C'_{Ai}$$

where:

$\boldsymbol{C_A}$ - is the concentration of a key reactant

$\boldsymbol{T}$ - is the temperature in the reactor

$\boldsymbol{T_{Cin}}$ - is the coolant temperature

$\boldsymbol{C_{Ai}}$ - is the reactant concentration in the reactor feed

$\boldsymbol{a_{ij}}$ and $\boldsymbol{b_{ij}}$ are constants.

$$x = \begin{bmatrix} C'_A \\ T' \end{bmatrix} \qquad u = \begin{bmatrix} T'_C \\ C_{Ai} \end{bmatrix} \qquad y = \begin{bmatrix} T' \\ C'_A \end{bmatrix}$$

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \qquad B = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix}$$

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

The following code shows how to define such a model for some specific values of the a_{ij} and b_{ij} constants. The constants are calculated using the formula from earlier (17) to (29):

```
A = [-0.0285 -0.0014
    -0.0371 -0.1476];
B = [-0.0850   0.0238
     0.0802   0.4462];
C = [0 1
    1 0];
D = zeros(2,2);
CSTR = ss(A,B,C,D)
CSTR.InputName = {'T_c', 'C_A_i'};
CSTR.OutputName = {'T', 'C_A'};
CSTR.StateName = {'C_A', 'T'};
CSTR.InputGroup.MV = 1;
CSTR.InputGroup.UD = 2;
CSTR.OutputGroup.MO = 1;
CSTR.OutputGroup.UO = 2;
CSTR
```

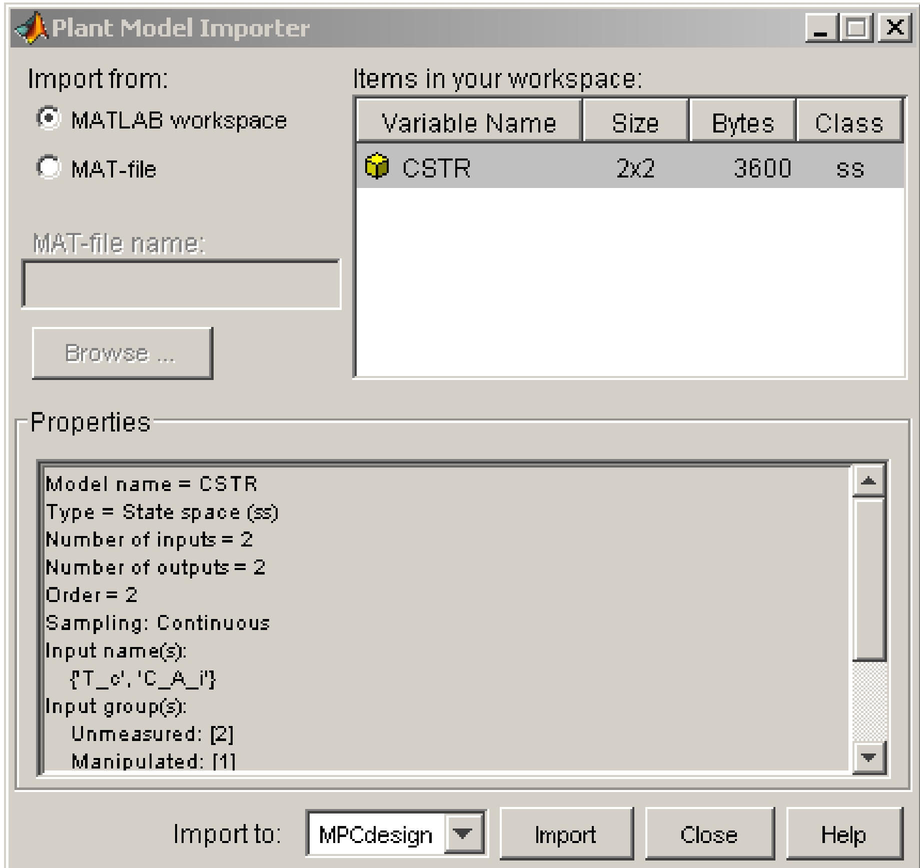

Figure 7: Plant Model Importer

The state-space model is named as CSTR (Continuous Stirred Tank Reactor). Then, the plant is loaded into the Plant Model Importer.

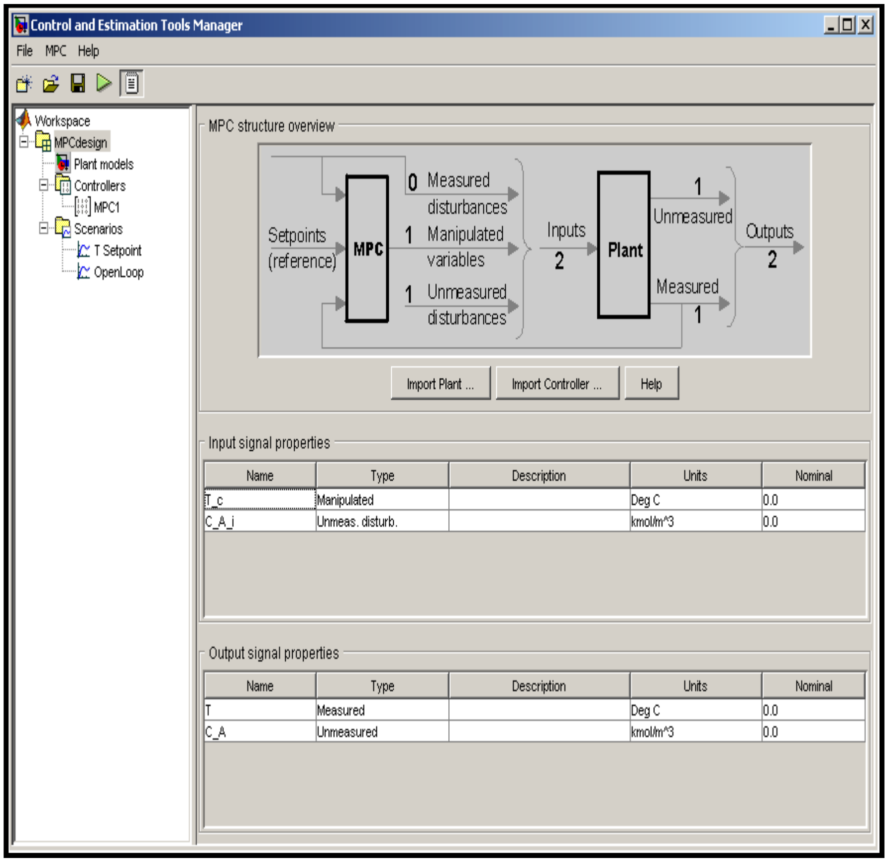

Figure 8: Control and Estimation Tools Manager

Figure 8 indicates the imported plant model and it is showing the number of inputs and outputs with the number in each subclass. As we can see in the picture, there are 2 inputs and 2 outputs:

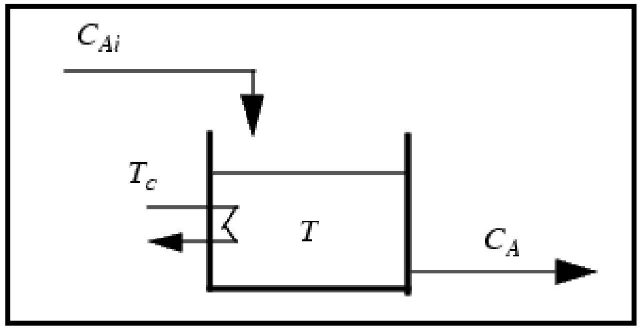

Figure 9: CSTR Diagram

Table 1: CSTR parameters and descriptions

Parameters	Description
Setpoints	We set temperature in the reactor (T) to achieve 2°C
Measured disturbance	No input (0)
Manipulated variable	The coolant temperature T_c (Deg C)
Unmeasured disturbance	The reactant concentration in the reactor feed C_{Ai} (kmol/m^3)
Inputs	Two (T_c and C_{Ai})
Unmeasured output	Output concentration from reactor (C_A)
Measured output	Temperature in the reactor (T)
Outputs	Two (C_A and T)

All the parameters in the Table 1 above are key in into the Control and Estimation Tools Manager as in Figure 10 below.

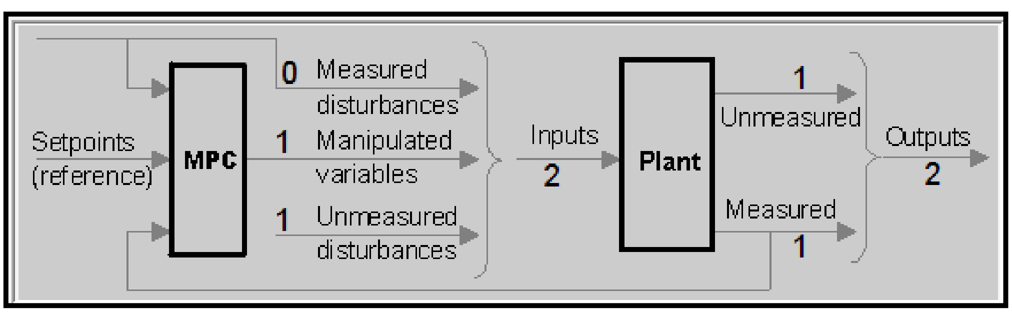

Figure 10: Control and Estimation Tools Manager

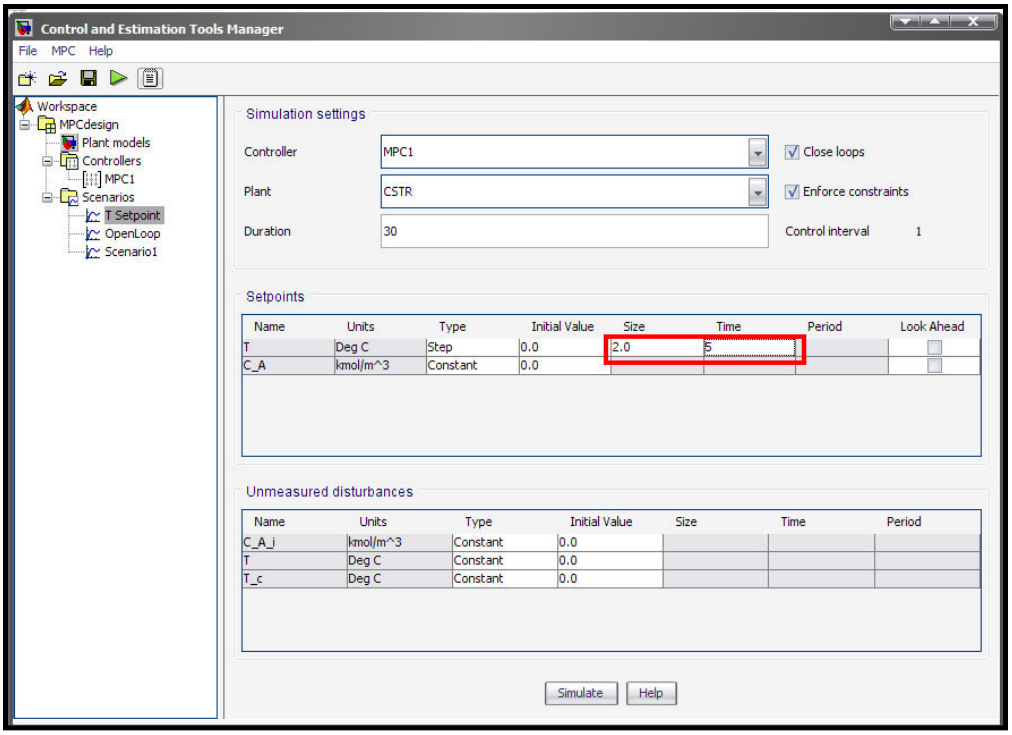

Figure 11: Control and Estimation Tools Manager

To simulate the plant model, the tabular data defining the reactor temperature is set:

- The Duration of data is set to 30.
- The set point is set to 2 for the temperature of the reactor.
- The time for x-axis is set to 5.

4.2 Results for 2 inputs

Inputs:

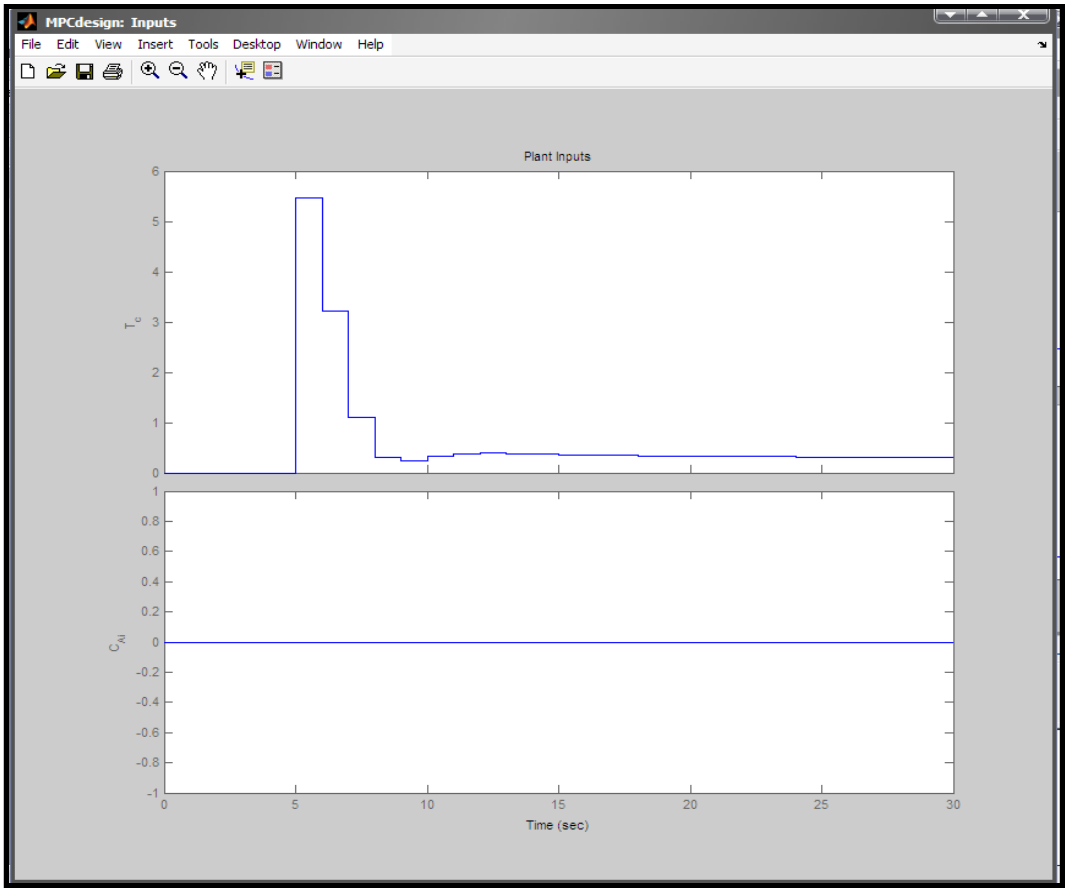

Figure 12: Input graph

From the Figure 12, the window is where we want to set the conditions for the plant. In the window, the reactor temperature set point is set to 2°C and the change is set to occur at T = 5s.

Outputs:

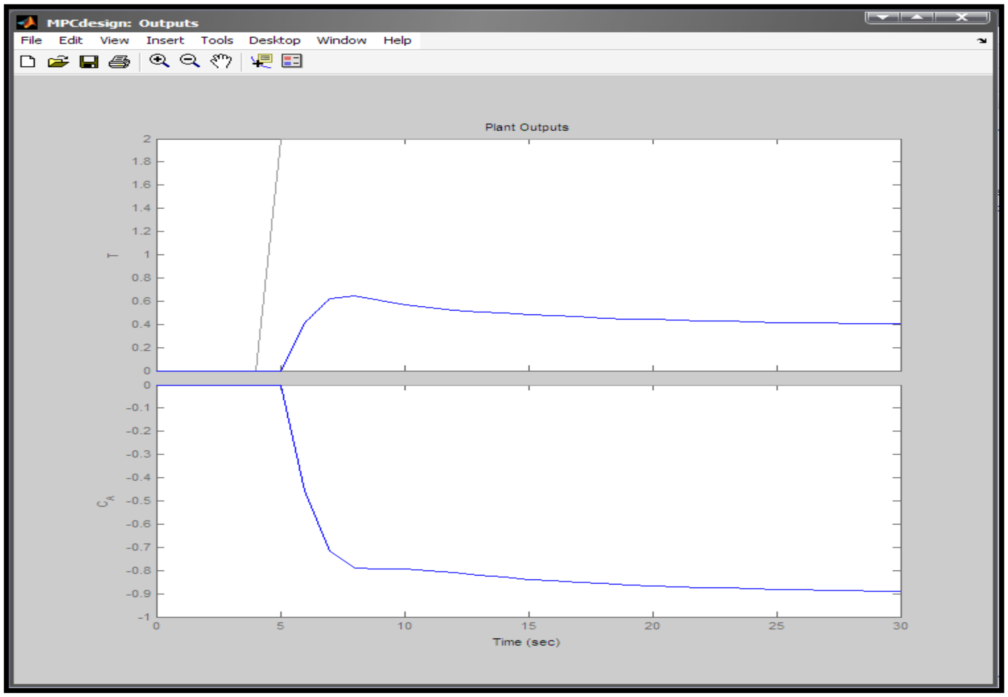

Figure 13: Output graph

After defining the simulation condition, we run the simulation and found the graph as in Figure 13. In the graph, the temperature does not track the set point very well as we set it to be 2°C earlier. The response found to settle at 0.4°C which results in error of 1.6°C at the end of the simulation.

Until this part, the simulation will consider a new set of inputs which contain 4 types on inputs. From the previous report (Progress Report I), the experiment had considered 2 types of inputs with 2 outputs.

For 4 types of inputs and 2 outputs, there are new parameters which are involved and can be represented as the following diagram below:

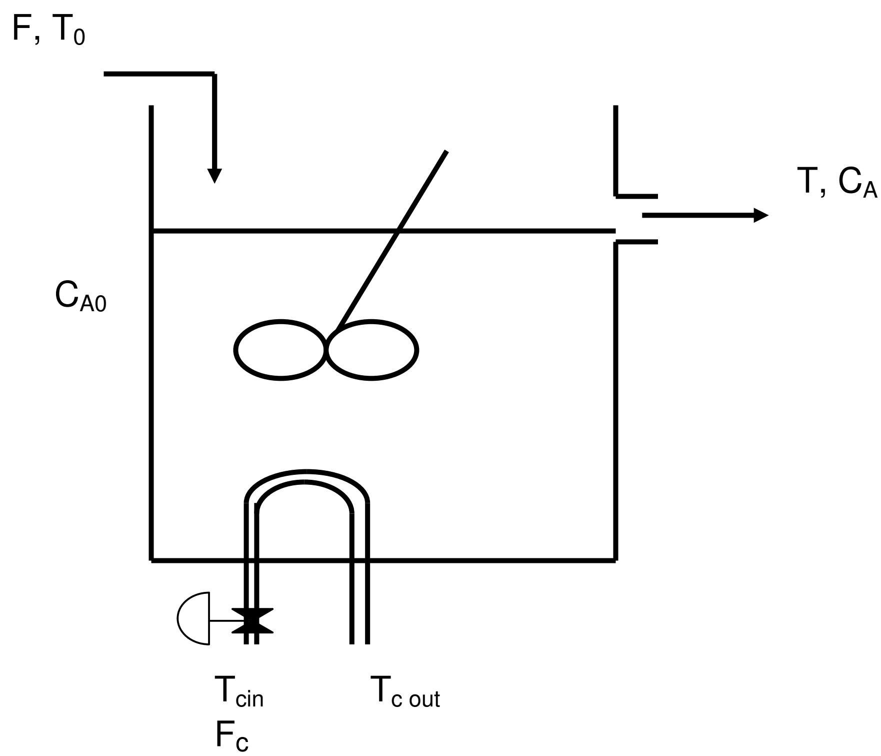

Figure 14: Non-isothermal CSTR with 4 inputs

Table 2: CSTR parameters and descriptions for 4 inputs and 2 outputs

Parameters	Description
Setpoints	We want temperature in the reactor (T) to reach a steady state temperature of 395.3 K
Measured disturbance	No input (0)
Manipulated variable	The coolant temperature T_c (Deg C)
Unmeasured disturbance	The reactant concentration in the reactor feed C_{Ai} (kmol/m^3)
Inputs	Four (F, T_0, F_c and C_{A0})
Unmeasured output	Output concentration from reactor (C_A)
Measured output	Temperature in the reactor (T)
Outputs	Two (C_A and T)

As for the new set of inputs, we need to set a new linearized equation in order to be used as a model for simulation. The new linearized equationfor the 4 inputs (F, T_0, F_c and C_{A0}) and the outputs (C_A and T) are :

$$\frac{dC'_A}{dt} = a_{11}C'_A + a_{12}T' + a_{13}C'_{A0} + a_{14}F'_c + a_{15}T'_0 + a_{16}F' \quad (30)$$

$$\frac{dT'}{dt} = a_{21}C'_A + a_{22}T' + a_{23}C'_{A0} + a_{24}F'_c + a_{25}T'_0 + a_{26}F' \quad (31)$$

Next, to fill in the constant from a_{11} to a_{26} the formula (17) to (29) are calculated using this data:

Table 3: CSTR Data

F = 1.0 m3/min	C_p = 1.0 cal/(g K)
V = 1.0 m3	$\rho = 10^6$ g/m^3
C_{a0} = 2.0 kmol/m3	$T_{c\,in}$ = 365 K ≈ 92 °C
T_0 = 323 K	F_c = 15 m^3/min
k_0 =1.0 x 10^{10} min-1	C_{pc} = 1.0 cal/ (g K)
E/R =8330.1 K	$\rho_c = 10^6$ g/m^3
ΔH_{rxn} = -1.30 x 10^8 cal/kmol	

The constants are calculated and their values are as follows:

a_{11}= -7.576253

a_{12}= -7.3706 x 10^4

a_{13}= 1

a_{14}= 0

a_{15}= 0

a_{16}= 1735

a_{21}= 855.1082

a_{22}= -2.0688 x 10^{12}

a_{23}= 0

a_{24}= -1.9852

a_{25}= 1

a_{26}= -71

4.3 Results for 4 inputs

The new equations with the values (30) and (31) are put into matrix form in order to be used as the plant model in the Model Predictive Control Toolbox. We load the new plant model into the Control and Estimation Tools Manager as below :

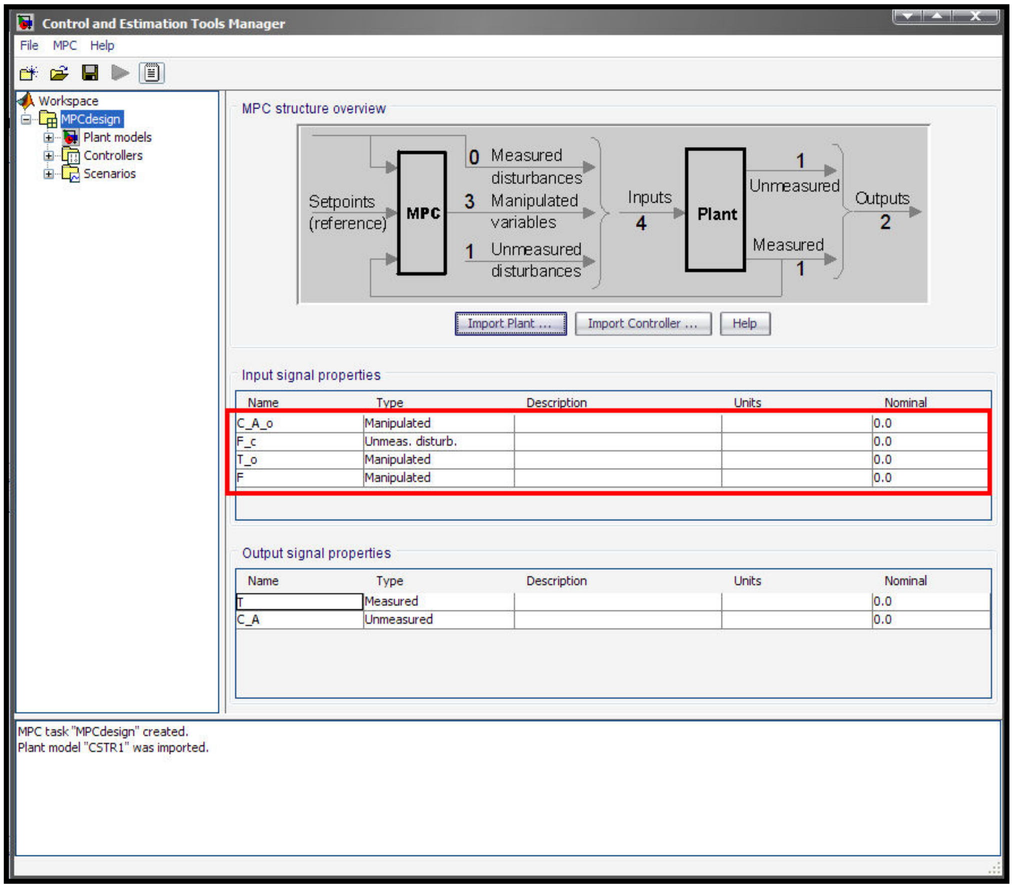

Figure 15: Control and Estimation Tools Manager

From the figure above the red coloured box indicated the 4 new inputs parameters that will be consider in order to get the outputs.

The plant model is simulated but for now the graph contains error. The output graphs do not indicate any change in the temperature and concentration (C_A and T) and only the set point are visible. The actual graphs needed to be achieved are in the next page.

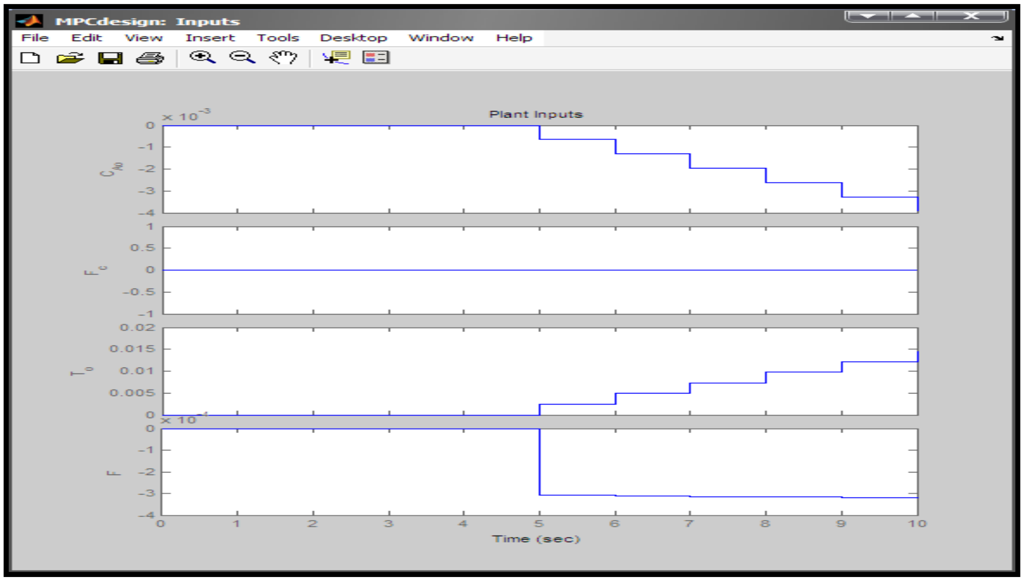

Figure 16: Graph for 4 inputs

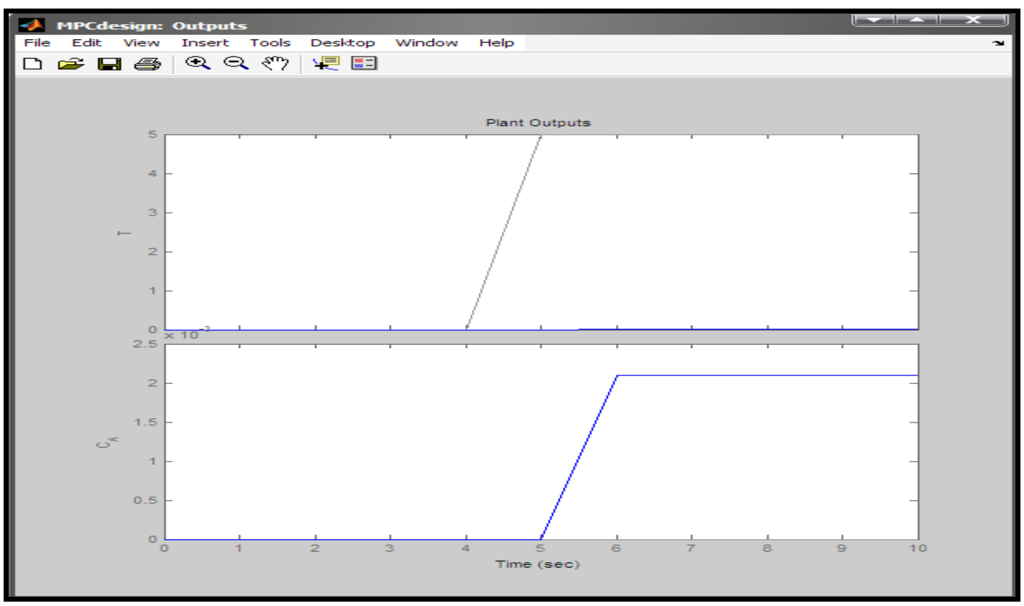

Figure 17: Graph for 2 outputs

Here are the actual graph that need to be achieved and the objectives are to increase the chemical reactor to its steady state 395.3 K and the output concentration to 0.265 kmole/m^3. The actual desired outputs are expected to be as follow:

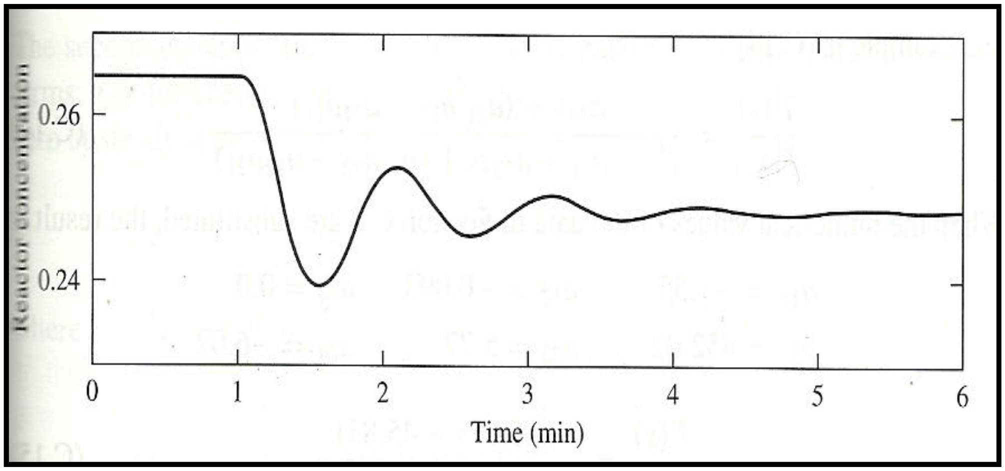

Figure 18: Expected Graph for Output Concentration, C_A

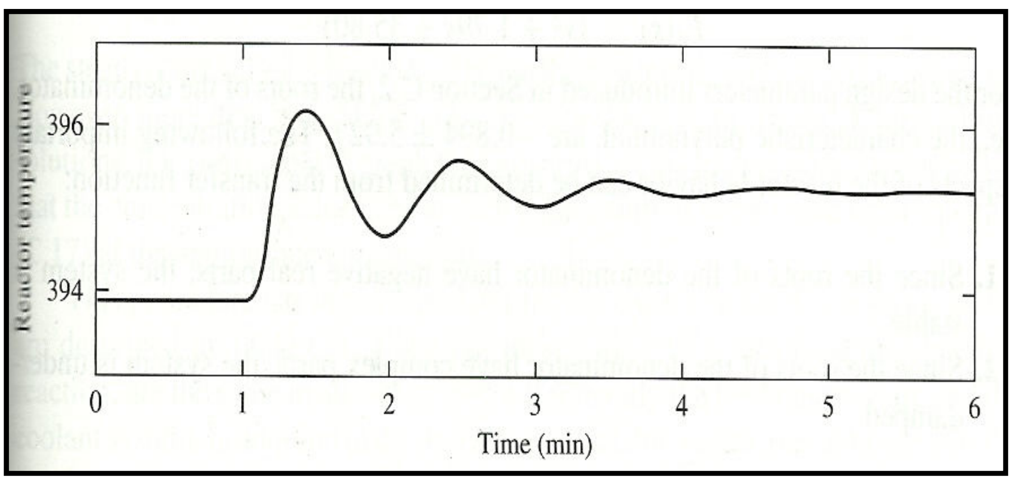

Figure 19: Expected Graph for Reactor Temperature, T

CHAPTER 5
CONCLUSION AND RECOMMENDATIONS

5.1 Conclusion

It was found that the model that would be obtained follows the behavior that is a combination of trends processes. However, there would be some irregularities in the simulation results that could not be predicted by both process trends. The mathematical software, MATLAB was chosen as the means to simulate the resulting model, due to its greater flexibility. Simulations would then be performed in order to study the behavior of the resulting optimization production output. Many studies are being conducted on this process in order to improve understanding of its behavior by mathematical modeling and simulation using computers. This method of study is more effective compare to experimental studies.

5.2 Recommendations

For the future works, I hope to find other suitable plant model that suitable for this project. Furthermore, I would like to simulate multiple inputs and produce multiple output products (MIMO). Lastly, is to optimize the output after the plant model is successfully simulated. Another thing to add is the type of chemical reactant that are usually used in the CSTR.

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APPENDIX