JIMMA UNIVERSITY

JIMMA INSTITUTE OF TECHNOLOGY

FACULTY OF ELECTRICAL AND COMPUTER ENGINEERING

TITLE:

MODEL AND DESIGN OF SELF-TUNING REGULATOR BASED CASCADE CONTROL OF EXOTHERMIC STIRRED TANK REACTOR

A Thesis submitted to the School of graduate studies of Jimma University in partial Fulfillment of requirements for the Degree of Master of Science in Control and Instrumentation Engineering

Prepared by:

Tesfabirhan Shoga

RM 0138/08

Jan, 2018

Jimma, Ethiopia

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Main Advisor: Dr. Prashanth Alluvada

Co-Advisor: Mr. Mengistu Fentaw

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DECLARATION

The undersigned agrees to accept responsibility for the scientific ethical and technical conduct of the research project and for provision of required progress reports as per terms and conditions of the Jimma Institute of Technology in effect at the time of Grant is forwarded as the result of this application.

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ABSTRACT

Exothermic reaction process releases energy during mixing of different substances within the stirred tank reactor. The nature of reacting substances may exhibit different chemical properties that lead for an exothermic reaction to be occurring. The generated heat on the stirred tank reactor due to exothermic process should be regulated properly as the system shows non-linear and uncertain process. In this thesis the design of cascade control of exothermic stirred tank reactor is only using adaptive self-tuning regulator. The purpose of self-tuning regulator is to make online parameter estimation for the uncertain plant. It has both ordinary feedback control loop and parameter estimation block. For parameter estimation recursive least square algorithm is used to estimate the plant parameters. The control system has two controlled outputs the concentration of feed stream and temperature of the reactor. The flow rate of water through the cooling jacket around the reactor is a common manipulated input variable. The controlled outputs have two disturbance variables like inlet feed temperature and the inlet feed concentration to the reactor. By considering the stirred tank reactor as ideal and assuming perfect mixing of the reactant in reacting medium, the volume of reactor will be constant. On the other hand, the concentration of reactant inside the reactor is also the same with that of the output concentration. The cascade stirred tank reactor processes presented involves two internal control loop stages for each controlled outputs. Each control loop has its own slave controller and the corresponding plant dynamics. For the two outputs of the cascade exothermic stirred tank reactor, a PI controller was used for controlling the secondary internal loop plant of the system under the desired condition. Such loops will be considered as secondary control loops for the each controlled outputs. On the other hand the self-tuning controller is used as a master controller for each controlled variables. So far a PID controller based designs of cascade CSTR were made to the linear plant models so as to analyze the control action and the stability of the system. But the PID controller does not have the ability to estimate the parameters of the plant exhibiting non-linear characteristics. .Thus self-tuning regulator control technique used in this thesis allows a more stable output of for the plant having dynamic behavior.

Key words- Exothermic CSTR, Cascade control, RLS Algorithm, Self-tuning controller

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LIST OF ABBREVIATIONS AND SYMBOLS

CSTR	Continuous stirred tank reactor
PI	Proportional and integral
PID	Proportional, integral and derivative
STR	Self-tuning regulator
MPC	Model predictive control
RLS	Recursive least squares
k_0	Frequency factor
k_r	Arrhenius law
τ_R	Residence time
τ_C	Composition time constant
τ_T	Thermal time constant
K_{CT}	Gain for the effect of temperature on concentration
K_{TC}	Gain for the effect of concentration on temperature
K_{ht}	Gain of heat transfer
ξ	damping ratio
C_A	Concentration of reactant A in reactor tank
C_{Ai}	Concentration of reactant A in inlet feed stream
r_A	Rate of reaction for reactant A
Q	Heat energy of reaction
ρ	Product density

ρ_c	Water density
V	Reactor volume
C_p	Thermal capacity
E	Activation energy
R	Perfect gas constant
ΔH_R	Reaction heat
h_i	Inner surface heat transfer barrier
h_{ir}	Reference Inner surface heat transfer barrier
h_0	Outer surface heat transfer barrier
A_0	Outer heat transmission surface
U_{0r}	Heat transmission coefficient
F	Feed flow rate
T	Reactor Temperature
T_{cr}	Reference temperature of cooling jacket
T_{ir}	Reference inlet feed temperature
T_{ci}	Steady state cooling water input temperature
F_{cr}	Reference flow rate of water in cooling jacket
T_r	Reference reactor temperature
T_i	Inlet feed stream temperature
C_{AR}	Reference feed concentration
C_{pc}	Water thermal capacity

β_r	Number of transfer units
θ_1	Parameter of temperature plant
θ_2	Parameter of concentration plant
φ_1	Regression matrix for temperature plant parameters
φ_2	Regression matrix for concentration plant parameters
P_1	Covariance Matrix for temperature plant
P_2	Covariance Matrix for concentration plant
λ_1	Exponential forgetting factor for temperature plant parameters estimator
λ_2	Exponential forgetting factor for concentration plant parameters estimator
ε_1	Temperature plant parameters estimation error
ε_2	Concentration plant parameters estimation error

CHAPTER ONE

1.1. INTRODUCTION

The development and advancement of chemical industries has been providing environment-friendly technology on the area of manufacturing process of chemical products. A chemical reactor is the one which plays a vital role in the production of significant chemical products. It is an equipment unit in a chemical process (plant) where chemical transformations (reactions) take place to generate a desirable product at a specified production rate, using a given chemistry. A chemical reaction is a process that leads to the transformation of one substance to another. Classically, chemical reactions encompass changes that involves electrons positions in forming and breaking of a chemical bond among atoms with no change to the nuclei (no change to the elements present) [1].

The reactor configuration and its operating conditions are selected to achieve certain objectives such as maximizing the profit of the process, and minimizing the generation of pollutants, while satisfying several design and operating constraints (safety, controllability, availability of raw materials, etc.). Usually, the performance of the chemical reactor plays a pivotal role in the operation and economics of the entire process since its operation affects most other units in the process (separation units, utilities, etc.).

Chemical reactors are expected to fulfill three main requirements such as providing appropriate contacting of the reactants, allowing the necessary reaction time for the formation of the desirable product and providing the heat-transfer capability required to maintain the specified temperature range [2].

In many instances these three requirements are not complimentary, and achieving one of them comes at the expense of another. Chemical reaction engineering is concerned with achieving these requirements for a wide range of operating conditions—different reacting phases (liquid, gas, solid), different reaction mechanisms (catalytic, non-catalytic), and different operating temperature and pressure (low temperature for biological reaction, high temperature for many reactions in hydrocarbon processing).

A chemical reactor tank is the one that plays an important role in process control by providing an environment for the reaction of reactants. It has two important parts in order to make effective chemical reaction to be occurred. The first part is an internal feed reacting element while the outer part is the cooling element which has a series of cooling pipes of different thickness and cross section. The cooling water will flow through the respective pipes around the reactor tank so that the heat generated on the surface of the tank will be regulated. The heat is caused by the nature, inlet concentration and temperature of reactants in the given chemical reaction.

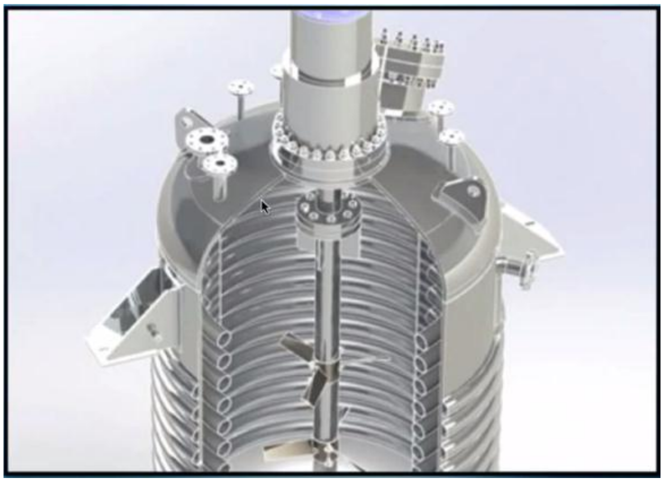

Figure 1.1. Configuration of chemical reactor [3]

The operation of a chemical reactor is affected by a multitude of diverse factors. In order to select, design, and operate a chemical reactor, it is necessary to identify the phenomena involved, to understand how they affect the reactor operation, and to express these effects mathematically.

The control of chemical reactors is one of the most challenging problems in control processes. A continuous stirred tank reactor can be considered as the heart of many chemical reaction processes. The stability and performance of the system will be effectively analyzed to ensure that the entire process is operating within optimum range [**4**].

Many reactors are inherently unstable. The un-stability appears when irreversible exothermic reactions are carried out in a CSTR. Proper management and monitor of reactor systems have the potential to achieve controlling certain parameters around it. The CSTR control strategy is based on the fact that concentrations of components of reactions taking place in the reactor depend on the reactant temperature. Then, in the cascade control-loop, the concentration and flow rate of a main product of the reaction is considered as the primary controlled variable, and, the reactant temperature and level of fluid as the secondary controlled variable. The coolant flow rate represents a common control input [**5**].

The parameters of the reactor dynamics which are going to be controlled using an adaptive self-tuning regulator is the main task to be performed which involves a real time parameters adjustment using adaptive self-tuning regulator control scheme significantly employed for chemical industrial applications under this research.

Cascade control is commonly used in the control of chemical processes to reject disturbances that have a rapid effect on a secondary measured variable, before the primary controlled variable is affected. In this paper, cascade control strategy is used to control the temperature inside a jacketed exothermic continuous stirred tank reactor [**6**].

Basically an adaptive self-tuning regulator can be designed for a given chemical reactor system dynamics having adjustable plant and controller parameters. A different scheme is obtained if the estimates of the process parameters are updated and the controller parameters are obtained from the solution of a design problem using the estimated parameters.

An adaptive control strategy is a helpful tool in the process control industries which has a controller with adjustable parameters. In the sense of control theory and engineering, an adaptive controller can modify its behavior in response to the variations in the dynamics of the process and the character of the disturbances. It is understood that the task of controller design for a process is very much domain specific. First the model of the process is linearized around a certain nominal point and the controller is designed on the basis of the linearized model and finally implemented on the process. Hence, the controller is applicable for certain domain around the nominal operating point around which the model has been linearized using Taylor series. However, if the process deviates from the nominal point of operation, controller will lose its efficiency. In such cases, the parameters of the controller need to be re-tuned in order to retain the efficiency of the controller. When such retuning of controller is done through some “automatic updating scheme”, the controller is termed as adaptive controller.

Usually there are four types of adaptive control schemes: self-tuning regulators, model-reference adaptive control, gain scheduling and stochastic control. This section focuses on self-tuning regulators.

1.2. STATEMENT OF PROBLEM

The stirred tank reactor allowing exothermic reaction releases heat energy so that the reactor temperature will increase so fast. Due to the production of large increment in temperature, the heat generated on the reactor highly affects the safety and the lifetime of the reactor. This may result in unexpected loss of product. The rising of reactor temperature should be controlled by applying certain appropriate control mechanism a more stable output.

To avoid the damage of the tank due to the heat generated and further loss of products, it is often important to keep the stability of reactor temperature and making a continuous online regulation of parameter in the range of operation of using self-tuning regulator control algorithm.

The parameters have to be adjusted or estimated so as to obtain a more stable reactor output temperature that corresponds with the range by which the chemical reactor intermediate processes are going to be monitored. The un-stability of reactor process parameters influences the smooth activities and performances of several industrial chemical reactor machineries.

This study is tending to provide a solution by enhancing the stability of the temperature of the chemical reactor through its intermediate process dynamics control. It involvesonline monitoring and controlling of process parameters like temperature, flow rate and concentration with important modelling structure using adaptive self-tuning regulator.

1.3. SCOPE AND LIMITATIONS OF THE STUDY

This study discusses a design of self-tuning regulator based cascade control of exothermic stirred tank reactor for the reactor process control that involves:

- Developing the material and energy balance model based on the chemical engineering principle of reaction.
- Designing the controller and reference plant model for both concentration and reactor temperature plant dynamics using pole placement design analysis.
- Designing the plant parameter estimator for both output concentration and reactor temperature.
- Analyzing the stability of the two controlled variables using Jury stability analysis.

In the control system, PI controller is used as slave controller and self-tuning controller was used as primary controller for both controlled output temperature and feed concentration.

The control strategy is based on the fact that the temperature of the reactor expressed in terms of inlet feed temperature, inlet feed concentration and flow rate of cooling jacket around the reactor. The other task was computing the stability of the desired plant model under each sub-system and the entire control process dynamics which was followed by designing the reference plant model, the primary self-tuning controller and parameter estimator for both controlled outputs.

On the other hand, there were certain limitations that challenged on the completion this study like there was no enough time due to time consuming and complex design nature of the study, the absence required hardware materials for having experiment. Since the study included requirement of careful design and modeling of the entire system having many parameters to be analyzed.

1.4. SIGNIFICANCE OF THE STUDY

For the sake of having better control of process variables, this study provided ways

- To perform Continuous regulation of controlled variables
- To determine updates or estimation of the past and present time slot plant parameters adjustment.
- To control both linear and non-linear plant dynamics having uncertain characteristic under different circumstances.
- To make Online or continuous update of parameter of both plant dynamics and controller.
- To obtain an accurate result in finding the extent that the plant model to be stable or not.

Besides achieving the above purposes this study allows the chemical reactor to be effective in its operation by reducing the heat generated on its surface. This enables for chemical factories to avoid unnecessary loss or wastage of products and to deliver good quality of products to the community at any time and place. This depends on how the chemical reacting system is more effective and efficient in its operation of reacting two streams of mixtures having different concentration. Since a continuous stirred tank reactor has a constant height that can react two mixtures at constant volume. Besides the improvement of product quality, due to online process parameters adjustment, the factors influencing on the inlet mixture of the reactor will be easily adjusted to enhance the stability of the system.

1.5. OBJECTIVES OF THE STUDY

1.5.1. GENERAL OBJECTIVE

- The main objective of this study is to design cascade control of exothermic continuous stirred tank chemical reactor using self-tuning regulator.

1.5.2. SPECIFIC OBJECTIVES

- To design the plant model and controller for concentration and temperature plants.
- To design the RLS estimator for both concentration and temperature plants.
- To determine the stability of reactor temperature and feed concentration.

CHAPTER TWO

LITERATURE REVIEW

The study of cascaded continuous stirred tank reactor temperature control has been studied in different literatures. For example the S. Nagammai. K, Dhanalakshmi and S. Latha first reviewed literature [7] presented an internal Model based cascade controller design for controlling the temperature of the reactor. The paper described the control of reactor temperature, PID controller based on the feed and jacket temperature changes. In this design, the response of the simple feedback control were improved by measuring jacket temperature and taking control action before its effect has been observed on the output. In such control system, the jacket cooling water flow rate was considered as manipulated variable. The process control involves measurements of single disturbance and manipulated variable. In this case manipulated variable was ultimately adjusted so as to regulate the temperature of reactor.

In such literature, the design analysis of an internal model based cascade control has used filter tuning parameter adjustment for varying the speed of response and for making the controller realizable in the closed loop system. In such design it was found that the stability of the desired reactor temperature and it cooling temperature determined on the basis of transient characteristics of the system response.

However, in such model, cascade control strategy, the effect of an inlet feed concentration and inlet feed temperature on the stability of reactor is not clearly recognized. The system will not continuously optimize the controlled output when there are certain undesired situations or uncertain factors influencing the expected output variable.

Compared with the above literature the system design and analysis in this study, involve consideration of the disturbance variables inlet feed concentration and temperature. By having flow rate of cooling system as manipulated variable and PI slave controller as a secondary internal controller as well as a primary controller that provides a self-tuning regulator for appropriate plant parameters adjustment of controlled output reactor temperature and concentration.

The stability of such controlled output variables is determined due to an online plant parameters adjustment by using RLS algorithm and pole placement based model following between the process and its reference model.

The Suman Debnath and V.K. Tripathi reviewed paper to this study is written in [8] so that the cascade control based continuous stirred tank reactor providing control of a non-linear process with the co-ordination of multiple model predictive controllers. In this control system, the control action was done by using multiple model predictive controllers so as to reduce the effect of undesired noise from the input. Such control technique tried to regulate the state of the reactor and the rate of exothermic reaction by adjusting the coolant temperature of the coolant jacket to have further control for reactor temperature and composition.

Since the approach was to obtain linear models for designing a controller on the basis of dynamic characteristics of the plant by switching the MPC controller block to make transition between multiple MPC controllers within the entire operating-range. In such system design the coordination of MPC controllers was used for optimizing the current time slot for predicting events in the future.

However, the MPC controllers will not necessarily control the output temperature and composition when similar response time is needed due to its transitional control action and its operation only with similar conditions. Even though MPC controllers provide prediction of future events by optimizing the present one, the computational response time for the controlled variable is long due to the interdependence of each controller to apply the necessary action. Due to this some sort of model error will be encountered so that it may reduce the stability of the entire system.

Compared with the second literature, this study has the common goal to achieve better control of the temperature and concentration of exothermic stirred tank reactor with common disturbance variable, inlet feed concentration. The control system will effectively optimize the effect of variable volumetric flow rate of cooling water on the reactor temperture and composition.

In this study by using online parameter estimation with adaptive self-tuning regulator, the desired plant will be updated further in the controller.

The NDZANA Benoît and BIYA MOTTO reviewed literature [9] explained the technique of controlling the temperature of a non-isothermal continuous stirred tank reactor using adaptive PID controller. In this paper, the system controller regulates the feed reaction temperature by manipulating the feed flow rate in the process control dynamics using PID controller. Such process control provides separate modes of tracking and regulatory response of the entire system based on the analysis of both the input and output tracking errors in the corresponding plant model.

The controller was designed to provide a tracking and regulatory response of the plant based on the mass and energy balance principle of inlet feed stream in the chemical reaction processes under the reactor. In this control system design the reactant concentration and initial feed temperature were considered to be disturbance variables while flow rate of liquid inside the cooling jacket was assumed to be manipulated variable. Thus in this paper, the cascade structure of these variables would lead for controlling the temperature of the reaction using PID controller.

In such paper it was found that the process parameters were estimated to make further tuning of PID controller parameters in order to regulate the temperature of non-isothermal chemical reactor. On the other hand, both tracking and regulation model were developed based on the model dynamics so as to provide a response having well damping with minimum time delay.

However, the problem observed in such paper was the PID controller will not perform online update or prediction of the entire parameters for the plant having dynamic characteristics. Since parameter estimator loop will estimate the plant parameters for every period of time so that the controller needs an algorithm to keep adjustment of the parameters for further change in the plant parameters.

Compared with this literature, self-tuning regulator based process control fills the above gap by responding in online tuning of the controller parameters for non-linear or uncertain plant that shows dynamic characteristics.

The ANURAG M. DEULKAR and AJAY B. PATIL reviewed literature to this study is given at [10] whose objective was to develop a Model Predictive Control (MPC) to control the temperature in Continuous Stirred Tank reactor (CSTR) exhibiting highly nonlinear dynamics. The paper described the temperature control process based on comparative analysis between conventional control of PID and MPC control through servo and regulatory response of CSTR model.

In the conventional control analysis, it was found that the PID controller tuning of parameters for plant exhibiting non-linear dynamic characteristic did not provide good performance of the entire system due to the parameters of these nonlinear process varies with all operating conditions. In such case for the non-linear process temperature control of CSTR, the PID controller has given high overshoot and settling time to the entire system in the time domain response.

On the other hand, the analysis on the basis of the model predictive control, the desired control algorithm was applied for controlling the non-linear process dynamics problem and it has provided desired performance to the entire system. It was done by the control system to predict the future values of the output over a certain time horizon. The prediction was performed based on the future instant values which were computed to result in minimum cost function.

The optimized control was then applied to the plant as well as the plant outputs which were measured by making measurements of the plant states as the initial states of the model to perform the next iteration. The MPC controller allowed the plant to provide lower settling time and peak overshoot in the time domain response of the system.

However in this literature, the control system did not provide necessary information about the effect of disturbance variables on CSTR such as inlet feed temperature and concentration as well as flow rate of liquid through the cooling jacket. The MPC controller used in such design might not effectively respond well for large disturbance to the system due to its poor ability of dead time compensation. There is the effect of overshoot on the output of rector temperature due to such problem. So the temperature needed to be controlled so as to achieve the main objective

Compared with such paper, the effect of an overshoot caused by the dead time compensation is totally remove in a self-tuning control technique for exothermic tank reactor.

The P. Dostál, V. Bobál, and J.Vojtěšek, literature which is related with to the study is given in [11]. The paper described the cascade adaptive control of a continuous stirred tank reactor of an exothermic reaction so that the control action was performed on the basis of primary and secondary control-loops. In the control system, the primary controlled output of the reactor was the concentration of the reaction product while the secondary output was the inlet reactant temperature. A jacket surrounding the reactor assumed to have feed and exit streams so that it was assumed to be perfectly mixed at lower temperature. The control objective was to keep the temperature of the reacting mixture to be constant at desired value.

In this paper, the control loops were used for measuring the temperature of reactor and cooling jacket but was sharing liquid flow rate as a common manipulated variable. In this strategy the reactor temperature controller was the primary controller while the jacket temperature controller was the secondary controller. An inner loop disturbance such as jacket feed temperature will be felt by the jacket temperature before it has a significant effect on the reactor temperature.

In this paper, it was found that in cascade design of stirred tank chemical reactor a saturation problem has been happened due to automatic reset in both primary and secondary controllers. Such conditions were considered to be the causes for the occurrence of overshoot on the expected system output. Thus, the control system used an anti-reset windup compensation technique for avoiding such constraints.

On the other hand the system contains a PID controller for both primary and secondary cascade control loops so that, it does not have ability to predict and estimate for responding dynamic characteristics of plant which may cause large time delay to be happen in the system output.

Compared with the third literature, in this study non-linear plants will be easily controlled in terms of increasing the stability of the entire process its parameters. The plant having dynamic property is going to be continuously monitored and better transient response can be achieved effectively.

CHAPTER THREE

3.1. SYSTEM DESIGN PROCEDURES AND METHODS

There are certain basic methods to design the self-tuning regulator based cascade control of exothermic reactor. The procedures were followed to analyse the system design are:

- Understanding an exothermic stirred tank reactor system operation
- Identifying both the input and output variables to the system
- Derive a mathematical model that relates such variables using mass balance equation of exothermic continuous stirred tank reactor.
- Identifying the manipulated, controlled and disturbance variables of the system.
- Developing transfer function model related with controlled variables.
- Drawing the block diagram for cascade continuous stirred tank reactor system having secondary slave controller and primary self-tuning controller as master controller.
- Designing the internal loop slave controller
- Determining the internal closed loop transfer function model for each plant
- Designing the internal loop controller and desired plant model using minimum degree pole placement algorithm and model following technique.
- Analysing the stability of the desired internal loop plant models using Jury stability test.
- Making the Simulink design of the entire system and simulating the observing the results through Matlab software.

3.2. METHOD FOR ANALYZING THE SYSTEM DESIGN

The method which is going to be used for controlling feed concentration and temperature of chemical reactor is adaptive self-tuning regulator. It adjusts the parameters of the dynamic plant model under the control system of cascade feedback loops having slave controllers.

3.2.1. SELF-TUNING REGULATORS (STR)

Self-tuning regulator can be thought of as being composed of two loops. The inner loop consists of the process and an ordinary feedback controller and the other loop is a parameter adjustment loop. The parameters of the controller are adjusted by the outer loop, which is composed of recursive parameter estimator and design calculation.

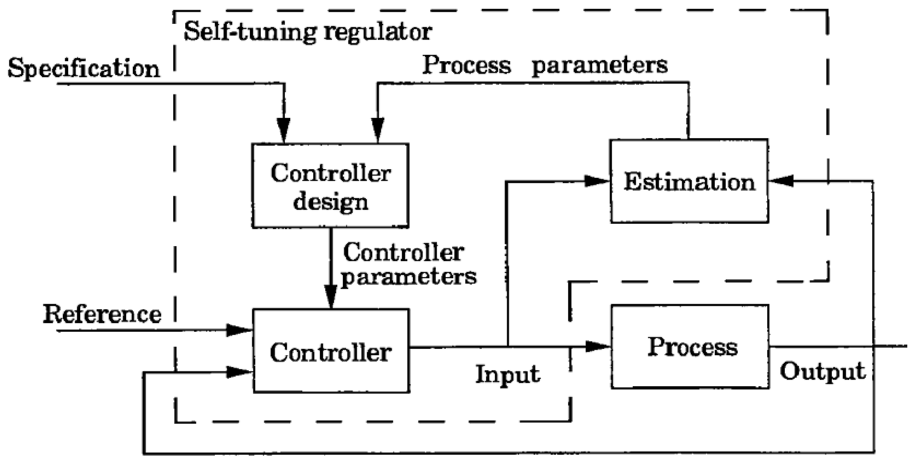

Figure 3.1. Self-tuning regulator block diagram [12]

The block labeled "Estimator" represents an on-line estimation of the process parameters using least-squares or projection algorithms. The block labeled "Controller Design" represents an on-line solution to a design problem for a system with known parameters or with estimated parameters. The block labeled "Controller" is to calculate the control action with the controller parameters computed by its proceeding block. The system can be viewed as an automation of processing modeling/estimation and design, in which the process model and the control design are updated at each sampling interval. Sometimes the STR algorithm can be simplified by re-parametizing and directly estimating the controller parameters, not the process parameters alone. It is flexible in that the STR scheme can be implemented by different choices of the underlying design and estimation methods.

The parameter adjustment loop is often slower than the normal feedback loop. The unknown and un-measurable variations of the process parameters degrade the performances of the control systems. Similarly to the disturbances acting upon the controlled variables, the variations of the process parameters are caused by disturbances acting upon the parameters.

Output of the adaptation mechanism will act upon the parameters of the controller and in order to modify the system performance accordingly.

3.2.2. ESTIMATION ALGORITHMS

It is important to estimate the process parameters on-line in adaptive control. For an adaptive control system, the adaptive mechanism is based on identifying the system first. A self-tuning regulator in Fig. 2 explicitly includes a recursive parameter estimator. Simply speaking, the process parameters estimation is a part of system identification. In a broader sense, system identification is selection of model structure, experiment design, parameter estimation, and validation.

3.2.3. LEAST-SQUARES ESTIMATION ALGORITHM

The least-square method is commonly used in system identification. Its principle is that the unknown parameters of a mathematical model should be chosen by minimizing the sum of the square of the difference between the actually observed and the analytically predicted output values with possible weighting that measure the degree of precision. The least-squares criterion is quadratic, so an analytic solution to the least-squares problem exists as long as the measured variable is linear in the unknown parameters.

In adaptive control system the observations are obtained sequentially in real time. Recursive estimation algorithm is desirable. It saves the computation time by using the results obtained at previous time to get the estimates at present time. Hence, the recursive least-square (RLS) estimation method is used in this section.

3.3. EXOTHERMICSTIRRED TANK REACTOR PROCESS CONTROL

The reactor temperature and concentration are monitored on the basis of the cascade control of the cooling water flow rate with the inlet feed temperature and concentration. So that, the reactor is equipped with a heat transfer surface that contains a flow of cooling water. It is required to know how the output concentration and temperature may vary with time.

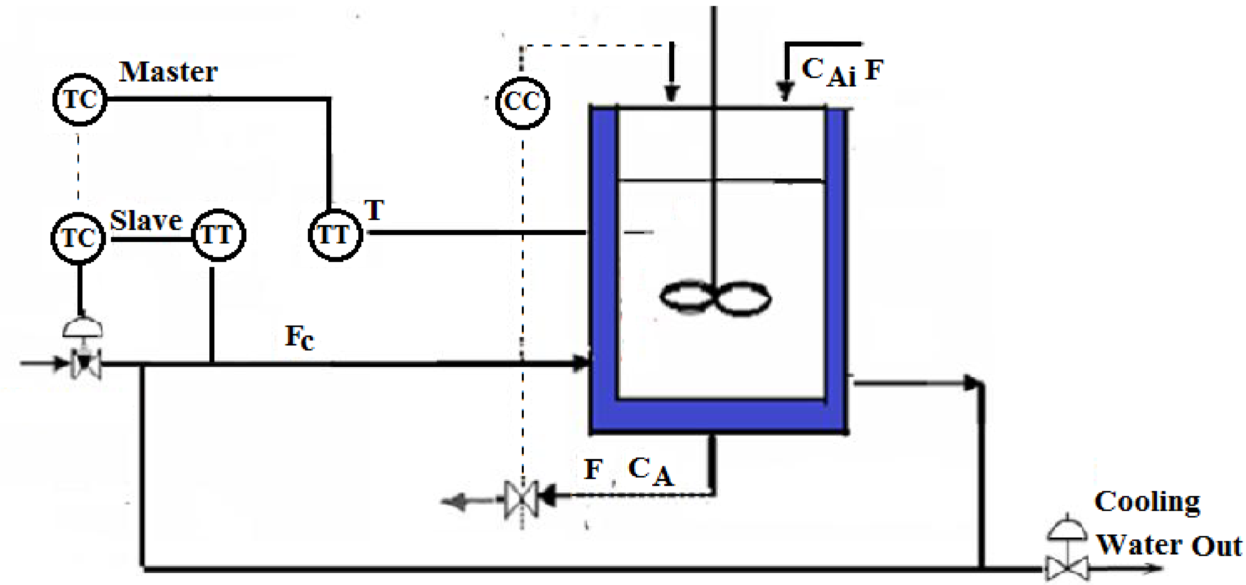

Figure 2.2. Schematic diagram of stirred tank chemical reactor [3]

A stirred tank reactor with an exothermic reaction requires a more elaborated system model, in terms of controlled variables like temperature and concentration. Furthermore, the model is nonlinear, which forces us to make a linear approximation to solve it.

3.4. DYNAMIC MODEL OF THE REACTOR

With two output variables, there will be two balances models having several supporting relationships. The mole balance on the given reactant A can be represented as

$$V\frac{dC_A}{dt} = FC_{Ai} - FC_A - V(-r_A) \qquad (1)$$

The equation takes a second-order kinetic rate expression for the rate of disappearance of reactant A, according to Arrhenius temperature dependence.

$$-r_A = -\frac{1}{V}\frac{dN_A}{dt} = kC_A^2 = k_0 e^{-E/RT} C_A^2 \qquad (2)$$

The energy balance is applied for the reaction process and heat transfer.

$$V\rho C_p \frac{dT}{dt} = F\rho C_p (T_i - T_{ref}) - F\rho C_p (T - T_{ref}) - \Delta H_R V(-r_A) - Q \qquad (3)$$

Now by considering that the physical properties as independent of temperature, enthalpies are going to be defined with respect to an arbitrary thermodynamic reference temperature. For an exothermic reaction, the heat of reaction ΔH_R will be a negative quantity, and will thus tend to raise the reactor temperature T. The rate of heat transfer Q depends on the logarithmic temperature difference in which the well-mixed tank temperature T is uniform and the coolant temperature T_c varies from inlet to outlet.

$$\mathrm{Q} = \mathrm{U}_0 A_0 \frac{(T - T_{ci}) - (T - T_{c0})}{\ln \dfrac{(T - T_{ci})}{(T - T_{c0})}} \qquad (4)$$

Now assuming that the coolant supply temperature T_{ci} is quite stable and it is not considered as a disturbance. The overall heat transfer coefficient depends on the film coefficients on the inner and outer surfaces of the heat transfer barrier. Assuming that there is no any conduction resistance the barrier will be neglected.

The outer film coefficient h_0 depends on the rate of stirring in the tank, as well as the variation of physical properties with temperature. With constant physical properties, there is no reason for h_o to be varied instantaneously. On the other hand the inner coefficient h_i is necessarily depends on the rate of flow of cooling water in the cooling jacket of the reactor tank.

$$U = \left(\frac{1}{h_0} + \frac{A_0}{A_i h_{ir}} \right)^{-1} \qquad (5)$$

At a reference condition, we can express the flow dependence of h_i as:

$$h_i = h_{ir} \left(\frac{F_c}{F_{cr}} \right)^n \qquad (6)$$

For flow in tubes, n is an impurity factor which is often about 0.8.

The main structure of the model is given by the balances (1) and (3). These relate the outlet temperature and concentration to their inlet values. Supplementary equations are needed to describe the reaction kinetics and heat transfer. The two balances will be coupled through the temperature dependence of the reaction rate parameter k in equation (2).

Heat transfer is performed by equipment has been given in equations (4) and (6) as convective heat transfer in conduits.

These latter equations show how the coolant flow F_c influences the reactor outlet temperature T. Here is better to consider the outlet coolant temperature T_{co} given in (4) that can be represented by energy balance model.

$$V_c\rho_c C_{pc}\frac{d\Delta T_c}{dt} = F_c\rho_c C_{pc}(T_{ci} - T_{ref}) - F_c\rho_c C_{pc}(T_{c0} - T_{ref}) + Q \qquad (7)$$

where ΔT_c is the average coolant temperature in the coolant volume.

$$h_i = h_{ir}\left(\frac{F_c}{F_{cr}}\right)^n \qquad (8)$$

In proceeding with (7), the average temperature is expressed in terms of the inlet and outlet temperatures. Now assuming that heat exchanger outlet temperature adjusts much more quickly than does the tank temperature T, the accumulation term in (7) can be neglected and written as:

$$F_c\rho_c C_{pc}(T_{c0} - T_{ci}) = Q \qquad (9)$$

As it is already noted, the rate of heat transfer depends on the instantaneous values of the inlet and outlet temperatures according to a relationship derived at the steady state.

The equations of this section describe how the outlet temperature and concentration vary with time due to disturbances in inlet temperature, inlet concentration, and coolant flow rate.

3.4.1. APPROXIMATIONS TO BE USED

To linearize the previous non-linear balances, the Taylor series linear approximation technique is used.

According to this approach, using a function f, the reference value of independent variables is specified and thus the function in the neighborhood of that reference point is represented in a series of terms. For a function of one variable:

$$f(x) = f(x_r) + \left.\frac{df}{dx}\right|_{x_r}(x - x_r) + O(x - x_r)^2 \qquad (10)$$

For a function of more than one variable:

$$f(x, y, ...) = f(x_r y_r, ...) + \left.\frac{df}{dx}\right|_{x_r, y_r \ldots}(x - x_r) + \left.\frac{df}{dy}\right|_{x_r, y_r \ldots}(y - y_r) + ... + O(x - x_r)^2, O(y - y_r)^2 \qquad (11)$$

3.4.2. LINEARIZATION OF MATERIAL BALANCE

Let us apply the Taylor series linearizing approach at equation (11) to the material balance given at equation (1).

$$V\frac{dC_A}{dt} = FC_{Ai} - FC_A - V(-r_A)_r - V\left.\frac{\partial(-r_A)}{\partial C_A}\right|_r (C_A - C_{Ar}) - V\left.\frac{\partial(-r_A)}{dT}\right|_r (T - T_r) \qquad (12)$$

At the reference (steady state) (12) becomes:

$$V\frac{dC_A}{dt} = 0 = FC_{Air} - FC_{Ar} - V(-r_A)_r \qquad (13)$$

Now let us subtract equation (13) from (12) and define the deviation variables.

$$V\frac{dC_A}{dt} = FC_{Ai} - FC_A - V\left.\frac{\partial(-r_A)}{\partial C_A}\right|_r C_A - V\left.\frac{\partial(-r_A)}{\partial T}\right|_r T \qquad (14)$$

The partial derivatives variables in equation (14) can be obtained using equation (2).

$$\frac{\partial(-r_A)}{\partial C_A} = 2k_0 e^{-E/RT} C_A \tag{15}$$

$$\left.\frac{\partial(-r_A)}{\partial C_A}\right|_{r} = 2k_0 e^{-E/RT_r} C_{Ar} = 2k_r C_{Ar} \tag{16}$$

$$\frac{\partial(-r_A)}{\partial T} = k_0 \frac{E}{RT^2} e^{-E/RT} C_A^2 \tag{17}$$

$$\left.\frac{\partial(-r_A)}{\partial T}\right|_{r} = k_0 \frac{E}{RT_r^2} e^{-E/RT_r} C_{Ar}^2 = C_{Ar}^2 k_r \frac{E}{RT_r^2} \tag{18}$$

Here k_r is the rate constant at the reference condition.

$$k_r = k_0 e^{-E/RT_r} \tag{19}$$

Now let us substitute equation (16) and (18) into the linearized material balance at equation (14).

$$V\frac{dC_A}{dt} = FC_{Ai} - FC_A - 2Vk_r C_{Ar} C_A - TE\frac{k_r V C_{Ar}^2}{RT_r^2} \tag{20}$$

This is a first-order lag equation, which is more apparent if it is placed into standard form

$$\tau_c \frac{dC_A}{dt} + C_A = \frac{\tau_c}{\tau_R} C_{Ai} + K_{CT} T, C_A(0) = 0 \tag{21}$$

$$\begin{aligned} \tau_R &= \frac{V}{F} \\ \tau_C &= \frac{\tau_R}{1 + 2\tau_R k_r C_{Ar}} \\ K_{CT} &= \frac{E C_{Ar}^2}{RT_r^2} k_r \tau_C \end{aligned} \tag{22}$$

The residence time, τ_R, of reactor tank is representing the time taken by reactor to make conversion of reactant into desirable product. The time constant τ_C characterizes the dynamics of concentration change which is smaller than τ_R.

On the other hand the group K_{CT} is the gain for the effect of temperature on concentration in the reactor.

3.4.3. LINEARIZATION OF ENERGY BALANCE

Here we also apply equation (11) to the energy balance given at equation (3).

$$V\rho C_p \frac{dT}{dt} = F\rho C_p T_i - F\rho C_p T - \Delta H_R V(-r_A)_r - \Delta H_R V \left.\frac{\partial(-r_A)}{\partial C_A}\right|_r (C_A - C_{Ar}) - \Delta H_R V \left.\frac{\partial(-r_A)}{\partial T}\right|_r (T - T_r) - Q_r \quad (23)$$

$$-\left.\frac{\partial Q}{\partial T}\right|_r (T - T_r) - \left.\frac{\partial Q}{\partial F_c}\right|_r (F_c - F_{cr})$$

At the reference condition equation (23) becomes:

$$V\rho C_p \frac{dT_r}{dt} = 0 = F\rho C_p T_{ir} - F\rho C_p T_r - \Delta H V(-r_A)_r - Q_r \quad (24)$$

We subtract (24) from (23) and define deviation variables.

$$V\rho C_p \frac{dT}{dt} = F\rho C_p T_i - F\rho C_p T - \Delta H_R V \left.\frac{\partial(-r_A)}{\partial C_A}\right|_r C_A - \Delta H_R V \left.\frac{\partial(-r_A)}{\partial T}\right|_r T - \left.\frac{\partial Q}{\partial T}\right|_r T - \left.\frac{\partial Q}{\partial F_c}\right|_r F_C \quad (25)$$

The reaction rate partial derivatives are given in (16) and (18). To obtain the heat transfer rate partial derivatives, the heat transfer expressions (4) through (6) with the coolant energy balance (9) can be combined to eliminate intermediate variable T_{co}.

$$Q = F_c \rho_c C_{pc}(T - T_{ci})\left[1 - \exp\left(-\frac{A_0}{F_c \rho_c C_{pc}}\left(\frac{1}{h_0} + \frac{A_0 F_{cr}^n}{A_i h_{ir} F_{cr}^n}\right)^{-1}\right)\right] \qquad (26)$$

The partial derivatives are

$$\frac{\partial Q}{\partial T} = F_c \rho_c C_{pc}\left[1 - \exp\left(-\frac{A_0}{F_c \rho_c C_{pc}}\left(\frac{1}{h_0} + \frac{A_0 F_{cr}^n}{A_i h_{ir} F_{cr}^n}\right)^{-1}\right)\right] \qquad (27)$$

$$\left.\frac{\partial Q}{\partial T}\right|_{r} = F_{cr} \rho_c C_{pc}[1 - \beta] \qquad (28)$$

$$\frac{\partial Q}{\partial T} = \rho_c C_{pc}(T - T_{ci})\begin{bmatrix} 1 - \exp\left(-\frac{A_0}{F_c \rho_c C_{pc}}\left(\frac{1}{h_0} + \frac{A_0 F_{cr}^n}{A_i h_{ir} F_{cr}^n}\right)^{-1}\right) - \frac{A_0 (T - T_{ci})}{F_c}\left(\frac{1}{h_0} + \frac{A_0 F_{cr}^n}{A_i h_{ir} F_{cr}^n}\right)^{-1} \\ \exp\left(-\frac{A_0}{F_c \rho_c C_{pc}}\right)\left(\frac{1}{h_0} + \frac{A_0 F_{cr}^n}{A_i h_{ir} F_{cr}^n}\right)^{-1}\left[1 - \left(\frac{1}{h_0} + \frac{A_0 F_{cr}^n}{A_i h_{ir} F_{cr}^n}\right)^{-1} \frac{n A_0 F_{cr}^n}{A_i h_{ir} F_{cr}^n}\right] \end{bmatrix} \qquad (29)$$

$$\left.\frac{\partial Q}{\partial F_c}\right|_{r} = \rho_c C_{pc}(T - T_{ci})[1 - \beta_r] - \frac{\beta_r U_{or} A_0}{F_{cr}}(T - T_{ci})\left[1 - \frac{n U_{or} A_0}{A_i h_{ir}}\right] \qquad (30)$$

where

$$U_{or} = \left(\frac{1}{h_0} + \frac{A_0}{A_i h_{ir}}\right)^{-1} \qquad (31)$$

And

$$\beta_r = \left(\frac{U_{or} A_0}{F_{cr} \rho_c C_{pc}}\right)^{-1} \qquad (32)$$

The argument of the exponential function in (32) is the "number of transfer units", used in models of heat exchangers.

We substitute equations (16), (18), (28), and (30) into linearized energy balance (25) to obtain another first order equation which can be represented as:

$$\tau_T \frac{dT}{dt} + T = \frac{\tau_T}{\tau_R} T_i + K_{TC} C_A^{'} + K_{ht} F_c, T(0) = 0 \qquad (33)$$

where

$$\tau_T = \frac{\tau_R}{1 + \frac{F_{cr}\rho_c C_{pc}}{F\rho C_p}(1-\beta_r) + \tau_R \frac{\Delta H_r}{\rho C_p} \frac{E}{RT_r^2} k_r C_{Ar}^2}$$

$$K_{TC} = -2\tau_T k_r C_{Ar} \frac{\Delta H_r}{\rho C_p} \qquad (34)$$

$$K_{ht} = \frac{\tau_T \rho_c C_{pc}(T_r - T_{ci})}{\tau_R F\rho C_p}\left[\frac{\beta_r U_{or} A_o}{F_{cr}\rho_c C_{pc}}\left(1 - \frac{nU_{or}A_o}{A_i h_{ir}}\right) - (1-\beta_r)\right]$$

Once again, standard-form parameters have been defined. The thermal time constant τ_T characterizes the dynamics of temperature change, and K_{TC} and K_{ht} are gains for concentration and heat transfer disturbances.

3.4.4. DERIVING TRANSFER FUNCTIONS BY LAPLACE TRANSFORM

The Laplace transform of the mole balance equation (21) and energy balance equation (33) is:

$$(\tau_c s + 1) C_A(s) = \frac{\tau_c}{\tau_R} C_{Ai}(s) + K_{CT} T(s) \qquad (35)$$

$$(\tau_T s + 1) T(s) = \frac{\tau_c}{\tau_R} T_i(s) + K_{TC} C_A(s) + K_{ht} F_c(s) \qquad (36)$$

Now the output concentration $C_A(s)$ is isolated either by eliminating output temperature T(s) between (35) and (36), or by tracing the dependency through the block diagram:

$$C_A(s)=\frac{\dfrac{\tau_c}{\tau_R(\tau_c s+1)}}{1-\dfrac{K_{CT}K_{TC}}{(\tau_c s+1)(\tau_T s+1)}}C_{Ai}(s)+\frac{\dfrac{K_{CT}\tau_T}{\tau_R(\tau_c s+1)(\tau_T s+1)}}{1-\dfrac{K_{CT}K_{TC}}{(\tau_c s+1)(\tau_T s+1)}}T_i(s)+\frac{\dfrac{K_{CT}K_{ht}}{\tau_R(\tau_c s+1)(\tau_T s+1)}}{1-\dfrac{K_{CT}K_{TC}}{(\tau_c s+1)(\tau_T s+1)}}F_c(s) \quad (37)$$

After simplifying the individual transfer functions in equation (37), we will get a second-order system in which the coefficients in the characteristic equation are:

$$C_A(s)=\frac{\dfrac{\tau^2(\tau_T s+1)}{\tau_R\tau_T}}{\tau^2 s^2+2\tau\xi\, s+1}C_{Ai}(s)+\frac{\dfrac{\tau^2 K_{CT}}{\tau_R\tau_c}}{\tau^2 s^2+2\tau\xi\, s+1}T_i(s)+\frac{\dfrac{\tau^2 K_{CT}K_{ht}}{\tau_T\tau_c}}{\tau^2 s^2+2\tau\xi\, s+1}F_c(s) \quad (38)$$

In which the coefficients in the characteristic equation are:

$$\tau^2=\frac{\tau_T\tau_c}{(1-K_{CT}K_{TC})} \quad (39)$$

$$2\tau\xi=\frac{(\tau_c+\tau_T)}{(1-K_{CT}K_{TC})} \quad (40)$$

Substituting equation (38) to (36) , the reactor temperature model T(s) is written as:

$$T(s)=\frac{\dfrac{\tau^2(\tau_c s+1)}{\tau_R\tau_c}}{\tau^2 s^2+2\tau\xi s+1}T_i(s)+\frac{\dfrac{\tau^2 K_{TC}}{\tau_R\tau_T}}{\tau^2 s^2+2\tau\xi s+1}C_{Ai}(s)+\frac{\dfrac{\tau^2 K_{ht}(\tau_c s+1)}{\tau_T\tau_c}}{\tau^2 s^2+2\tau\xi s+1}F_c(s) \quad (41)$$

Now using equations (38) and (41), the material and energy balances are combined to produce second-order dependence for both controlled variables. The characteristic equation and poles become the same for both variables.

By applying superposition principle to equations (38) and (41), the individual plant and disturbance transfer functions for the reactor temperature and output concentration will be determined as shown below.

Case 1

Plant Transfer function of Reactor Temperature

- From (41), the plant transfer function, $G_{p1}(s)=\dfrac{T(s)}{F_c(s)}$ of reactor temperature given

$$G_{p1}(s)=\frac{\dfrac{\tau^2 K_{ht}(\tau_c s+1)}{\tau_T\tau_c}}{\tau^2 s^2+2\tau\xi s+1} \qquad (42)$$

Disturbance transfer function for reactor temperature

- The first reactor disturbance, $G_{d1}(s)=\dfrac{T(s)}{T_i(s)}$ will be computed as:

$$G_{d1}(s)=\frac{\dfrac{\tau^2(\tau_c s+1)}{\tau_R\tau_c}}{\tau^2 s^2+2\tau\xi s+1} \qquad (43)$$

- Similarly the second disturbance $G_{d1}(s)=\dfrac{T(s)}{C_{Ai}(s)}$ will be determined as:

$$G_{d2}(s)=\frac{\dfrac{\tau^2 K_{TC}}{\tau_R\tau_T}}{\tau^2 s^2+2\tau\xi s+1} \qquad (44)$$

Case 2

Plant Transfer function of concentration of feed stream

- From equation (38), the second disturbance $G_{p2}(s)=\dfrac{C_A(s)}{F_c(s)}$ which will be determined as:

$$G_{p2}(s)=\frac{\dfrac{\tau^2 K_{CT}K_{ht}}{\tau_T\tau_c}}{\tau^2 s^2+2\tau\xi s+1} \qquad (45)$$

Disturbance transfer function for concentration

- The first input disturbance to concentration is $G_{ud1}(s) = \dfrac{C_A(s)}{T_i(s)}$ will be computed as:

$$G_{ud1}(s) = \frac{\tau^2 K_{CT}}{\dfrac{\tau_R \tau_c}{\tau^2 s^2 + 2\tau\xi\, s + 1}} \qquad (46)$$

- In similar way the second input disturbance to concentration is $G_{ud2}(s) = \dfrac{C_A(s)}{C_{Ai}(s)}$) will be computed as:

$$G_{ud2}(s) = \frac{\tau^2 (\tau_T s + 1)}{\dfrac{\tau_R \tau_T}{\tau^2 s^2 + 2\tau\xi\, s + 1}} \qquad (47)$$

The cascade design of the feed concentration and reactor temperature outputs which were expressed in terms of the three input variables can be represented with a block diagram as shown in the figure 5.

3.4.5. BLOCK DIAGRAM OF CASCADE STIRRED TANK REACTOR CONTROL

Using the model from equations (38) and (41), the block diagram of an exothermic cascade continuous stirred tank reactor is represented for both concentration of feed stream and reactor temperature. Self-tuning controller is used as a master controller which is connected to the closed loop control system of concentration and temperature plants. A PI controller is used as slave controller in the secondary control loop of both plants. As reference command signal we have set point for reactor temperature and concentration of feed stream.

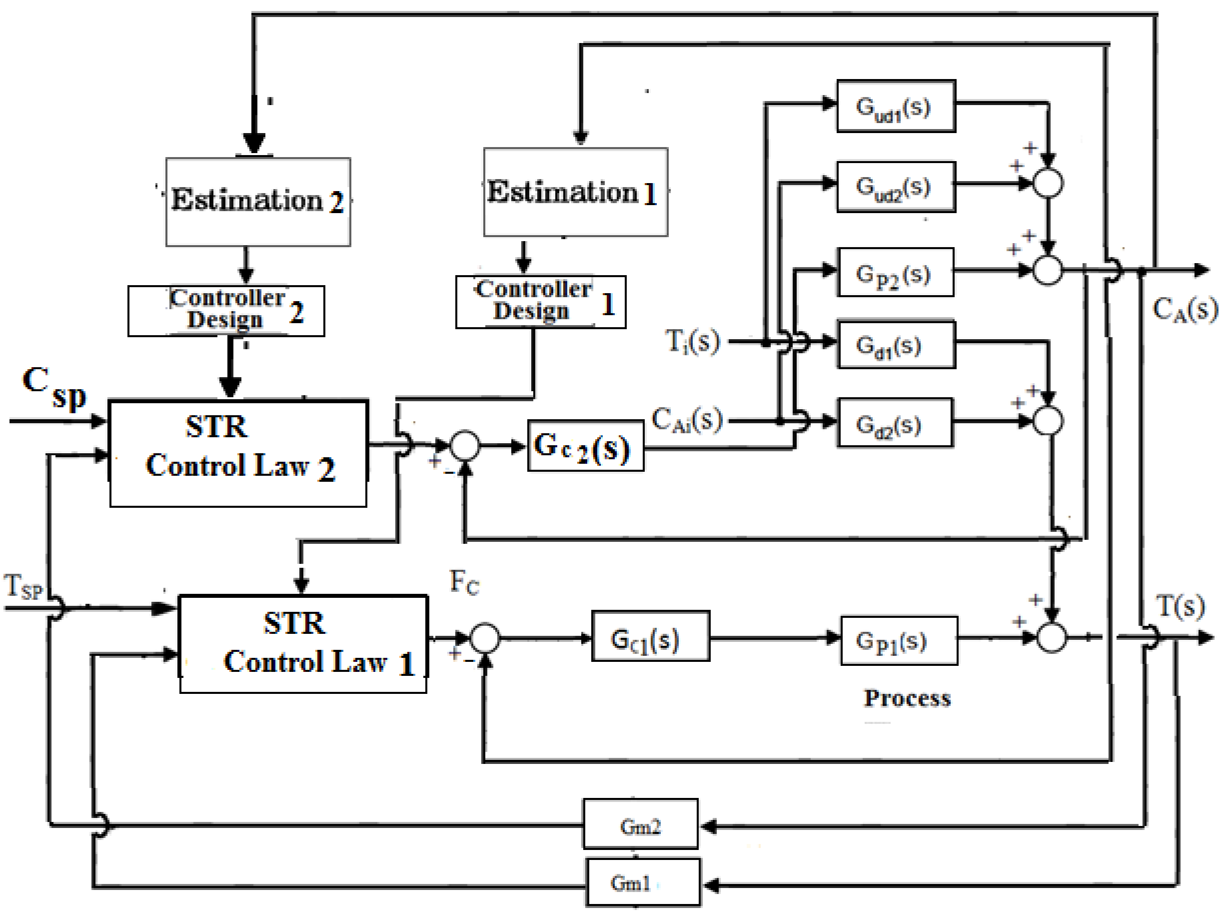

Figure 3.4. Block diagram of the entire system

where

The transfer functions, $G_{C1}(s)$ and $G_{C2}(s)$ are the PI controller transfer functions of the temperature and concentration plants respectively.

3.5. INTERNAL LOOP PLANT MODELS

For steady state operation of exothermic tank reactor, the above parameters are chosen for the sake of finding smooth reaction process of feed and having good performance of the reactor. The selected parameters in this case are shown in the given table.

Table 3.1. List of parameters value for better system operation [7]

Variable	unit	Value
ρ	$Kg/\ m^3$	800
ρ_c	$Kg/\ m^3$	1000
V	m^3	1.36
C_p	$KJ/Kg\ ^0K$	3.13
E	KJ/K mol	69815
R	$KJ/K\ mol\ ^0K$	8.314
$(-\Delta H_R)$	KJ/K mol	69815
A_0	m^2	18
U_{0r}	$KJ/hr\ \ m^{2\ 0}K$	3065
F	m^3/hr	1.13
T_{cr}	^0K	331.4
T_{ir}	^0K	330
F_{cr}	m^3/hr	1.41
T_r	^0K	335
C_{AR}	$K\ mol/m^3$	4.031
C_{pc}	$KJ/Kg\ ^0K$	4.18
T_{ci}	^0K	294.7
k_0	s^{-1}	1100

Now the plant model will be designed by substituting the numerical values parameters given in the above Table, so that the required parameters of equations (22), (31), (32), (33), (39) and (40) will have the following value.

$$k_r = 7.6x10^{-4},\ \tau_R = 52.33,\ \tau_c = 2.72,\ \tau_T = 33.93,\ K_{CT} = 2.64,$$
$$K_{TC} = 0.187,\ K_{ht} = 15.58,\ \tau = 13.5\ \&\ \xi = 2.68.$$
$$\mathrm{G_{m1} = G_{m2} = 1\ for\ unity\ feedback}$$

Now substituting these parameters values into equations (38) and (41) gives:

$$C_A(s) = \frac{(3.494s + 0.103)C_{Ai}(s)}{182.25s^2 + 72.36s + 1} + \frac{3.3803T_i(s)}{182.25s^2 + 72.36s + 1} + \frac{81.234F_c(s)}{182.25s^2 + 72.36s + 1} \qquad (48)$$

$$T(s) = \frac{(3.482s + 1.28)T_i(s)}{182.25s^2 + 72.36s + 1} + \frac{0.0192C_{Ai}(s)}{182.25s^2 + 72.36s + 1} + \frac{(83.69s + 30.77)F_c(s)}{182.25s^2 + 72.36s + 1} \qquad (49)$$

Using equations (42) and (45) the plant transfer function models for the controlled output concentration and reactor temperature become the following respectively:

$$G_{p2}(s) = \frac{C_A(s)}{F_c(s)} = \frac{81.234}{182.25s^2 + 72.36s + 1} \qquad (50)$$

$$G_{p1}(s) = \frac{T(s)}{F_c(s)} = \frac{(83.69s + 30.77)}{182.25s^2 + 72.36s + 1} \qquad (51)$$

Let's first rearrange equations (50) and (51) as

$$G_{p2}(s) = \frac{0.446}{s^2 + 0.397s + 0.0055} \qquad (52)$$

$$G_{p1}(s) = \frac{0.4592(s + 0.3676)}{s^2 + 0.397s + 0.0055} \qquad (53)$$

The secondary control loop for both concentration and reactor temperature has PI slave controllers which has a transfer function of:

$$G_{c1}(s) = K_{p1}\left(1 + \frac{1}{\tau_{i1}s}\right) \qquad (54)$$

$$G_{c2}(s) = K_{p2}\left(1 + \frac{1}{\tau_{i2}s}\right) \qquad (55)$$

Now using Routh's Stability analysis the characteristic equation for the secondary control loop of concentration.

It is known that

$$1+\frac{0.446K}{s^2+0.397s+0.0055}=0$$

This implies that:

$$\begin{aligned}
&s^2+0.397s+0.446K+0.0055=0\\
&0.446K=0.00556\\
&K=0.012\\
&k_{cr2}=K=0.012\\
&\omega_{n2}=\sqrt{0.012}=0.133
\end{aligned} \tag{56}$$

For the sake minimum overshoot and settling time, Tyreus Lubean tuning topology is used from other tuning topologies. Thus, the critical period and gain will be

$$\begin{aligned}
&K_{p2}=\frac{k_{cr2}}{3.2}=0.00375,\\
&P_{cr2}=\frac{2\pi}{\omega_{n2}}=47.22\\
&\tau_{i2}=\frac{P_{cr2}}{0.45}=\frac{47.22}{0.45}=104.93
\end{aligned} \tag{57}$$

The characteristic equation for the plant transfer function of reactor temperature is:

$$1+\frac{0.167K}{s^2+0.397s+0.0055}=0$$

$$\begin{aligned}
&s^2+0.8562s+0.0055+0.167K=0\\
&0.0055=0.167K\\
&K=0.457,
\end{aligned} \tag{58}$$

In similar approach it implies that:

$$\begin{aligned}
&k_{cr2} = K = 0.0329 \\
&\omega_{n1} = \sqrt{0.0329} = 0.1814 \\
&K_{p1} = \frac{k_{cr1}}{3.2} = 0.0102, \\
&P_{cr1} = \frac{2\pi}{\omega_{n1}} = 34.64 \\
&\tau_{i1} = \frac{P_{cr1}}{0.45} = \frac{15.05}{0.45} = 76.93
\end{aligned} \qquad (59)$$

The closed loop transfer function for the secondary concentration control loop is

$$G_2(s) = \frac{C_A}{U_2} = \frac{G_{p2}(s)G_{c2}(s)}{1+G_{p2}(s)G_{c2}(s)} \qquad (60)$$

Substituting equations (45) and (52) into equation (60) and let C_A=y_2.

$$G_2(s) = \frac{y_2}{U_2} = \frac{\tau^2 K_{p2} K_{CT} K_{ht}(\tau_{i2}s+1)}{\tau^2\tau_c\tau_{i2}\tau_T s^3 + 2\tau\xi\tau_c\tau_{i2}\tau_T s^2 + (\tau_c\tau_{i2}\tau_T + \tau^2 K_{p2}K_{CT}K_{ht}\tau_i)s + \tau^2 K_{p2}K_{CT}K_{ht}} \qquad (61)$$

Let us compute the values of the coefficients of characteristic polynomial by substituting parameters' value.

$$\begin{aligned}
&\tau^2\tau_c\tau_{i2}\tau_T = 195{,}129.3 \\
&2\tau\xi\tau_c\tau_{i2}\tau_T = 76{,}382.8 \\
&(\tau_c\tau_{i2}\tau_T + \tau^2 K_{p2}K_{CT}K_{ht}\tau_{i2}) = 23{,}063.1 \\
&\tau^2 K_{p2}K_{CT}K_{ht} = 1{,}264.4
\end{aligned} \qquad (62)$$

Substituting the parameters values determined at equation (62) into process model (61) we have:

$$G_2(s) = \frac{17{,}986.1s + 1{,}264.4}{195{,}129..3s^3 + 76{,}382.8s^2 + 21{,}063.1s + 1{,}264.4} \qquad (63)$$

Similar to secondary loop, the closed loop transfer function for the reactor temperature plant dynamics will be:

$$G_1(s) = \frac{T}{U_1} = \frac{G_{p1}(s)G_{c1}(s)}{1+G_{p1}(s)G_{c1}(s)}$$
$$G_1(s) = \frac{y_1}{U_1}, T = y_1 \qquad (64)$$

Substituting equations (42) and (53) into equation (64)

$$G_1(s) = \frac{\tau^2 K_{p1}K_{ht}(\tau_c s+1)(\tau_{i1}s+1)}{\tau^2\tau_{i1}\tau_c\tau_T s^3 + (2\tau\xi\tau_{i1}\tau_c\tau_T + \tau^2\tau_{i1}\tau_c K_{p1}K_{ht})s^2 + (\tau_{i1}\tau_c\tau_T + (\tau_c+\tau_T)\tau^2 K_{p1}K_{ht})s + \tau^2 K_{p1}K_{ht}} \qquad (65)$$

The coefficients can be calculated and become

$$\begin{aligned}
&\tau^2\tau_{i1}\tau_c\tau_T = 205{,}211.6\\
&(2\tau\xi\tau_{i1}\tau_c\tau_T + \tau^2\tau_{i1}\tau_c K_{p1}K_{ht}) = 107{,}837.2\\
&(\tau_{i1}\tau_c\tau_T + (\tau_c+\tau_T)\tau^2 K_{p1}K_{ht}) = 21{,}246.52\\
&\tau^2 K_{p1}K_{ht} = 549.4
\end{aligned} \qquad (66)$$

Substituting the values obtained at (66) into (65) we have:

$$G_1(s) = \frac{16{,}321.31s^2 + 7{,}974.28s + 549.4}{205{,}211.6s^3 + 107{,}837.2s^2 + 21{,}246.52s + 549.4} \qquad (67)$$

3.2.8. DESIGN OF REFERENCE PLANT MODEL

The desired internal loop plant model for both concentration and reactor temperature will be designed by specifying the denominator polynomial of the reference plant model whose coefficient values are somewhat related with coefficient values of the denominator of process model $G_1(s)$ and $G_2(s)$.

3.2.9. REFERENCE CONCENTRATION PLANT MODEL DESIGN

From equation (63), the simplified closed loop transfer function of concentration of feed stream of the reactor can be rearranged and written as:

$$G_2(s) = \frac{0.8922\,s + 0.00648}{s^3 + 0.391s^2 + 0.108\,s + 0.00648} \qquad (68)$$

Due to discrete values of parameters in the estimation block, it is possible to represent the z transform equivalent for $G_2(s)$ at equation (68) using bilinear transformation technique and choosing the sampling time at 0.1s and it becomes:

$$G_2(z) = \frac{0.09072\,z^2 - 0.0067\,z - 0.0514}{z^3 - 1.946\,z^2 + 1.231\,z - 0.254} \qquad (69)$$

Since

$$B_2(z) = 0.09072z^2 - 0.0067z - 0.0514$$

$$A_2(z) = z^3 - 1.946z^2 + 1.231\,z - 0.254$$

Now we specify the a closed loop characteristic polynomial of the desired plant model by which the process will be tracked and followed the model appropriately given at equation (69)

$$A_{m2}(z) = z^3 - 1.787\,z^2 + 1.119\,z - 0.321$$

As it can be seen from the transfer function there is no process zeros and pole cancellation zero cancellation, the numerator of the desired plant model transfer function $G_{m2}(z)$ can be obtained as:

$$B_{m2}(z) = \beta_2 B_2(z) \qquad (70)$$

where

$$\beta_2 = \frac{A_{m2}(1)}{B_2(1)} = 0.851$$

Thus

$$B_{m2}(z) = 0.851(0.09072z^2 - 0.0067z - 0.0514)$$
$$= 0.0772\,z^2 - 0.0057\,z - 0.0438$$

Therefore the desired plant model of the concentration dynamics is:

$$G_{m2}(z) = \frac{B_{m2}(z)}{A_{m2}(z)} = \frac{0.0772\;z^2 - 0.0057\,z - 0.0438}{z^3 - 1.787\,z^2 + 1.119\,z - 0.321} \qquad (71)$$

3.2.10. DESIGN OF REFERENCE MODEL OF TEMPERATURE PLANT

Rearranging $G_1(s)$ at equation (67) $G_1(s)$ can be written as:

$$G_1(s) = \frac{0.906\,s^2 + 0.404\,s + 0.00263}{s^3 + 0.483\,s^2 + 0.0987\,s + 0.00263} \qquad (72)$$

Representing the z transform equivalent for equation (72) by applying bilinear transformation technique and choosing the sampling time at 0.1s. Thus the discrete transfer function becomes:

$$G_1(z) = \frac{0.198\,z^2 - 0.012\,z - 0.0323}{z^3 - 1.727\,z^2 + 1.302\,z - 0.521} \qquad (73)$$

The closed loop characteristic polynomial of the desired plant model is specified for appropriate tracking model following with the process by considering the denominator of a closed loop transfer function given at equation (73)

$$A_{m1}(z) = z^3 - 1.687\,z^2 + 1.102\,z - 0.287$$

Here also it can be seen that there is no process zeros and pole cancellation, the numerator of the desired plant model transfer function $G_{m1}(z)$ can be obtained as:

$$B_{m1}(z) = \beta_1 B_1(z) \qquad (74)$$

where

$$\beta_1 = \frac{A_{m1}(1)}{B_1(1)} = 0.798$$

Thus,

$$\begin{aligned} B_{m1}(z) &= 0.798(0.198z^2 - 0.012z - 0.0323) \\ &= 0.158\,z^2 - 0.00943\,z - 0.0253 \end{aligned}$$

Therefore the desired plant model of the temperature dynamics is:

$$G_{m1}(z) = \frac{B_{m1}(z)}{A_{m1}(z)} = \frac{0.158\,z^2 - 0.00943z - 0.0253}{z^3 - 1.687\,z^2 + 1.102\,z - 0.2873} \tag{75}$$

3.3. CONTROLLER DESIGN

3.3.1. CONTROLLER DESIGN OF CONCENTRATION

The closed loop characteristic polynomial can be computed using Diophantine equation given by

$$A_{C2} = A_2 R_2 + B_2 S_2 \tag{76}$$

$$B_2 = B_2^+ B_2^- \tag{77}$$

Then it follows that

$$B_{m2} = B_2^- B_{m2}^{'} \tag{78}$$

The polynomial A_{m2} is also be a factor of A_{C2}

$$A_{C2} = A_{02} A_{m2} B_2^+ \tag{79}$$

where A_{02} is observer polynomial for the desired model of the plant

From equations (77) and (79) B_2^+ is a factor of B_2 and A_{C2} and chosen to be 1. And it also divides R_2

$$R_2 = B_2^+ R_2^{'} \tag{80}$$

Thus the Diophantine in (76) reduces to

$$A_2 R_2^{'} + B_2^- S_2 = A_{02} A_{m2} \tag{81}$$

From the compatibility condition, by assuming that no process zeros are canceled, we have

$$\begin{aligned} \deg A_{m2} &= \deg A_2 \\ \deg B_{m2} &= \deg B_2 \\ \deg A_{02} &= \deg A_2 - \deg B_2^+ - 1 \\ \deg R_2 &= \deg A_{C2} - \deg A_2 \\ \deg T_2 &= \deg S_2 \le \deg R_2 \end{aligned} \qquad (82)$$

As we can see the closed loop characteristic polynomial A_{C2} is 5th order thus based on (81) S_2, R_2 and A_{02} polynomials represented as shown below.

Let the observer polynomial be:

$$A_{02} = z^2 + a_0 z + a_1 \qquad (84)$$

The primary controller for output concentration y_2 has a control law algorithm which is given by:

$$R_2 u_2 = T u_{c2} - S_2 y_2 \qquad (85)$$

where

R_2, S_2 and T_2 are the desired parameters of the second self-tuning controller.

The primary controller for concentration of feed stream can be designed by computing the polynomials R_2 and S_2 by using the Diophantine equation given at equation (81). Let us assume the polynomials R_2 and S_2 as shown below

$$R_2^{'}(z) = z^2 + r_0 z + r_1 \qquad (86)$$

$$S_2(z) = s_0 z^2 + s_1 z + s_2 \qquad (87)$$

Let

$$A_{02}(z) = (z + 0.4)(z + 0.8) = z^2 + 1.2z + 0.32$$

Substituting (86) and (87) into equation (81) we have

$$(z^3 - 1.946z^2 + 1.231z - 0.254)(z^2 + r_0 z + r_1) + (0.09072z^2 - 0.0067z - 0.0514)(s_0 z^2 + s_1 z + s_2)$$
$$= (z^2 + 1.2z + 0.32)(z^3 - 1.787z^2 + 1.102z - 0.2873) \qquad (88)$$

Equating coefficients with equal power of z, we have the following equations:

$$\begin{aligned} &r_0 + 0r_1 + 0.0907s_0 + 0s_1 + 0s_2 = -0.587 \\ &-1.946r_0 + r_1 - 0.0067s_0 + 0.0907s_1 + 0s_2 = -0.7054 \\ &1.1231r_0 - 1.946r_1 - 0.0514s_0 - 0.0067s_1 + 0.09072s_2 = 0.45 \\ &-0.254r_0 + 1.231r_1 + 0s_0 - 0.0514s_1 - 0.0067s_2 = -0.0271 \\ &0r_0 - 0.254r_1 + 0s_0 + 0s_1 - 0.0514s_2 = -0.1027 \end{aligned} \qquad (89)$$

Solving the unknowns in (89) simultaneously, we get

$$\begin{aligned} &r_0 = -1.212 \\ &r_1 = 0.271 \\ &s_0 = 0.623 \\ &s_1 = -0.0463 \\ &s_2 = 0.3234 \\ &S_2(z) = 0.623z^2 - 0.0463z + 0.3234 \\ &R_2(z) = z^2 - 1.21z + 0.271 \\ &T_2(z) = \beta_2 A_{02}(z) \\ &\qquad = 0.851(z^2 + 1.2z + 0.32) \\ &\qquad = 0.851z^2 + 1.0212z + 0.272 \end{aligned} \qquad (90)$$

Control law can obtained using equation (85) which is computed as shown below

$$\begin{aligned} u_2(t) = &-1.212u_2(t-1) - 0.271u_2(t-2) + 0.851u_{C2}(t) + 1.021u_{C2}(t-1) + 0.272u_{C2}(t-2) \\ &- 0.623y_2(t) + 0.0463y_2(t-1) - 0.3234y_2(t-2) \end{aligned} \qquad (91)$$

Overall transfer function for concentration of feed stream

$$\frac{y_2}{u_{c2}} = \frac{B_2T_2}{A_2R_2 + B_2S_2} = \frac{0.0772z^4 + 0.08694z^3 - 0.0341z^2 - 0.0543z - 0.01398}{z^5 - 0.587z^4 - 0.7054z^3 + 0.45z^2 - 0.0271z - 0.1027} \qquad (92)$$

3.3.2. CONTROLLER DESIGN OF REACTOR TEMPERATURE

The primary controller for output temperature y_1 has a control law algorithm which is given by:

$$R_1 u_1 = T_1 u_{C1} - S_1 y_1 \qquad (93)$$

where

R_1, S_1 and T_1 are the desired parameters of the first self-tuning controller.

Similar to equation 81 the Diophantine for reactor temperature represented as:

$$A_1 R_1^{'} + B_1^{-} S_1 = A_{01} A_{m1} \qquad (94)$$

The primary controller for temperature of feed stream can also be designed by computing the polynomials R_1 and S_1 by using the Diophantine equation given at equation (94).

Similarly let us assume the polynomials R_1 and S_1 as shown below

$$R_1^{'}(z) = z^2 + p_0 z + p_1 \qquad (95)$$

$$S_1(z) = q_0 z^2 + q_1 z + q_2 \qquad (96)$$

Let

$$A_{01}(z) = (z+0.4)(z+0.8) = z^2 + 1.2z + 0.32$$

Substituting (95) and (96) into equation (94) we have:

$$(z^3 - 1.727z^2 + 1.302\ z - 0.521)(z^2 + p_0 z + p_1) + (0.198\, z^2 - 0.012\, z - 0.0323)(q_0\, z^2 + q_1\, z + q_2)$$
$$= (z^2 + 1.2z + 0.32)(z^3 - 1.687\, z^2 + 1.102\ z - 0.2873) \qquad (97)$$

Equating coefficients with equal power of z we have the following equations:

$$\begin{aligned}
&p_0 + 0p_1 + 0.198q_0 + 0q_1 + 0q_2 = -0.687 \\
&-1.627p_0 + p_1 - 0.012q_0 + 0.198q_1 + 0q_2 = -0.425 \\
&1.302p_0 - 1.627p_1 - 0.0323q_0 - 0.012q_1 + 0.198q_2 = 0.5448 \\
&-0.521p_0 + 1.302p_1 + 0q_0 - 0.0323q_1 - 0.012q_2 = -0.111 \\
&0p_0 - 0.521p_1 + 0q_0 + 0q_1 - 0.0323q_2 = -0.0459
\end{aligned} \tag{98}$$

Solving the unknowns in (98) simultaneously, we get

$$\begin{aligned}
p_0 &= -1.482 \\
p_1 &= 0.524 \\
q_0 &= 1.687 \\
q_1 &= 0.643 \\
q_2 &= -0.123 \\
S_1(z) &= 1.687z^2 + 0.643z - 0.123 \\
R_1(z) &= z^2 - 1.482z + 0.546 \\
T_1(z) &= \beta_1 A_{01}(z) \\
&= 0.798(z^2 + 1.2z + 0.32) \\
&= 0.798\ z^2 + 0.958z + 0.255
\end{aligned} \tag{99}$$

Control law can be obtained using equation (93) which is computed as shown below

$$\begin{aligned}
u_1(t) &= 1.482u_1(t-1) - 0.524(t-2) + 0.798u_{c1}(t) + 0.798u_{c1}(t-1) + 0.128u_{c1}(t-2) \\
&-1.687y_1(t) - 0.643y_1(t-1) + 0.123y_1(t-2)
\end{aligned} \tag{100}$$

The overall transfer function of reactor temperature become:

$$\frac{y_1}{u_{c1}} = \frac{B_1T_1}{A_1R_1 + B_1S_1} = \frac{0.158z^4 + 0.1484z^3 - 0.036z^2 - 0.02731z - 0.004131}{z^5 - 0.687z^4 - 0.425z^3 + 0.5448z^2 - 0.111z - 0.04597} \tag{101}$$

3.4. PARAMETER ESTIMATOR DESIGN

3.4.1. ESTIMATOR DESIGN OF CONCENTRATION PLANT DYNAMICS

The parameter estimation is done by using recursive least square parameter estimation algorithm that helps to determine the unknown plant model parameters.

The Process model in (69) can be rewritten explicitly as:

$$\begin{aligned} y_2(t) = {} & 1.946y_2(t-1) - 1.231y_2(t-2) + 0.254y_2(t-3) + 0.09072u_2(t-1) - 0.0067u_2(t-2) \\ & - 0.0514u_2(t-3) \end{aligned} \tag{102}$$

where

$$\begin{aligned} a_1 &= -1.946 \\ a_2 &= 1.231 \\ a_3 &= -0.254 \\ b_0 &= 0.09072 \\ b_1 &= -0.0067 \\ b_2 &= -0.0514 \end{aligned}$$

The model is linear in the parameters and can be written in the vector form as

$$y_2(t) = \varphi_2^T(t)\theta_2(t) \tag{103}$$

where

$$\varphi_2^T(t) = [-y_2(t-1) \quad -y_2(t-2) \quad -y_2(t-3) \quad u_2(t-1) \quad u_2(t-2) \quad u_2(t-3)] \tag{104}$$

$$\theta_2^T = [0.09072 \quad -0.0067 \quad -0.0514 \quad -1.946 \quad 1.231 \quad -0.254] \tag{105}$$

Computation of the least squares estimate can be arranged in such a way that the results obtained at time t − 1 can be used to get estimates at time t.

The new parameter estimate for the desired internal plant model can be obtained as

$$\theta_2(t) = \theta_2(t-1) + K_2(t)\varepsilon_2(t) \tag{106}$$

where

$$\varepsilon_2(t) = y_2(t) - \varphi_2^T(t)\theta_2(t-1) \tag{107}$$

$$\theta_2(t-1) = \begin{bmatrix} 0.09072 \\ -0.0067 \\ -0.0514 \\ -1.946 \\ 1.231 \\ -0.254 \end{bmatrix}$$

$$\begin{aligned} K_2(t) &= P_2(t)\varphi_2(t) \\ P_2(t) &= \left(\lambda_2 - K_2(t)\varphi_2^T(t)\right)P_2(t-1) \Big/ \lambda_2 \\ K_2(t) &= P_2(t-1)\varphi_2(t)\left(\lambda_2 + \varphi_2^T(t)P_2(t-1)\varphi_2(t)\right)^{-1} \end{aligned} \tag{108}$$

Where λ_2 exponential forgetting factor for concentration plant. The value of λ_2 varies between 0 and 1. The parameters $K_2(t)$ and $P_2(t)$ can be computed by choosing the initial matrix, $P_2(t-1)$ as larger value within estimation algorithm.

3.4.2. ESTIMATOR DESIGN OF TEMPERATURE PLANT DYNAMICS

The reactor temperature Process model (73) can also be rewritten as:

$$\begin{aligned} y_1(t) = {} & 1.727y_1(t-1) - 1.302y_1(t-2) + 0.521y_1(t-3) + 0.198u_1(t-1) - 0.012u_1(t-2) \\ & -0.0323u_1(t-3) \end{aligned} \tag{109}$$

where

$$\begin{aligned} a_1 &= -1.727 \\ a_2 &= 1.302 \\ a_3 &= -0.521 \\ b_0 &= 0.198 \\ b_1 &= -0.012 \\ b_2 &= -0.0323 \end{aligned}$$

The model is linear in the parameters and can be written in the vector form as:

$$y_1(t) = \varphi_1^T(t)\theta_1 \qquad (110)$$

where

$$\varphi_1^T(t) = [-y_1(t-1) \quad -y_1(t-2) \quad -y_1(t-3) \quad u_1(t-1) \quad u_1(t-2) \quad u_1(t-3)] \qquad (111)$$

$$\theta_1^T = [0.198 \quad -0.012 \quad -0.0323 \quad -1.727 \quad 1.302 \quad -0.521] \qquad (112)$$

The new parameter estimate for the desired internal plant model can be obtained as

$$\theta_1(t) = \theta_1(t-1) + K_1(t)\varepsilon_1(t) \qquad (113)$$

where

$$\varepsilon_1(t) = y_1(t) - \varphi_1^T(t)\theta_1(t-1)$$
$$\theta_1(t-1) = \begin{bmatrix} 0.198 \\ -0.012 \\ -0.0323 \\ -1.727 \\ 1.302 \\ -0.521 \end{bmatrix} \qquad (114)$$

$$\begin{aligned} K_1(t) &= P_1(t)\varphi_1(t) \\ P_1(t) &= \left(\lambda_1 - K_1(t)\varphi_1^T(t)\right)P_1(t-1) \Big/ \lambda_1 \\ K_1(t) &= P_1(t-1)\varphi_1(t)\left(\lambda_1 + \varphi_1^T(t)P_1(t-1)\varphi_1(t)\right)^{-1} \end{aligned} \qquad (115)$$

where

λ_1 is exponential forgetting factor for temperator plant. Its value is also chosen between 0 and 1.

The initial covariance matrix $P_1(t-1)$ is necessarily chosen as large value for further computing the matrices $K_1(t)$ and $P_1(t)$ in the estimation algorithm.

3.5. STABILITY ANALYSIS

The stability of the two controlled quantities will be determined by applying Jury stability test.

3.5.1. STABILITY OF SUB-SYSTEM OF FEED CONCENTRATION

The stability analysis is beginning from determining the stability of the sub-system of concentration plant output.

From equation (69) the discrete characteristic polynomial of sub-system of the concentration plant is given by:

$$f_2(z) = z^3 - 1.946z^2 + 1.231z - 0.254 \qquad (116)$$

Since it a degree of, n=3 thus, the sub-system stability can be determined using jury stability test as follows:

$$\begin{aligned} f_2(1) &= 1 - 1.946 + 1.231 - 0.254 \\ &= 0.031\,\& \\ (-1)^n f_2(-1) &= (-1)^3[-1 - 1.946 - 1.231 - 0.254] \\ &= 4.431 \end{aligned} \qquad (117)$$

From equation (117) it can be seen that both $f_2(1)$ and $(-1)^n f_2(-1)$ are greater than zero. Therefore, the sub-system of concentration plant $G_2(z)$ is stable.

3.5.2. STABILITY OF ENTIRE SYSTEM OF CONCENTRATION PLANT

The stability of the entire system of concentration plant can also be determined using jury stability test. First the stability of the each controller parameters should 2be checked.

From equation (90)

$$\begin{aligned} &R_2(1) = 0.061 > 0, \ (-1)^2 R_2(-1) = 2.481 > 0 \\ &S_2(1) = 0.9001 > 0, \ (-1)^2 S_2(-1) = 0.9927 > 0 \\ &T_2(1) = 2.144 > 0, \ (-1)^2 T_2(-1) = 0.1018 > 0 \end{aligned} \qquad (118)$$

On the other hand using equation (92), the characteristic polynomial of the entire concentration plant will be:

$$f_1(z) = z^5 - 0.587z^4 - 0.7054z^3 + 0.45z^2 - 0.0271z - 0.1027 \qquad (119)$$

$$\begin{aligned} f_1(1) &= 1 - 0.587 - 0.7054 + 0.45 - 0.0271 - 0.1027 \\ &= 0.0278 > 0 \\ (-1)^n f_1(-1) &= (-1)^5[-1 - 0.587 + 0.7054 + 0.45 + 0.0271 - 0.1027] \\ &= 09572 > 0 \end{aligned} \qquad (120)$$

From equation (118) and (120) it is clear be that the total system of concentration plant is stable.

3.5.3. STABILITY OF SUB-SYSTEM OF TEMPERATURE PLANT

Here also the stability analysis for temperature plant is started from determining the stability of the sub-system.

From equation (73) the discrete characteristic polynomial of sub-system of the Temperature plant is given by:

$$W_2(z) = z^3 - 1.727\,z^2 + 1.302\,z - 0.521 \qquad (121)$$

It has a degree of, n=3 thus, the sub-system stability can be determined using jury stability test as follows:

$$\begin{aligned} W_2(1) &= 1 - 1.727 + 1.302 - 0.254 \\ &= 0.321\,\& \\ (-1)^n W_2(-1) &= (-1)^3[-1 - 1.727 - 1.302 - 0.521] \\ &= 4.55 \end{aligned} \qquad (122)$$

From equation (122) it can be seen that both $W_2(1)$ and $(-1)^n W_2(-1)$ are greater than zero. Therefore, the sub-system of temperature plant $G_1(z)$ is stable.

3.5.4. STABILITY OF ENTIRE SYSTEM OF TEMPERATURE PLANT

The stability of the entire system of concentration plant can also be determined using jury stability test. First the stability of the each controller parameters should be checked.

From equation (90)

$$\begin{aligned} &R_1(1) = 0.064 > 0,\ (-1)^2 R_1(-1) = 3.028 > 0 \\ &S_1(1) = 2.207 > 0,\ (-1)^2 S_1(-1) = 0.921 > 0 \\ &T_1(1) = 2.011 > 0,\ \ (-1)^2 T_1(-1) = 0.095 > 0 \end{aligned} \qquad (123)$$

From equation (101) the characteristic polynomial of the entire system temperature plant will be:

$$W_1(z) = z^5 - 0.687\,z^4 - 0.425\,z^3 + 0.5448\,z^2 - 0.111z - 0.04597 \qquad (124)$$

$$\begin{aligned} W_1(1) &= 1 - 0.587 - 0.7054 + 0.45 - 0.0271 - 0.1027 \\ &= 0.0278 > 0.2759 \\ (-1)^n W_1(-1) &= (-1)^5[-1 - 0.687 + 0.425 + 0.5448 + 0.111 - 0.04597] \qquad (125) \\ &= 1.197 > 0 \end{aligned}$$

From equation (124) and (125) it is clear that the total system of temperature plant is also stable.

CHAPER FOUR

4.1. RESULT AND DISCUSSION

As it is shown in the following block diagram the entire system of cascade control of stirred tank reactor has controller and plant model with estimator block for both concentration and temperature outputs. The estimator blocks used an RLS parameters estimation algorithm. On the other hand the controllers regulated the entire system by using self-tuning control algorithm.

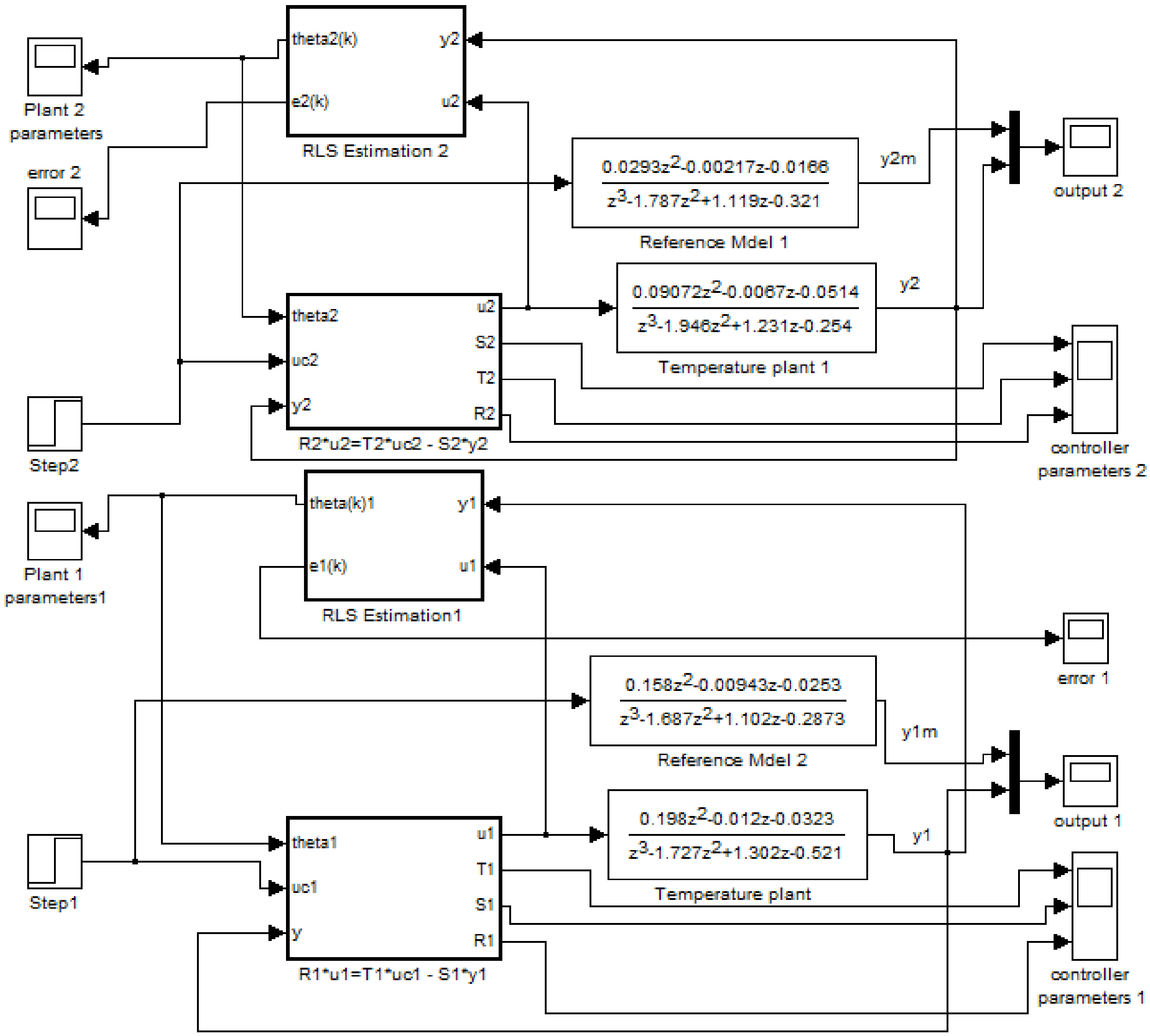

Figure 4.1. Simulink design of the entire system

RECURSIVE LEAST SQUARE ESTIMATOR

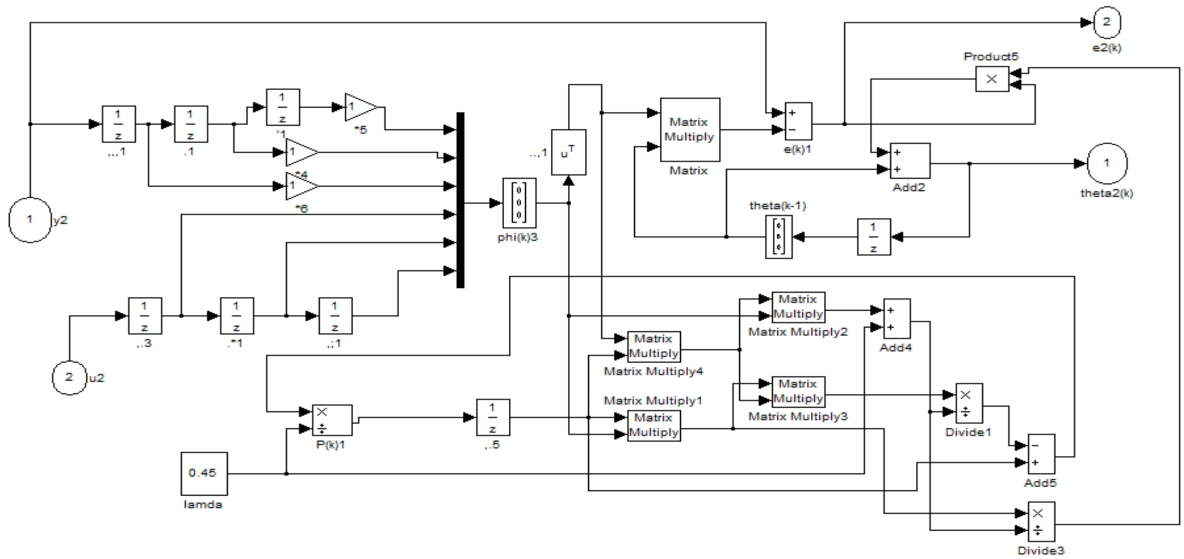

Figure 4.2. Parameters estimation block for Concentration and Temperature Plants

PRIMARY SELF-TUNING CONTROLLER

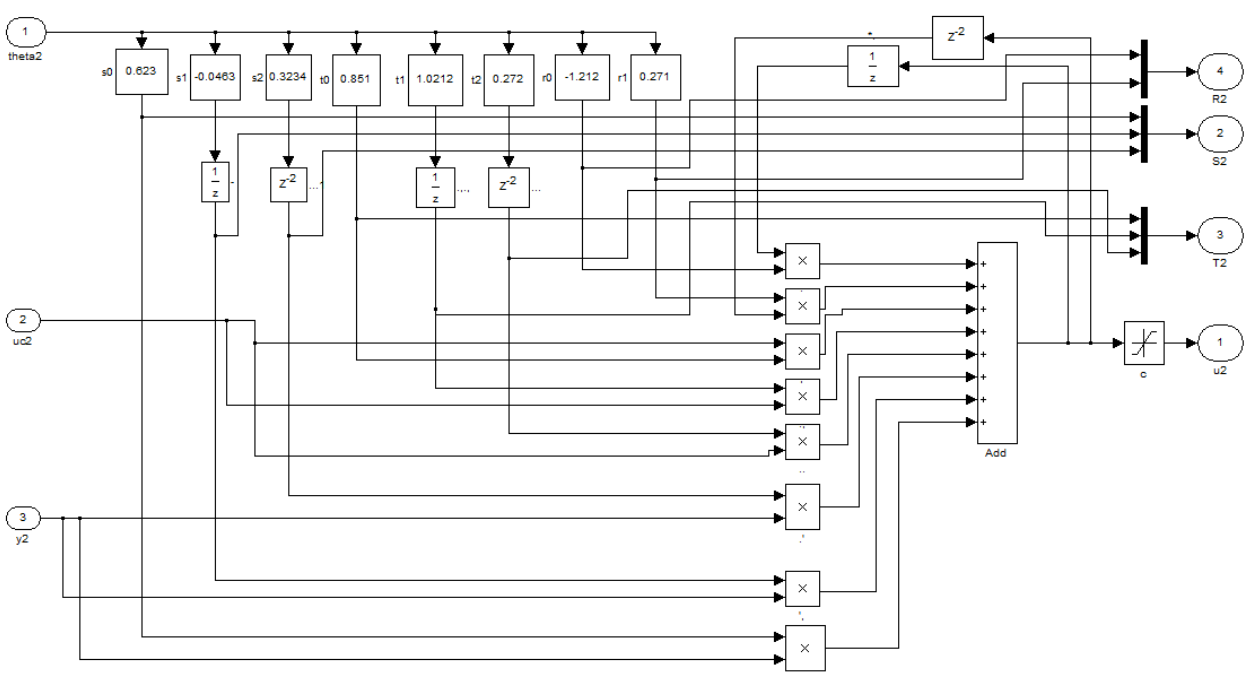

Figure 4.3. Primary Self-tuning controller of Concentration and Temperature Plants

4.2. CONCENTRATION OUTPUT OF THE REACTOR

In this section we can see that the concentration plant dynamics provides an output that follows the corresponding model as the set point of the input.

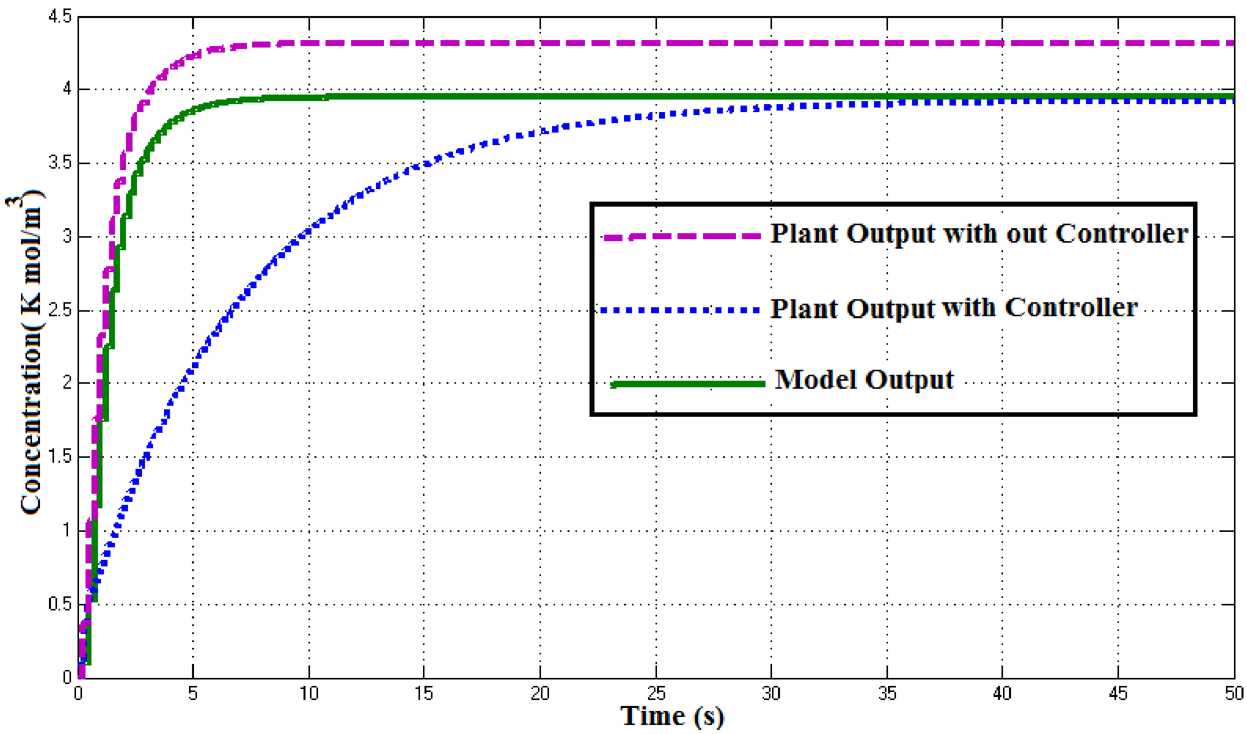

Figure 4.4. Simulation result of output of concentration plant and its reference model

From the above simulation figure it can be seen that understand that the concentration plant model output y_2 follows the saturated reference model output y_{2m} for the corresponding step reference input signal.

4.3. SELF-TUNING CONTROLLER PARAMETERS OF CONCENTRATION PLANT

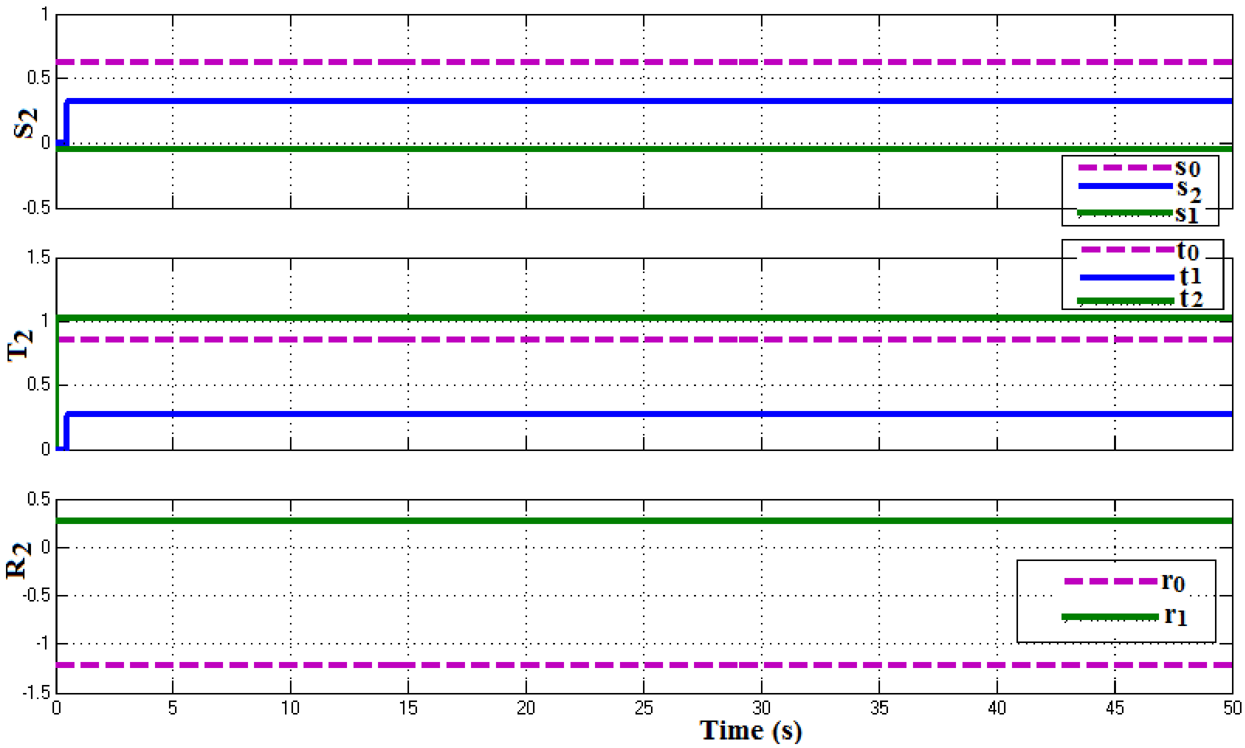

Figure 4.5. Concentration Plant Master Controller Parameters

Table 4.1. Outputs of concentration plant and its controller at different period of time

Time(s)				Concentration Plant Output y_2 (K mol/m^3)				Output of controller(u_2)			
t	t-1	t-2	t-3	$y_2(t)$	$y_2(t-1)$	$y_2(t-2)$	$y_2(t-3)$	$u_2(t)$	$u_2(t-1)$	$u_2(t-2)$	$u_2(t-3)$
3	2	1	0	1.5	1.3	0.85	0	0.1	0.1	0.1	0.1
5.5	4.5	3.5	2.5	2.3	1.75	1.6	1.4	0.1	0.1	0.1	0.1
8	7	6	5	2.8	2.5	2.2	2.1	0.1	0.1	0.1	0.1
10.5	9.5	8.5	7.5	3.2	2.9	2.85	2.65	0.1	0.1	0.1	0.1
13	12	11	10	3.45	3.37	3.3	2.95	0.1	0.1	0.1	0.1
18	17	16	15	3.8	3.7	3.58	3.5	0.1	0.1	0.1	0.1

4.4. CONCENTRATION PLANT ESTIMATION ERROR

Under this result of concentration plant dynamics error analysis its nature of non-linearity has reduced due to the minimum amount of error in the estimation of parameters. From the following simulation figure it can be observed that the error in the concentration plant parameters estimation become zero from the time t>2s. This shows that the concentration plant and its reference model exhibit better model following on the entire system.

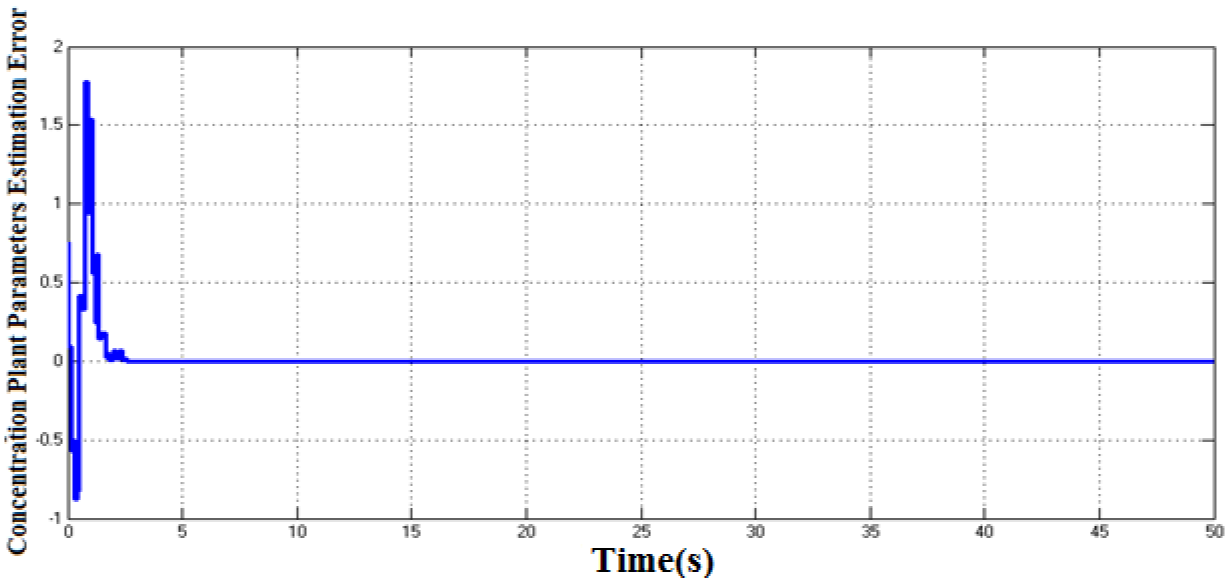

Figure 4.6. Simulation result for parameter estimation error of concentration plant

Table 4.2. Parameters Estimation Error of Concentration plant at different times

Time(s)				Estimation error(ε_2)			
t	t-1	t-2	t-3	ε_2(t)	ε_2(t-1)	ε_2(t-1)	ε_2(t-3)
3	2	1	0	0.006	0.25	0.4	0
5.5	4.5	3.5	2.5	0	0	0	0.0025
8	7	6	5	0	0	0	0
10.5	9.5	8.5	7.5	0	0	0	0
13	12	11	10	0	0	0	0
18	17	16	15	0	0	0	0

4.5. PARAMETER ESTIMATOR FOR CONCENTRATION PLANT DYNAMICS

This section tells that the estimator block of the concentration plant dynamics will displays out plant parameters. There were six parameters which were estimated by the parameter estimation block of the concentration plant using recursive least square algorithm. In such case the estimator block the plant used an exponential forgetting factor which was chosen to be λ=0.45.

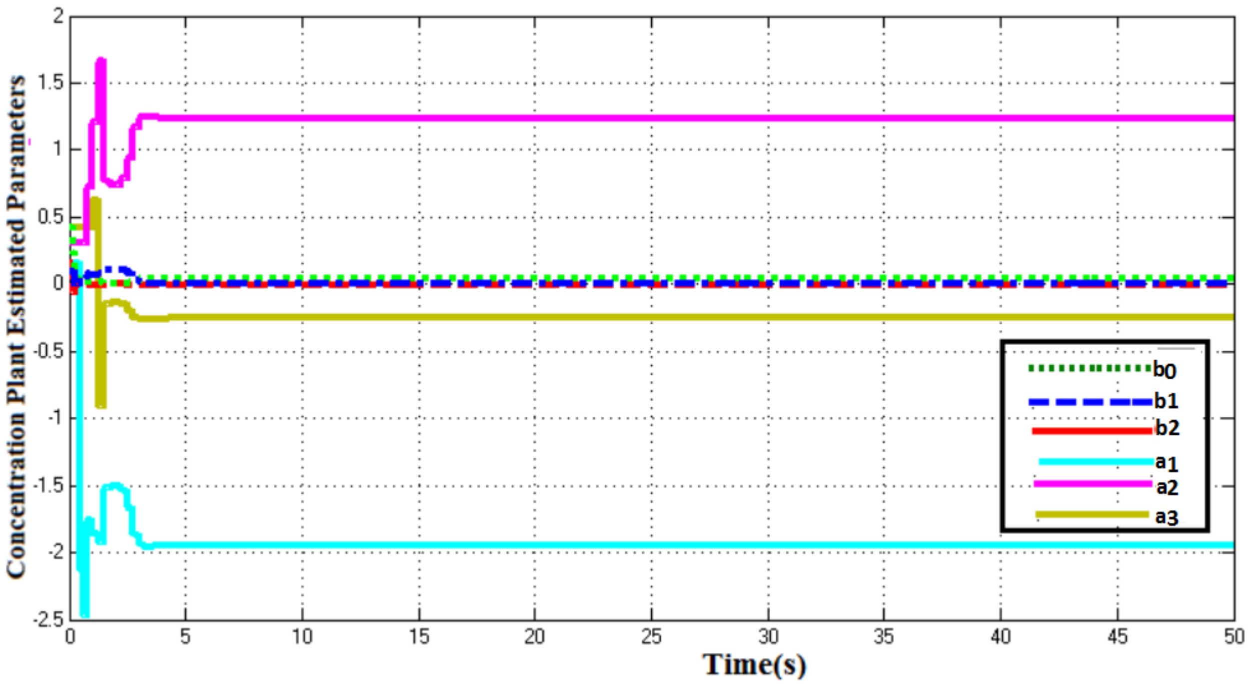

Figure 4.7. Simulation result of parameters of concentration plant dynamics

As we can see in the figure the estimator block estimated the six parameters a_1, a_2, a_3, b0, b_1 and b_2 of the concentration plant dynamic. These parameters of the concentration plant updated and become stable from time t>3s.

The concentration plant parameters are estimated for various times based on the estimation output obtained in the above graph.

For the given initial covariance matrix $P_2(t-1)$ and exponential forgetting factor $\lambda_2 = 0.45$, the regression vector $\varphi_2^T(t)$, $K_2(t)$ and $P_2(t)$ can be estimated as shown in the table:

Table 1.3. Regression and Covariance Matrix of Concentration plant Estimator

parameters	Result
$P_2(t-1)$	$\begin{bmatrix} 50 & 0 & 0 & 0 & 0 & 0 \\ 0 & 50 & 0 & 0 & 0 & 0 \\ 0 & 0 & 50 & 0 & 0 & 0 \\ 0 & 0 & 0 & 100 & 0 & 0 \\ 0 & 0 & 0 & 0 & 100 & 0 \\ 0 & 0 & 0 & 0 & 0 & 100 \end{bmatrix}$
$\varphi_2^T(t)$	$\begin{bmatrix} -0.714 & -0.15 & 0 & 0.1 & 0.1 & 0.1 \\ -0.46 & -0.4 & -0.26 & 0.1 & 0.1 & 0.1 \\ -0.65 & -0.6 & -0.5 & 0.1 & 0.1 & 0.1 \\ -0.85 & -0.78 & -0.75 & 0.1 & 0.1 & 0.1 \\ -1.15 & -1.1 & -1 & 0.1 & 0.1 & 0.1 \\ -1.52 & -1.5 & -1.45 & 0.1 & 0.1 & 0.1 \end{bmatrix}$
$K_2(t)$	$\begin{bmatrix} -2.242 & 0.76 & 0.63 & -0.86 & -1.22 & 0.89 \\ -0.561 & -2.14 & -0.531 & 3.86 & -0.74 & -1.05 \\ 1.95 & 1.57 & 0.016 & -2.93 & 1.57 & -0.374 \\ 0.31 & 1 & 1.38 & 2.19 & -1.68 & -0.754 \\ 0.155 & 0.5 & 0.692 & 1.093 & -0.84 & -0.377 \\ 0.155 & 0.5 & 0.692 & 1.093 & -0.84 & -0.377 \end{bmatrix}$
$P_2(t)$	$\begin{bmatrix} -27.8 & -75.4 & -15.24 & 45.45 & 22.72 & 22.72 \\ -75.4 & 4.16 & -42.18 & 0.84 & 0.418 & 0.418 \\ -15.25 & -42.2 & -67.8 & -40.17 & -20.08 & -20.08 \\ 45.45 & 0.836 & -40.17 & 45.6 & -27.14 & -27.14 \\ 22.72 & 0.418 & -20.08 & -27.14 & 36.38 & -13.6 \\ 22.72 & 0.418 & -20.08 & -27.14 & -13.6 & 36.38 \end{bmatrix}$

4.6. REACTOR TEMPERATURE PLANT OUTPUT

In this case the output of temperature plant dynamics followed the reference model as the step reference input to the entire system. Its parameter estimation element estimated the plant parameters online using RLS estimation algorithm.

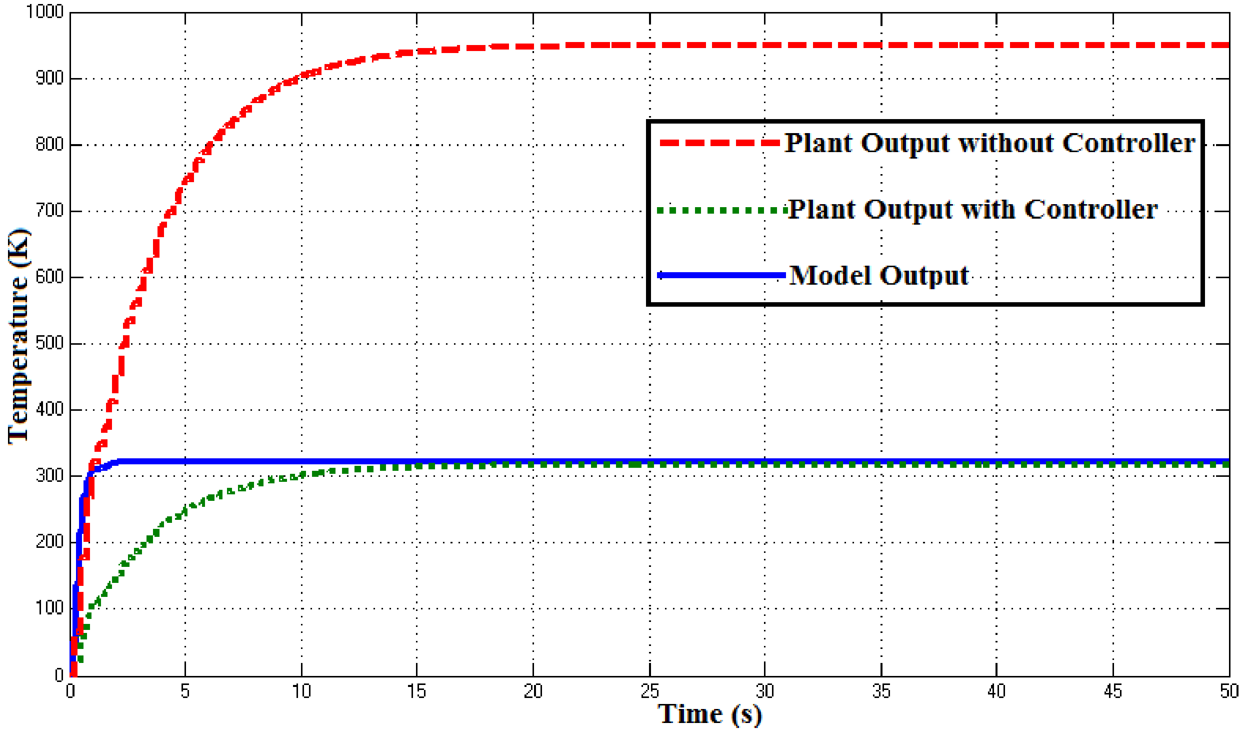

Figure 4.8. Simulation result for output of temperature plant and its reference model

From the above simulation graph, the temperature plant output without controller exceeds the required steady state temperature value 335K. But in the case of the plant with controller the plant output approaches to the steady state value.

4.7. SELF-TUNING CONTROLLER PARAMETERS OF TEMPERATURE PLANT

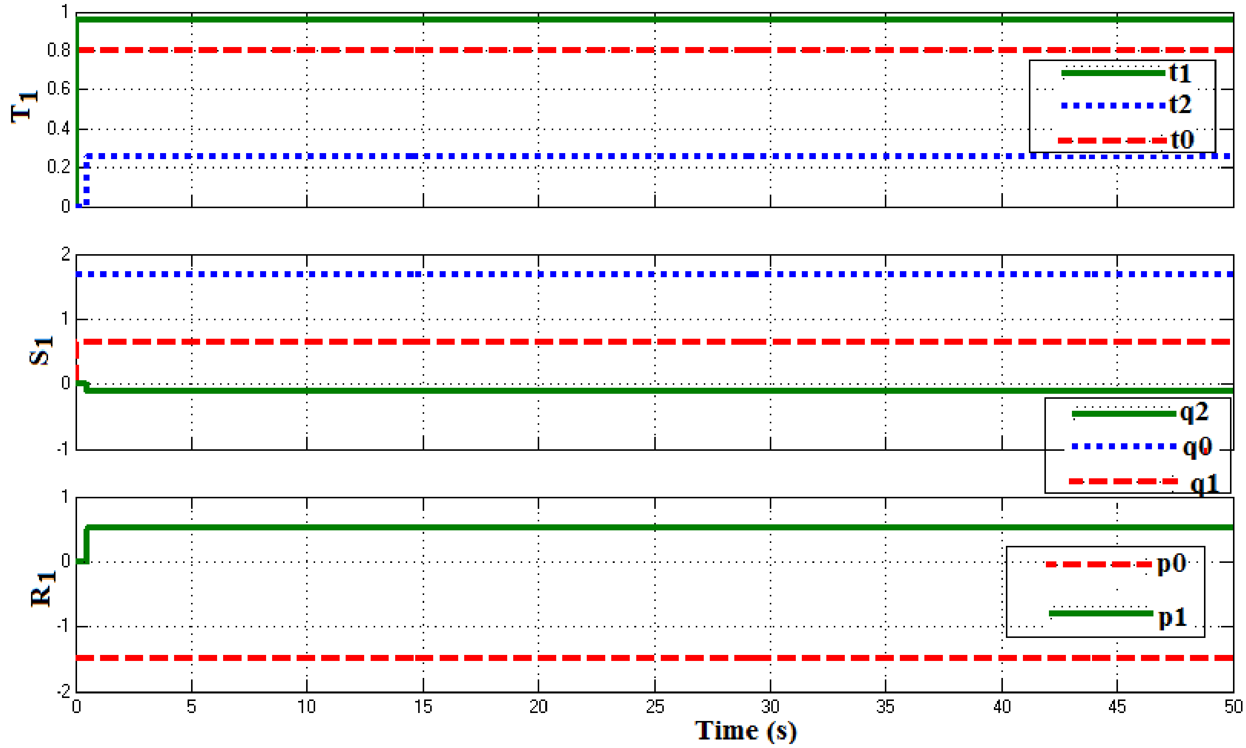

Figure 4.9. Temperature Plant Master Controller Parameters

Based on the above graphs the following data has been collected as shown in the table.

Table 4.4. Outputs of Temperature plant and its controller at different period of time

Time(sec)				Temperature plant output y_1 (K)				Output of controller(u_1)			
t	t-1	t-2	t-3	$y_1(t)$	$y_2(t-1)$	$y_1(t-2)$	$y_1(t-3)$	$u_1(t)$	$u_1(t-1)$	$u_1(t-2)$	$u_1(t-3)$
3	2	1	0	275	110	35	0	316	316	316	316
5.5	4.5	3.5	2.5	265	310	300	260	316	316	316	316
8	7	6	5	309	285	275	250	316	316	316	316
10.5	9.5	8.5	7.5	318	314	306	300	316	316	316	316
13	12	11	10	330	320	315	316	316	316	316	316
18	17	16	15	334	334	334	334	316	316	316	316

4.8. REACTOR TEMPERATURE PLANT ESTIMATION ERROR

As it can be observed in the following simulation diagram, with appropriate model following between the output of temperature plant dynamics and its reference model the error become zero for time t>5s. In such case non-linearity nature of reactor temperature plant slightly reduced so as to approach plant output to the output of the reference model.

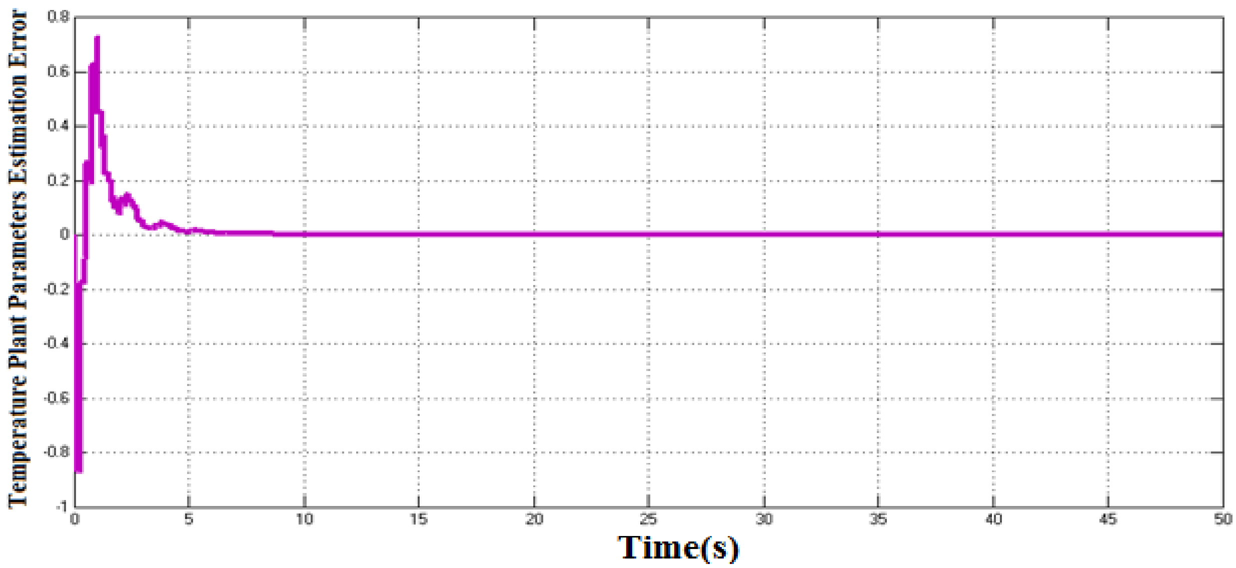

Figure 4.10. Simulation result for parameter estimation error of temperature plant

Based on the above graph of estimation error, the following data can be estimated.

Table 4.5. Parameters Estimation Error of Temperature plant at different times

Time(s)				Estimation error(ε_1)			
t	t-1	t-2	t-3	$\varepsilon_1(t)$	$\varepsilon_1(t-1)$	$\varepsilon_1(t-2)$	$\varepsilon_1(t-3)$
3	2	1	0	0.12	0.5	0.2	-0.83
5.5	4.5	3.5	2.5	0	0.02	0.08	0.17
8	7	6	5	0	0	0	0
10.5	9.5	8.5	7.5	0	0	0	0
13	12	11	10	0	0	0	0
18	17	16	15	0	0	0	0

4.9. PARAMETER ESTIMATOR FOR TEMPERATURE PLANT DYNAMICS

In this section there is also an estimator block that estimate or adjust the plant parameters of the reactor temperature. Similar to the concentration plant, the estimator displayed the six plant parameters using recursive least square algorithm.

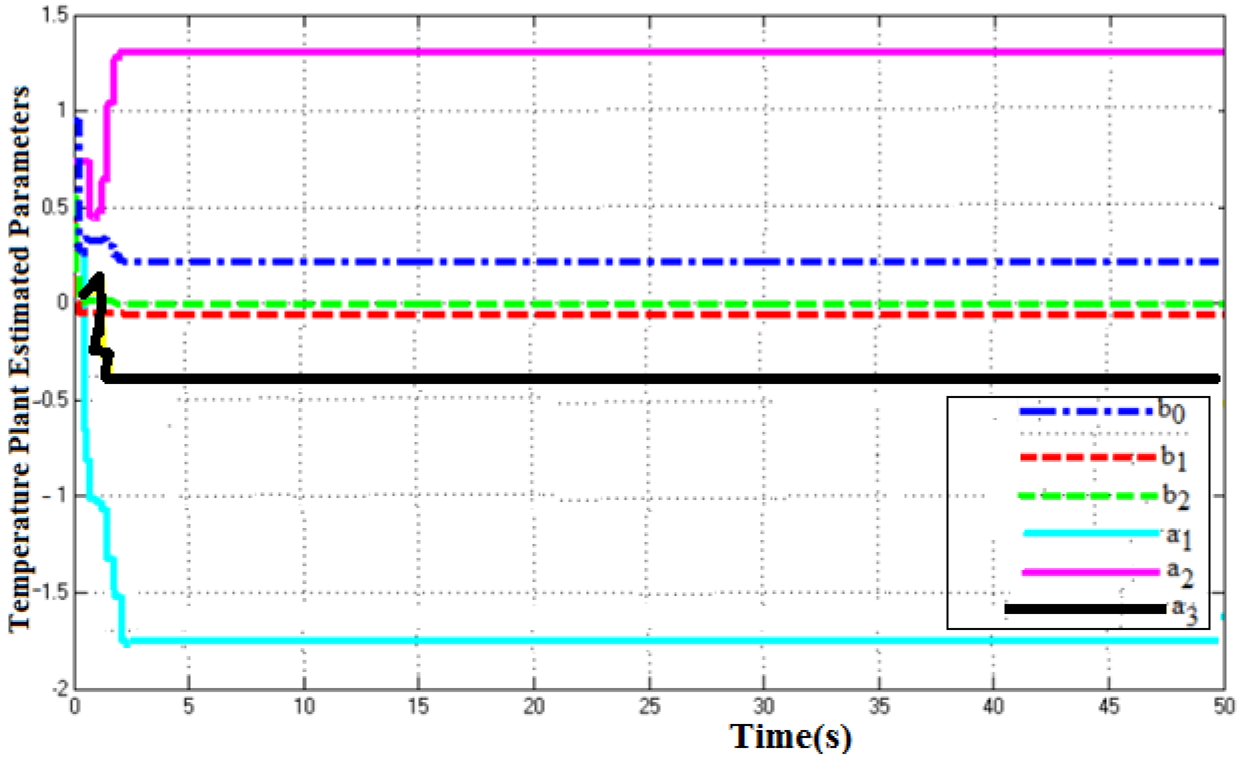

Figure 4.11. Simulation result for parameters of temperature plant dynamics

As it can be seen from the simulation graph, until the time t=2s the response of the estimated parameters of temperature plant show variation and become stable from this time.

For the temperature plant, using the given initial covariance matrix $P_1(t-1)$ and exponential forgetting factor $\lambda_1 = 0.6$, the regression vector $\varphi_1^T(t)$, $K_1(t)$ and $P_1(t)$ become:

Table 4.6. Regression and Covariance Matrix of Temperature plant Parameters Estimator

parameters	Result
$P_1(t-1)$	$\begin{bmatrix} 50 & 0 & 0 & 0 & 0 & 0 \\ 0 & 50 & 0 & 0 & 0 & 0 \\ 0 & 0 & 50 & 0 & 0 & 0 \\ 0 & 0 & 0 & 100 & 0 & 0 \\ 0 & 0 & 0 & 0 & 100 & 0 \\ 0 & 0 & 0 & 0 & 0 & 100 \end{bmatrix}$
$\varphi_1^T(t)$	$\begin{bmatrix} -110 & -35 & 0 & 316 & 316 & 316 \\ -310 & -300 & -260 & 316 & 316 & 316 \\ -334 & -334 & -334 & 316 & 316 & 316 \\ -334 & -334 & -334 & 316 & 316 & 316 \\ -334 & -334 & -334 & 316 & 316 & 316 \\ -334 & -334 & -334 & 316 & 316 & 316 \end{bmatrix}$
$K_1(t)$	$\begin{bmatrix} 0.009 & -0.04 & 0.011 & 0.0063 & 0.0063 & 0.0063 \\ 0 & 0 & -0.009 & 0.003 & 0.003 & 0.003 \\ -0.003 & 0.026 & 0.0005 & -0.008 & -0.008 & -0.008 \\ 0.003 & -0.007 & 0.0015 & 0.0013 & 0.0013 & 0.0013 \\ 0.002 & -0.0034 & 0.007 & 0.0006 & 0.0006 & -0.0006 \\ 0.002 & -0.0034 & 0.0007 & 0.0006 & 0.0006 & 0.0006 \end{bmatrix}$
$P_1(t)$	$\begin{bmatrix} -66.8 & 0 & -0.0012 & 0.0003 & 0.0002 & 0.0002 \\ 0 & -66.8 & -0.0001 & 0 & 0 & 0 \\ -0.0012 & -0.0001 & -66.8 & -0.0002 & -0.0001 & -0.0001 \\ 0.0003 & 0 & -0.0002 & 16.8 & -41.8 & -41.8 \\ 0.0002 & 0 & -0.0001 & -41.8 & 29.23 & -20.86 \\ 0.0002 & 0 & -0.0001 & -41.8 & -20.86 & 29.23 \end{bmatrix}$

CHAPTER **FIVE**

5.1. CONCLUSION

An exothermic chemical reactor allows release of heat energy in the production of desired chemical products from the entire chemical reaction. An exothermic continuous stirred tank is an important vessel in which reactants are fed continuously and products are withdrawn continuously from it. Cascade control is usually used in the control of chemical processes to reject disturbances that have a rapid effect on a secondary measured variable, before the master controlled variable is affected. An adaptive self-tuning controller is used as a master who allows online and continuous update of the parameters of un-certain reactor temperature and outlet concentration plants. The temperature of the reactor is properly monitored so that it’s steady state value is kept around 335K. On the other hand an outlet concentration of feed is regulated appropriately to 4.2 K mol/m^3 which is the desired steady state value. The parameter estimation unit enables the parameters of both the temperature and concentration plants to be estimated online using RLS algorithm. An online update of the parameters in both plants result in a further update of parameters of the master self-tuning controller so as to make both controlled variables stable. Generally regarding performance of the system, a comparative determination of transient characteristics is done along with the case with classical controllers used in the previous designs.

Table 4.7. Comparison between Self-tuning Regulator based design result and previous design

Plant	Transient Characteristics			
	Peak Overshoot	Settling Time	Rise time	Peak Time
Concentration plant	0.05	0.317	0.193	0.74
Temperature plant	0.042	0.22	0.204	0.822
IMC based	0.12	0.512	0.248	0.95
MPC based	0.74	0.621	0.345	0.94
Conventional based	0.08	21	9.85	50

5.2. FUTURE WORK

The self-tuning regulator design approach in this thesis has been applied the determination of the present time slot parameter estimation based on the previous estimation of plant parameters using recursive least square algorithm with exponential forgetting factor. In this study such control approach has also used for increasing the stability of the plant output and estimated parameters. The main future works to this thesis are:

- Analyzing the effect of variable volumetric flow rate of inlet feed reactant on the reactor temperature and concentration.
- Performing a future slot estimation of parameters for both temperature and concentration plants parameters in self-tuning regulator.
- Analyzing estimation of the effect of disturbance variables on the non-linear plant dynamics outputs.

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APPENDIX

SIMULATION PROGRAM

%% Inputs of self-tuning regulator process control:

% u_c: input signal to the system

% y: output signal to the system

% n_a: order of the denominator of the transfer function of the system

% n_b: order of the numerator of the transfer function of the system

% n_c: order of the numerator of the transfer function of the system noise if any if not put n_c=0

% d: order of delay of the system

% T_s: sampling time (ms)

%% Outputs of the plant in the control system:

% A: denominator of the discrete transfer function of the system

% B: numerator of the discrete transfer function of the system

% S: numerator of the discrete feedback controller

% R: denominator of the discrete feedback controller

% T: numerator of the discrete feed forward controller if any if not T=0

%using exponential forgetting factor, lambda

% A_m_ploes: required ploes in z-domain

% A_0_ploes: observer poles in z-domain

%Model following without zero cancelation

% T=β*A0;

% Control signal: u=T/R u_c - S/R y

% for model output y(m)

```
y1(m1) = 0;
for j1=1:na1
    if m1-j1 >0
        y1(m1) =y1(m1)+A1(j1)*y1(m1-j1);
    end
```

```
        elseif
          end
          for J1=0:length(B1)-1
              if m1-J1-d1 > 0
                  y1 (m1) =y1 (m1) +B1 (J1+1)*u1 (m1-d1-J1);
              end
         elseif
          end
          y_output1=y1(m1);
                 end
% Reference model denominator polynomial (Am)
              Am2=1;
              for i2=1:length(Am_poles2)
                  Am2=conv(Am2,[1,-Am_poles2(i2)]);
              end
   % Observer polynomial A0
              A02=1;
              for i2=1:length(A0_poles2)
           if i2 <= nalpha2-length (Am_poles2)
           A02=conv (A02,[1,-A0_poles2(i2)]);
                  end
          elseif
           end
% Diophantine
              D2=zeros (nalpha2, nalpha2);
              for i2=1:nr2
                  D2 (i2: length (A2) +i2-1, i2) =A2';
              end
              for i2=1:nalpha2-nr2
                  D2 (d2+i2-1:nb2+d2+i2-1, nr2+i2) =B2';
              end
```

```
            alpha2=Am02 (2: end)';
            a2=zeros (1, nalpha2);
            a2 (1:na2) =A2 (2: end);
            I2=alpha2-a2';
                      RS2=inv (D2)*I2;   R2= [1, RS2 (1:nr2)'];
            S2=RS2 (nr2+1: end)';
                   else
if nalpha2 > length (Am_poles2) +length (A0_poles2)
display ('The Required Closed Loop Poles is not Enough')
 elseif nalpha2 < length (Am_poles2) +length (A0_poles2)
  display ('The Required Closed Loop Poles is excess')
                         end
                   end
             end
%% Start Point
N=max (na+1, nb+d+1); X=ceil (2/Ts/N);
      N=X*N;   uco=uc; lambda (1: N) =0.9;
      if nc == 0
             for L=1: N
                   P {L} =eye (na+nb+1)*10^ (8);
             end
             theta_hat (:, 1: N) =zeros(na+nb+1, N);
             epslon (1: N) =0;
      else
             for L=1: N
                   P {L} =eye (na+nb+nc+1)*10^ (8);
             end
             theta_hat (:, 1: N) =zeros (na+nb+nc+1, N);
             epslon (1: N) =0;
             epslon_n (1: N) =0;
             epslon_p(1: N) =0;
```

```
    end
    e(1: N) =uc(1: N)-y (1:N);  u (1:N) =uc(1:N);
    ud(1:N) = uc(1:N);
    yd(1:N) = y(1:N);
    Dc_gain(1:N) = 1;
% RLS Parameter estimation
    for i = N/X:N-1
            for j=1:na
                if i-j <=0
                    phiT(i, j)=0;
                else
                    phiT(i,j)=[-y(i-j)];
                end
            end
            for j=0:nb
                if i-j-d <= 0
                    phiT(i,j+1+na)=0;
                else
                    phiT(i,j+1+na) = [u(i-j-d)];
                end
            end
            K{i}=P{i-1}*phiT(i,:)'*inv(1+phiT(i,:)*P{i-1}*phiT(i,:)');
            epslon(i)=y(i)-phiT(i,:)*theta_hat(:,i-1);
            theta_hat(:,i)=theta_hat(:,i-1)+K{i}*epslon(i);
            P{i}=(eye(length(K{i}*phiT(i,:)))-K{i}*phiT(i,:))*P{i-1};
            P{i}=(P{i}+P{i}')/2;
            AA{i}=[1 theta_hat(1:na,i)'];
            BB{i}=[theta_hat(na+1:end,i)'];
```