CERTIFICATION OF APPROVAL

Dynamic Modeling For a First Order Mixing Process Using Simulink in Matlab

By

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Approved by,

Nasser Mohammad Ramli

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 acknowledgement, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

Mohd Redza Harriz Zainal

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CHAPTER 1

ABSTRACT

1. ABSTRACT

This assessment reports the research made on the dynamic modeling for a first order system of a mixing process using Simulink in Matlab. The research project consists of two main tasks. The tasks are to develop a mathematical model of the process and also to find and use an appropriate controller tuning design based on the transient response criteria.

The research project conducted is meant to achieve three objectives. The objectives are:-

1. to develop the mathematical model that describes the mixing process
2. to study the response of the mixing process in manual mode
3. to study the step response of the process in automatic mode

Currently, there was not much information regarding the response's characteristic of the outlet concentration of a mixing process. Thus, the problem statement of this research project is to investigate how the characterization of response for the outlet concentration of the mixing process.

For this study, the scope would be only to study the response characteristic of several step responses in manual and automatic mode. This would be done by doing some adjustment in setting up the valve opening or input flow before the responses is investigated or study.

At this point, there is not much information regarding the mathematical model of a first order reaction system of a mixing process. Through findings for this kind of a process,

there are a few parameters that should be taken into consideration which affects the characterization response.

Currently, the simulation of this study has been completed. The next step would be to investigate the characterization responses of the model. This will be done by adjusting the input flow, valve opening and height or level of the mixing in the tank.

CHAPTER 2

INTRODUCTION

2. INTRODUCTION

2.1. BACKGROUND OF STUDY

The dynamic response of a process is of prime consideration in the design, analysis and implementation of process control system. It is important to know all this in order to understand the response characterization. The dynamic response will be described through the use of mathematical models, transfer functions and also block diagrams.

The transfer function of a process comes from the mathematical model that was developed starting from the first principles. This transfer functions would then reveal the terms that describes the process response. The process response consists of gain, time constant and dead time or time delay.

Through this dynamic modeling, the process could be control automatically by using an automatic mode. Thus, giving the appropriate adjust tuning automatically for what ever process done.

2.2. PROBLEM STATEMENT

Currently, there was not much information regarding the response's characteristic of the outlet concentration of a mixing process. There are few parameters that could be taken into consideration that affecting the characterization of response of this process.

This report later on will consist of a developed mathematical model of the process in Matlab and the use of appropriate tuning design based on the transient response criteria. The transient response would be obtained through the developed mathematical model.

This study will identify the characteristic of response that could be obtained through the mixing process. The study will also identify the mathematical model developed for a first order system of a mixing process. Including of that, the appropriate use of controller tuning design will also be described.

The problem statement also can be explained as below of a mixing process.

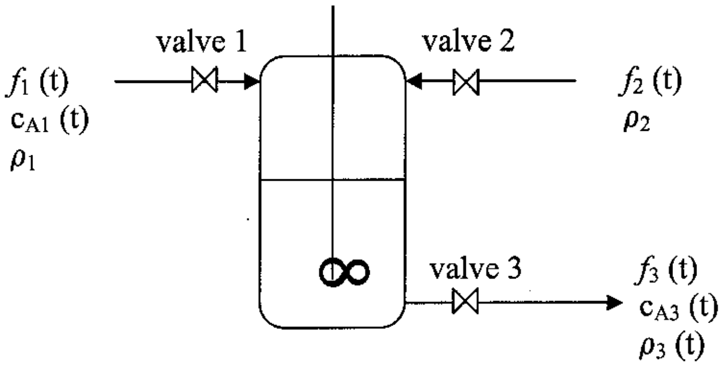


Fig. 1 Mixing process

A mixing process is an unsteady state process. Thus, a first-order system must be use for modeling this process. Considering the mixing process shown above (Fig. 1), the purpose of this process is to blend two streams with a different concentration. The density of the outlet stream should be a function of concentration which is given by,

$$\rho_3(t) = a_3 + b_3 c_{A3}(t)$$

Where a_3, b_3 = known constant

Besides that, the setting up of the valve opening also plays an important role. This is because the opening of the valve controls the flow inlet of the solution.

The flow through valve 1 can be given by

$$f_1(t) = C_{v1}\, v\rho_1(t)\, \sqrt{(\Delta P_1/G_1)}$$

The flow through valve 2 is given by

$$f_2(t) = C_{v2}\, v\rho_2(t)\, \sqrt{(\Delta P_2/G_2)}$$

Meanwhile the flow inlet through valve 3 could be given by

$$f_3(t) = C_{v3}\, \sqrt{(\Delta P_3(t)/G_3(t))}$$

Where $v\rho$ = valve opening

G = specific gravity

To find how the outlet concentration changers when either of the inputs, inlet concentration of c_{A1} or c_B, is changed, we use the general first-order transfer function

$$\frac{Y(s)}{X(s)} = \frac{K}{\tau s + 1}$$

Where K is the process gain and τ is the time constant. From this, the particular forms of input X(s) can be investigate, expressions for Y(s) and the response, y(t) can be derived.

2.3. OBJECTIVES

This project is relevant in nature because of a mixing process is a standard chemical reaction where most industries in the world do. Without proper process control, it's hard to determine an ideal and constant concentration of a mixture. This is where the dynamic response takes place, which is to determine what the appropriate step to take for. From this, a suitable controller tuning design based on the response criteria obtained could be design in order to control the process.

Thus, the objectives of this study are listed as follows:-

- To develop the mathematical model that describes the mixing process
- To study the response of the mixing process in manual mode
- To study the process in automatic mode.

2.4. SCOPE

The scope of the research project will mainly be: -

- To develop the mathematical model that describes the mixing process

  - The model will be a model of a simple mixing process which does not take any effect of any thermal reaction that uses heat or complicated chemical reactions

- To study the response of the mixing process in manual mode

  - The characterization response will be studied base on the resulting graph obtained from applying the simulation to the real test

- To study the step response process in automatic mode.

- The characterization response if a second order underdamped process is studied based on the results obtained from applying the simulation to a test.

CHAPTER 3
LITERATURE REVIEW

3. LITERATURE REVIEW

Recently, a research project on mixing of viscous liquid has been done. The project can be summarized when a quiescent binary mixture is instantaneously brought from two- to one-phase region of its phase diagram, the resulting mixing process is driven both by diffusion and by convection. Applying the diffuse interface model, here we show by numerical simulation that the bulk motion that is induced during phase transition effectively slows down the mixing process. In fact, in our model convection is induced by a non-equilibrium body force that is proportional to the chemical potential gradients, expressing the tendency of the demixing system to minimize its free energy. In liquid systems, as this driving force induces a material flux which is much larger than that due to pure molecular diffusion, drops tend to coalesce and form larger domains which eventually must dissolve by diffusion.

Therefore, in the absence of any external agitation, mixing is slower in mixtures with larger viscosities, contrary to common thinking. In addition, as expected, the mixing rate decreases as the Margules parameter ψ increase, where ψ describes the relative weight of enthalpic versus entropic forces.

3.1 Introduction

In most of the previous numerical studies on mixing, mixing of two fluids A and B has been considered as the result of the chaotic advection of one fluid into the other, assuming that the instantaneous velocity of a fluid particle (of either A or B type) is the solution of the Navier–Stokes equation for a single-phase fluid. Clearly, this is rigorously true only in the dilute limit and when the fluid mixture is ideal, which means that the enthalpic properties of the fluid mixture are neglected, assuming that the interparticle forces between A and A are equal to those between B and B and those between A and B.

This approximation seems to be justified when the flow is turbulent, so that convection dominates any diffusive process resulting from the thermodynamic properties of the system. In general, however, at low Reynolds numbers this approximation ceases to be valid and the physico-chemical properties of the fluid mixture have to be taken into account.

In this work, we present a series of simulations of the mixing process occurring after heating a quiescent and initially phase-separated liquid mixture to a temperature T well above its critical point of miscibility, showing that the process is strongly influenced by the interplay between convection and diffusion. The latter is induced by the velocity fluctuations of the molecules that compose the system at thermal equilibrium and consists of their incoherent, random motion, with no specific preferential direction. On the contrary, convection, when it is not imposed from the outside, can exist only for a system far from equilibrium, as it consists of the collective, coherent motion of its molecules, and is therefore a much faster process than diffusion.

As explained by the so-called diffuse interface model (otherwise called model H), convection arises as the system tends to minimize its free energy and, in fact, is induced by a (non equilibrium) body force that is proportional to the gradient of the chemical potential. At the late stages of phase separation, after the system has developed well-defined phase interfaces, this body force reduces to the more conventional surface tension, so that the driving force can be thought of as a non-equilibrium attractive force among drops.

The diffuse interface model provides a description of two-phase systems that is alternative to the classical fluid-mechanical approach, where phase interfaces are modeled as free boundaries that evolve in time. In fact, Jacqmin (2000), performing a careful matched asymptotic expansion, showed that the motion of sharp interfaces between immiscible fluids, obtained as the outer expansion of the velocity field calculated using the diffuse interface approach, satisfies the usual Marangoni-type boundary conditions at the interfaces.

By applying the diffuse interface model, it showed by numerical simulation that spinodal decomposition of fluid mixtures strongly depends on the relative importance of convection and diffusion, and that the enhanced coarsening rate is due to the strong coupling between concentration and velocity fields.

Diffuse interface model predicts that the mixing process of two miscible liquids is driven by the convection induced by a non-equilibrium body force, which is proportional to the chemical potential gradients.

3.2 Theory

The motion of an incompressible binary fluid mixture composed of two species *A* and *B* is described here through a modification of the diffuse interface model. Here, *A* and *B* are assumed to have equal viscosities, η, densities, ρ, and molecular weights, M_w, with the composition of the system uniquely determined through the molar fraction ϕ of, say, species *A*, as a function of position *r* and time *t*.

If the flow is assumed to be slow enough to neglect the inertial terms in the Navier–Stokes equation, conservation of mass and momentum lead to the following system of equation,

$$\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = -\frac{1}{\rho} \nabla \cdot \mathbf{J}.$$

$$\eta \nabla^2 \mathrm{v} - \nabla p = \mathbf{F}\phi; \ \nabla \cdot \mathrm{v} = 0,$$

where **v** is the average local fluid velocity, **J** is the diffusion flux and **F**$\boldsymbol{\phi}$ is a body force. **J** is proportional to the gradient of the chemical potential through the relation,

$$J = -\rho\phi(1-\phi)D\nabla\mu$$

where D is the molecular diffusivity, and $\mu = \mu_A - \mu_B$ is the generalized (non-dimensional) chemical potential difference between the two species defined as $\mu = \delta(\Delta g / RT) / \delta\varphi$. Here Δg denotes the molar free energy of mixing, defined as,

$$\Delta g = RT\left[\phi\log\phi + (1-\phi)\log(1-\phi) + \psi\phi(1-\phi)\frac{1}{2}a^2(\nabla\phi)^2\right]$$

where R is the gas constant, a is a characteristic microscopic length and ψ is the Margules parameter, which describes the relative weight of enthalpic versus entropic forces.

Phase separation occurs whenever the temperature of the system T is lower than the critical temperature T_c. Imposing that at the critical point $d^2g/d\phi^2=0$ and $\phi=1/2$, we find that $\psi_c=2$ is the critical value of ψ.

Therefore, the single-phase region of the phase diagram corresponds to values $\psi<2$, while the two-phase region has $\psi>2$. At the end of the phase segregation process, a surface tension σ can be measured at the interface and from that, a can be determined as

$$a \sim \frac{1}{\sqrt{\tau}(\Delta\phi)^2_{eq}}\frac{\sigma M_w}{\rho RT},$$

where $\tau=(\Psi-2)/2$, while $(\Delta\phi)_{eq}$ is the composition difference between the two phases at equilibrium. This relation can be easily derived considering that $\sigma \sim \rho\ell(\Delta g)_{eq}/M_w$, where $(\Delta g)_{eq}$ is the jump in free energy across an interface at equilibrium, which can be estimated earlier and $\ell \sim a/\sqrt{\tau}$ is the characteristic interface thickness. In the following, we will assume that $\tau=O(1)$.

The body force $\mathbf{F}\phi$ equal the generalized gradient of the free energy, and therefore it is driven by the chemical potential gradients within the mixture.

$$\mathbf{F}_{\phi} = \frac{\rho}{M_w}\frac{\delta g}{\delta \mathbf{r}} = \left(\frac{\rho RT}{M_w}\right)\tilde{\mu}\nabla\phi = \left(\frac{\rho RT}{M_w}\right)[\nabla\tilde{p} - \phi\nabla\tilde{\mu}].$$

where $\tilde{p} = \phi\tilde{\mu}$ is a pressure term which does not play any role. In particular, when the system presents well-defined phase interfaces, such as at the late stages of phase separation, this body force reduces to the more conventional surface tension. Therefore, being proportional to $\tilde{\mu}$, which is identically zero at local equilibrium, $\mathbf{F}\phi$ can be thought of as a non-equilibrium interfacial force.

Since $\mathbf{F}\phi$ is driven by surface energy, it tends to minimize the energy stored at the interface driving, say, *A*-rich drops towards *A*-rich regions. The resulting non-equilibrium attractive force f_A between two isolated drops of radius R separated by a thin film of thickness d can be easily evaluated as $f_A \sim F\phi R^2 d \sim R^2\sigma/a$, where $F\phi \sim \sigma/d^2$.

The magnitude of this attractive force is much larger than that of any repulsive interaction among drops due to the presence of surface-active compounds, thus explaining why the rate of phase separation in deeply quenched liquid mixtures is almost independent of the presence of surfactants.

The ratio between convective and diffusive mass fluxes defines the Peclet number, $N_{Pe}=Va/D$, where V is a characteristic velocity, which can be estimated through (2) and (6) as $V \sim F\phi a^2/\eta$, with $F\phi \sim \rho RT/(aM_w)$. Finally we obtain,

$$N_{Pe} = \frac{a^2}{D}\frac{\rho}{\eta}\frac{RT}{M_w} \approx \frac{\sigma a}{\eta D}.$$

which coincides with the "fluidity" parameter defined by Tanaka and Araki (1998). For systems with very large viscosities, N_{Pe} is small and the model describes a diffusion-driven separation process, as in polymer melts and alloys. For most liquids, however, N_{Pe} is very large, typically $N_{Pe}>10^3$, showing that diffusion is important only in the vicinity of local equilibrium, when the body force $\mathbf{F}\phi$ is negligible. In general, therefore, for fluid mixtures that are in conditions of non-equilibrium, either phase-separating or mixing, convection dominates diffusion.

Although this approach has been developed for much idealized systems, it seems to capture the main features of real mixtures, at least during the phase separation process. This is why we did not add further terms to generalize our model, although they can be derived rather easily

3.3.Numerical results

Now we restrict our analysis to two-dimensional systems, so that the velocity **v** can be expressed in terms of a stream function ψ, i.e. $v_1=\partial\psi/\partial r_2$ and $v_2=-\partial\psi/\partial r_1$. Consequently, the equations of motion ((1), (2) and (3)) become

$$\frac{\partial\phi}{\partial t} = \nabla\psi \times \nabla\phi - \frac{1}{\rho}\nabla\cdot\mathbf{J},$$

$$\eta\nabla^4\psi = \left(\frac{\rho RT}{M_w}\right)\nabla\tilde{\mu}\times\nabla\phi,$$

where $\mathbf{A}\times\mathbf{B}=A_1B_2-A_2B_1$

Since material transport here is diffusion-limited, the length-scale of the process is the microscopic length a. Therefore, using the scaling,

$$\tilde{\mathbf{r}} = \frac{1}{a}\mathbf{r}, \quad \tilde{t} = \frac{D}{a^2}t, \quad \tilde{\psi} = \frac{1}{DN_{Pe}}\psi,$$

the equations of motion become

$$\frac{\partial\phi}{\partial\tilde{t}} = N_{Pe}\tilde{\nabla}\tilde{\psi}\times\tilde{\nabla}\phi + \tilde{\nabla}\cdot(\tilde{\nabla}\phi - \phi(1-\phi)[2\Psi + \tilde{\nabla}^2]\tilde{\nabla}\phi).$$

$$\tilde{\nabla}^4\tilde{\psi} = -\tilde{\nabla}(\tilde{\nabla}^2\phi)\times\tilde{\nabla}\phi.$$

This system of differential equations has been time-integrated on a L=1000a square domain with periodic boundary conditions using the finite difference scheme.

First, we simulated the mixing process between two fluids which are initially quiescent and separated by a plane interface, $r_1=L/2$. In this case, the body force, is identically zero, so that **v**=**0** and therefore the process does not depend on the Peclet number. In fact it is well approximated by the following equation:

$$\frac{\partial \phi}{\partial t} = D^* \frac{\partial^2 \phi}{\partial r_1^2},$$

with

$$D^*(\bar{\phi}) = D[1 - 2\Psi\bar{\phi}(1 - \bar{\phi})].$$

where $\bar{\Phi}$ represents the mean value of ϕ, as the neglected terms play a role only at the very beginning of the mixing process, when the interface is still sharp. As shown in Fig. 1, the results of our simulations are in perfect agreement with the above equation, confirming that the mixing process of two fluids separated by an initially plane sharp interface remains one-dimensional, does not depend on the Peclet number and is a purely diffusive process, with an effective diffusivity D^* that depends on the thermodynamic properties of the mixture, i.e. the value of the Margules parameter Ψ. The same result is obtained whenever the initial configuration is one-dimensional, as in the case of an isolated drop.

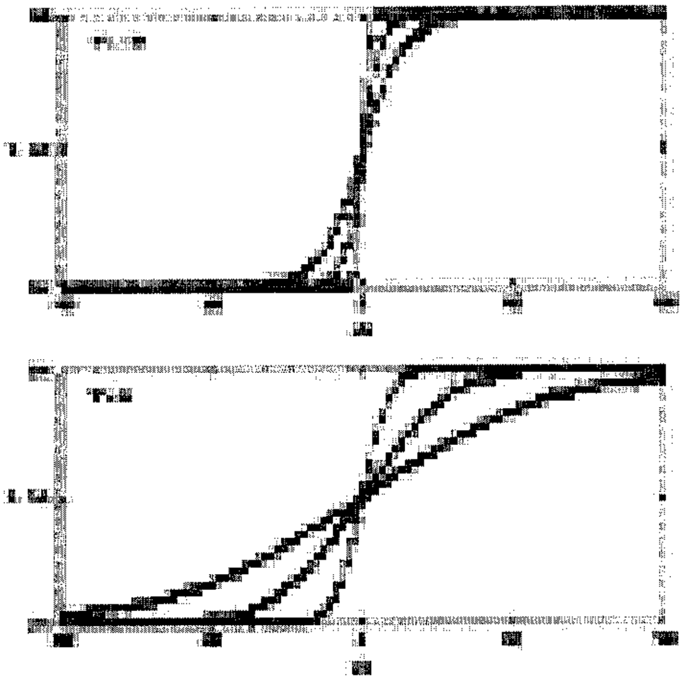


Fig. 1. Evolution of the concentration field assuming an initially plane interface for N_{Pe}=0 (circles) and N_{Pe}=10^4 (crosses) at time t=0.1, 1 and $5\times10^3 a^2/D$ for Ψ=0 (top) and Ψ=1.9 (bottom). The solid lines correspond to the solution of the diffusion equation (13), with $\Phi = \frac{1}{2}$ so that D^*=D(1-Ψ/2).

When we simulate the mixing process of a collection of drops immersed in a background field, while a single drop remains still as it is absorbed, two drops tend to attract each other and even coalesce, provided that the Peclet number is large enough and the drops are initially very close to each other.

This effect is further investigated in the simulations shown in Fig. 2, representing the evolution of two identical drops with Ψ=1.9 and radius 40a, that are placed within the quiescent bulk fluid at a distance of 120a from each other. When N_{Pe}=0, the drops do not move and are reabsorbed by diffusion, while when N_{Pe}=10^4, they rapidly coalesce and form a larger isolated single drop.

This latter, though, has to be reabsorbed by diffusion, too, and, being larger than the original drops, will take approximately twice as long to disappear. Consequently, mixing appears to be faster in the absence of convection.

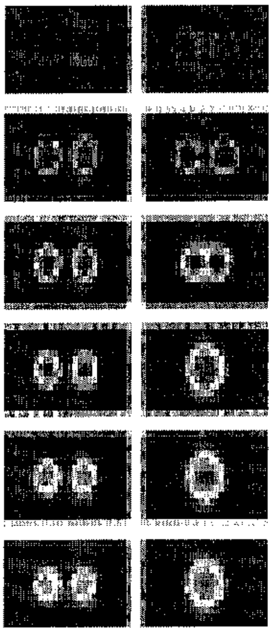


Fig. 2. Snapshots of the evolution of two identical drops with N_{Pe}=0 (left) and N_{Pe}=10^4 (right) at time t=0, 1, 2, 3, 4 and $5\times10^3a^2/D$. The drops have Ψ=1.9, an initial radius of 40a and are placed within the bulk fluid at a distance of 120a from each other.

This result is confirmed by the series of simulations shown in Fig. 3, where the initial concentration field is that resulting from a random distribution of 250 drops with radii between 5a and 20a and with Ψ=1.9.

The results of these simulations are summarized in Fig. 4 in terms of the degree of mixing δ_m, defined as

$$\delta_m(t) = \frac{\langle|\phi(\mathbf{r},t) - \phi_{av}|^2\rangle}{\langle|\phi_0(\mathbf{r}) - \phi_{av}|^2\rangle} = \frac{\phi^2_{rms}(t)}{\phi^2_{rms}(0)},$$

where the brackets indicate volume average. Comparing the behavior for N_{Pe}=0 with that for N_{Pe}=10^4, we see that δ_m decays exponentially as

$$\delta_m(t) = \exp\left(-10^3\frac{Dt}{a^2\tau}\right).$$

where τ=0.8 whenN_{Pe}=0 and τ=2.1 when $N_{Pe}=10^4$. This result shows that indeed δ_m decays faster in the absence of the convection that is induced by non-equilibrium interfacial forces, i.e. for very viscous liquids.

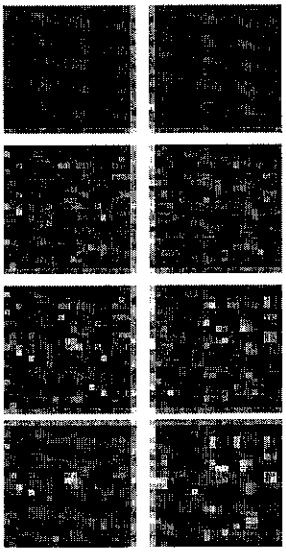


Fig. 3 Snapshots of the evolution of a random collection of 250 drops with N_{Pe}=0 (left) and $N_{Pe}=10^4$ (right), at time t=0, 1, 2 and $4\times10^3a^2/D$. The drops have Ψ=1.9 and initial radii between 5a and 20a.

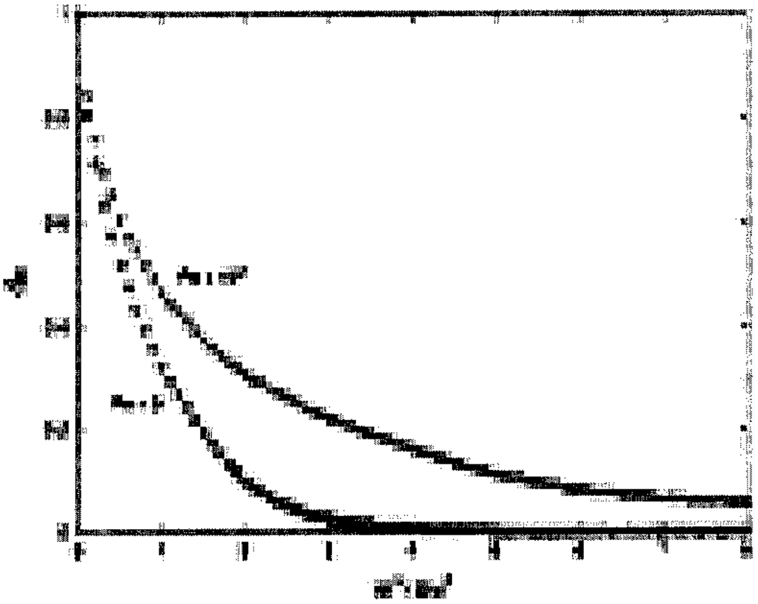


Fig. 4. Time evolution of the degree of mixing [cf. Eq. (15)] with N_{Pe}=0 and 10^4.

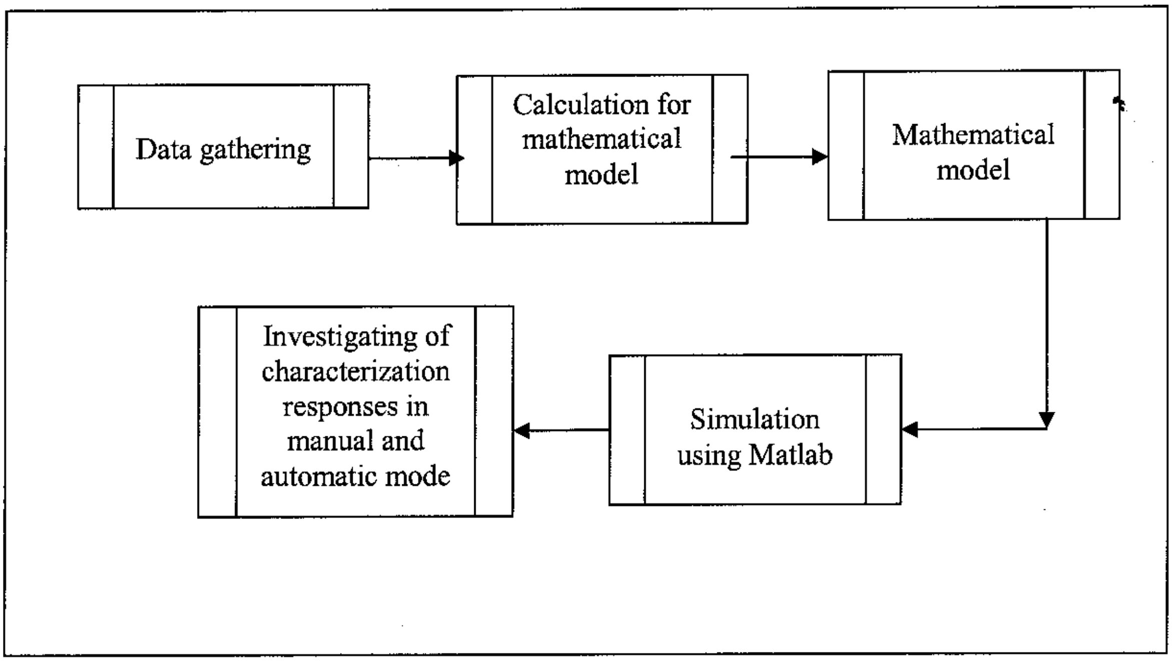


Fig. 2 Process flowchart for analysis of mathematical model for a mixing process

4.1.2. STEP PROCEDURES

In order to create a simulation which can be considered is developed from the root, many steps must be taken in order to achieve all the objectives. At least by the end of this research, this simulation will be ready to be used for any mixing application.

The procedures which to be taken are as explain below. This step procedure explains the step taken from the early stage of this research up to the simulation developed for this first order mixing process.

4.1.2.1. DATA GATHERING

All information regarding the mixing process was much referred from books which mainly talks about mixing processes. These include information regarding the valves equation, the mixing rates, the flowrate inlet for ideal mixing, and many more.

As for this research, a water base mixing process is being chosen just for simplicity understanding. The data gathered are represented as in figure 1 and in the literature review part.

The data that is taken into consideration are as follows: -

- $f_1(t) = C_{v1}\, v\rho_1(t)\, \surd(\Delta P_1 / G_1)$
- $f_2(t) = C_{v2}\, v\rho_2(t)\, \surd(\Delta P_2 / G_2)$
- $f_3(t) = C_{v3}\, \surd(\Delta P_3(t) / G_3(t))$
- $\rho_3(t) = a_3 + b_3 c_{A3}(t)$

4.1.2.2. MATHEMATICAL MODEL DERIVITION

The data gathered above is used to develop the mathematical model. Those equations will be equated to create a mathematical model which represents the mixing process.

The mixing process simulation that will be done is a water base process where in other words the process is a process to dilute a solution. Later on, in the mathematical derivation, it will explain why the concentration of solution 2 can be cancelled out.

Two equations could be developed based on the mixing process's flow. The two equations are: -

- overall mass balance of mixing
- component mass balance of mixing

By equating both the overall mass balance and also the component mass balance, a mathematical model that corresponds to the mixing process is developed. The mathematical model of this study was obtained by: -

$$in - out = accumulation$$
$$in = \rho_1(t)f_1(t) + \rho_2(t)f_2(t)$$
$$out = \rho_3(t)f_3(t)$$
$$accumulation = \frac{d}{dt}(\rho_3 Ah)$$

$$\Rightarrow \rho_1(t)f_1(t) + \rho_2(t)f_2(t) - \rho_3(t)f_3(t) = \frac{d}{dt}(\rho_3 Ah)$$
$$\Rightarrow \rho_1(t)f_1(t) + \rho_2(t)f_2(t) - \rho_3(t)f_3(t) = A\left[h\frac{d\rho_3}{dt} + \rho_3\frac{dh}{dt}\right]$$
$$where, \frac{d\rho_3}{dt} = 0$$

$$\frac{\rho_1(t)f_1(t) + \rho_2(t)f_2(t) - \rho_3(t)f_3(t)}{A\rho_3} = \frac{dh}{dt} \quad \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots(1)$$

Component mass balance (C_A)

$$in - out = accumulation$$
$$in = f_1(t)C_{A1}(t) + f_2(t)C_{A2}(t)$$
$$out = f_3(t)C_{A3}(t)$$
$$accumulation = A\frac{d}{dt}\left[C_{A3}(t)h(t)\right]$$
$$\Rightarrow f_1(t)C_{A1}(t) + f_2 C_{A2}(t) - f_3(t)C_{A3}(t) = A\frac{d}{dt}\left[C_{A3}(t)h(t)\right]$$
$$where, C_{A2} = 0$$
$$\therefore f_1(t)C_{A1}(t) - f_3(t)C_{A3}(t) = A\left(C_{A3}\frac{dh}{dt} + h\frac{dC_{A3}}{dt}\right)$$

$$\frac{f_1(t)C_{A1}(t) - f_3(t)C_{A3}(t)}{A} = C_{A3}\frac{dh}{dt} + h\frac{dC_{A3}}{dt} \quad \text{..............................(2)}$$

Known that; ρ_3 (t) = $a_3 + b_3 C_{A3}$

$$f_1 = C_{V1}\rho_1(t)V\sqrt{\frac{\Delta P_1}{G_1}}$$

$$f_2 = C_{V2}\rho_2(t)V\sqrt{\frac{\Delta P_2}{G_2}}$$

$$f_3 = C_{V3}\sqrt{\frac{\Delta P_3}{G_3}}$$

4.1.2.3. SIMULATION USING MATLAB

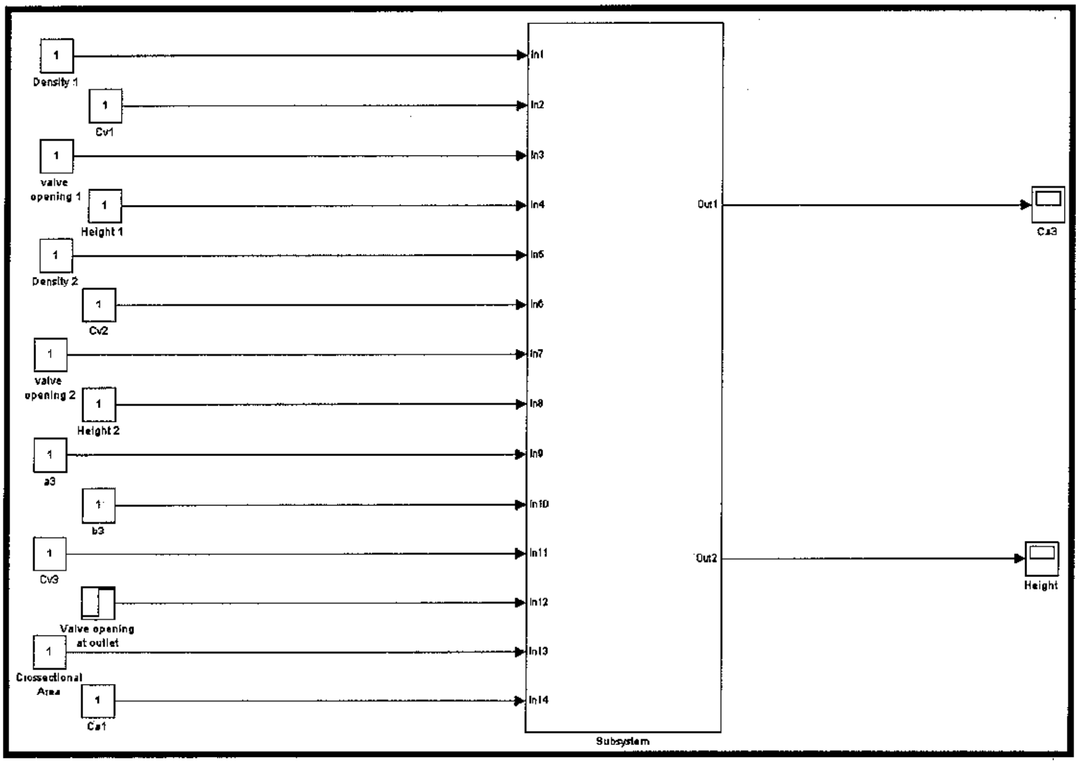


Fig. 4 Overall simulation of the process

Figure 1 shows the complete Simulink system of the mixing process. The boxes on the left hand side of the Simulink are the constant values that are needed to be keyed in. the values needed are: -

- density of solution to be diluted
- control valve 1 value
- valve 1 opening
- height of valve 1
- density of water (1 kg/m^3)
- control valve 2 value
- valve 2 opening
- height of valve 2
- cross-sectional area of tank
- concentration of solution to be diluted
- range of valve opening at the outlet of tank

Those are the constant values that are needed to be keyed into in order for the simulation to work.

Meanwhile, in figure 1 also shows the subsystem of the Simulink before the output results is obtained through graph results for concentration outlet (concentration 3) and solution level inside the tank. The subsystem consists of process flow which subsequently developed from the combination of the mathematical equations.

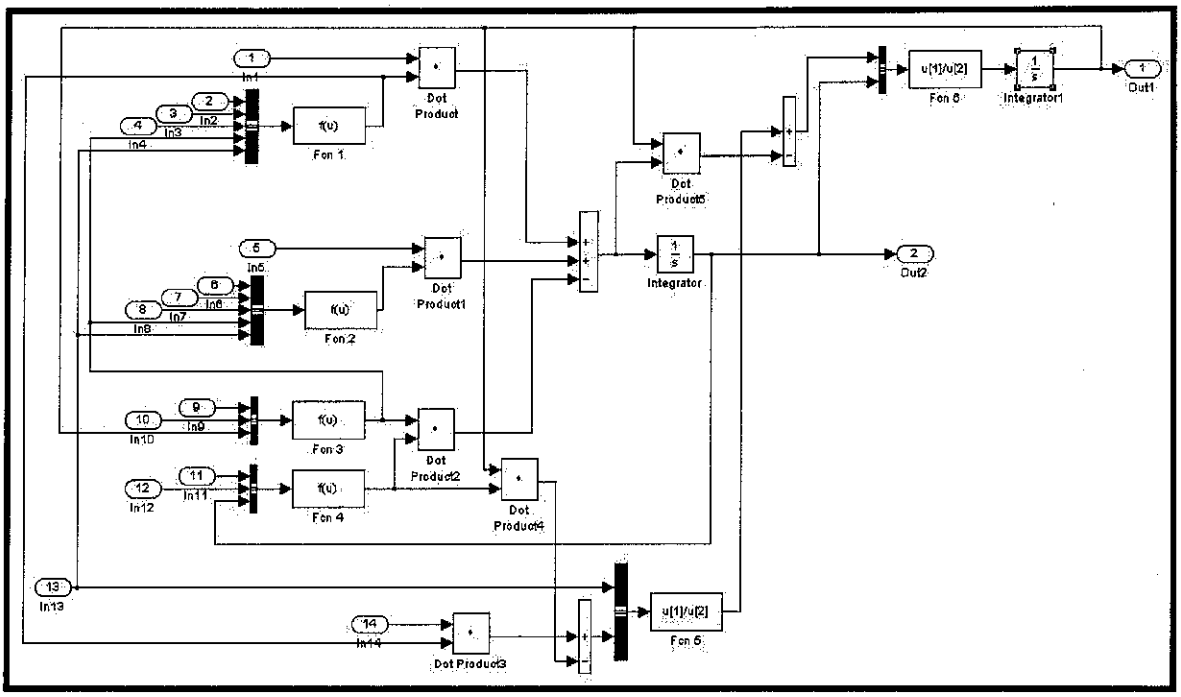


Fig. 3 Simulation process flow using Simulink in Matlab.

Figure 3 shows the inside of the subsystem. Basically the subsystem consists of developed mathematical model based on the derived mathematical equation above. This Simulink process flow shows both equated overall mass balance and also component mass balance.

In order to connect all the flows of the mathematical model is by making the mathematical model itself by using the Simulink terms. In another word, writing the mathematical model in terms of Simulink process.

Meanwhile, the PID controller for later use of automatic process control can be done by adjusting a little bit on the overall simulation process. By adding a PID controller device, the process now is already converted into automatic mode.

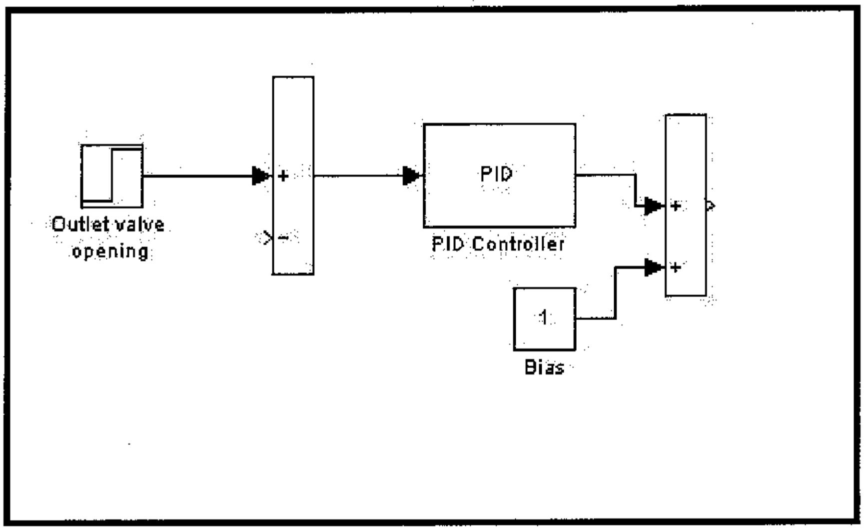


Fig. 5 PID Control Model

Figure 5 shows the PID controller model that is to be attached to the overall flow of the simulation. When this model is attached to the overall simulation model, the simulation now is called the automatic process control model. This is where the PID values are used to ensure the best controlling process.

Figure 6 shows the completed automatic simulation model. The automatic control model is attached through the input of outlet valve opening.

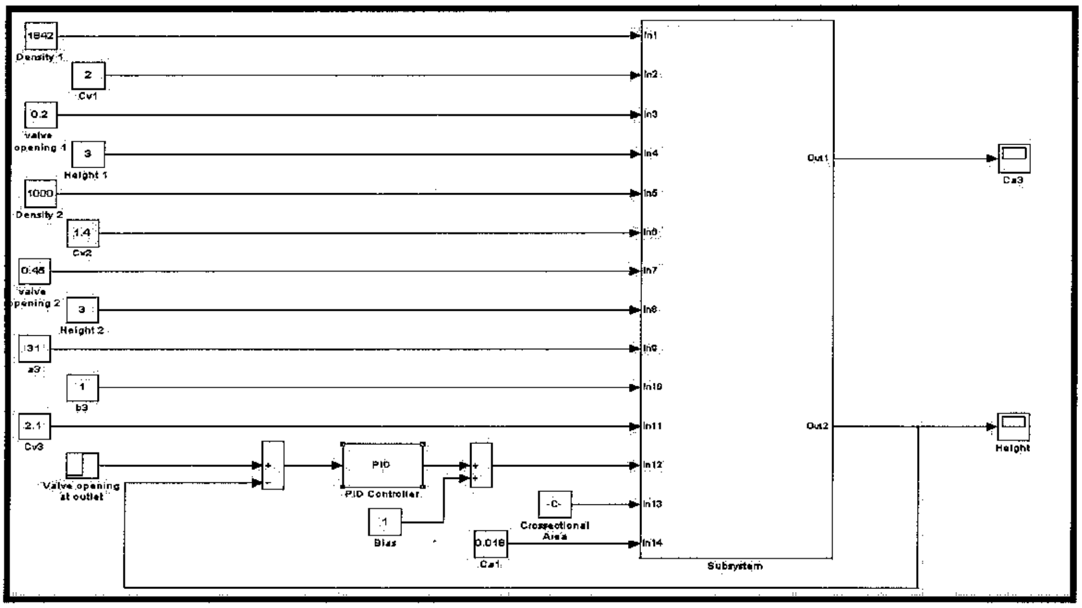


Fig. 6 Completed simulation process model

4.1.2.4. RESPONSES CHARATERIZATION STUDIES

Response characterization is obtained in graph form as results of using the simulation of the modeling. Basically, the trend line is studied in order to determine which of the best tuning control or method to be used to control the process.

Those resulting graph obtained is used to determine the values of gain value, time delay and also the time constant. Based on the calculated values, then it is easier to determine the best approach to be used to control the process.

In finding the appropriate control tuning using P, PI and PID there are a few methods that can be used to determining it. Among of the methods are The Ziegler and Nicholas method, Cohen Coon method, Decay Ratio method and others.

These are some examples of determining or calculating the PI and D values: -

i) Ziegler Nichols PID Tuning

Ziegler and Nichols have developed PID tuning methods back in the early forties based on open loop tests (less known than for example the Cohen-Coon formulas) and also based on a closed loop test, which is maybe their most widely known achievement.

The open loop method allows calculation of PID parameters from the process parameters. The procedures can be explained as below:

Step 1: Make an open loop plant test (e.g. a step test)

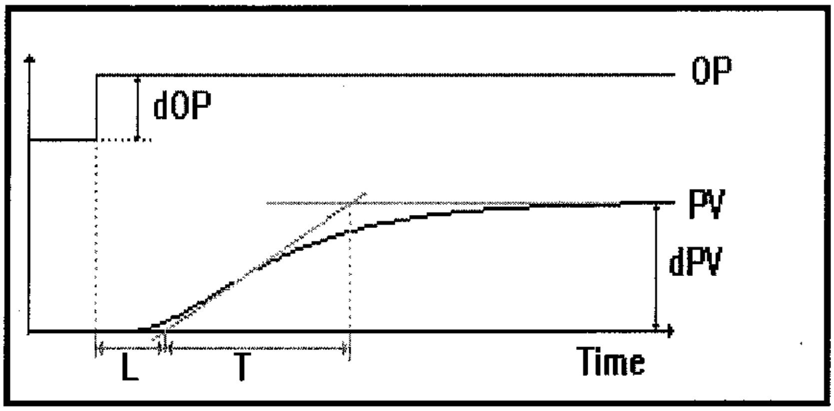
Step 2: Determine the process parameters: Process gain, time delay, time constant (see below: draw a tangent through the inflection point and measure L and T as shown.)

Step 3: Calculate the parameters according to the following formulas:

K = time constant / (process gain * time delay)

PI: Proportional gain = 0.9 * K, integral time = 3.3 * time delay

PID: Proportional gain = 1.2 * K, integral time = 2 * time delay, derivative time = 0.5 * time delay



Graph (ii) Tuning Procedure

Process gain = dPV / dOP, time delay = L, time constant = T

The closed loop method prescribes the following procedure:

Step 1: Disable any D and I action of the controller (--> pure P-controller)

Step 2: Make a set point step test and observe the response

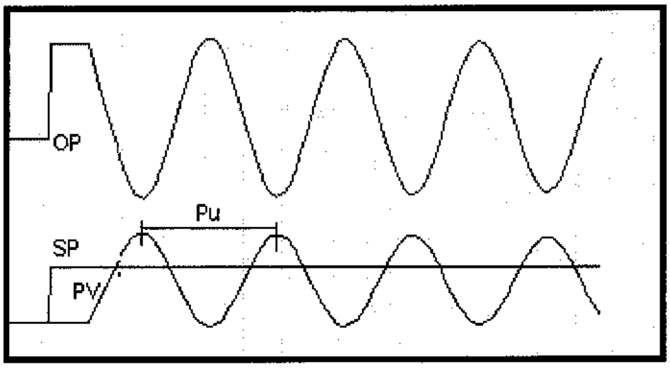
Step 3: Repeat the SP test with increased / decreased controller gain until a stable oscillation is achieved. This gain is called the "ultimate gain" Ku.

Step 4: Read the oscillation period Pu.

Step 5: Calculate the parameters according to the following formulas:

PI: Proportional gain = 0.45 * Ku, integral time =Pu / 1.2

PID: Proportional gain = 0.6 * Ku, integral time =Pu / 2, derivative time = Tu / 8



Graph (iii)   Ziegler Nichols test

Characterization:

Both methods give a good starting point but require further fine-tuning. The open loop method is based on a measurement range of 0-100 and continuous control. This requires adjustments for other measurement ranges and for the control interval in digital systems (the method was developed in the times when only analog controllers existed).

The closed loop methods does not require adjustments, a big advantage, since both process and controller are part of the test, but suffers from one major disadvantage: Bringing the loop into stable, sustained oscillation is simply out of the question for industrial processes.

Both methods are not determined between set point and load tuning and it is for self-regulating processes only, not for integrating processes like liquid level.

ii) Cohen Coon Tuning Method

Steps of using Cohen Coon tuning method:

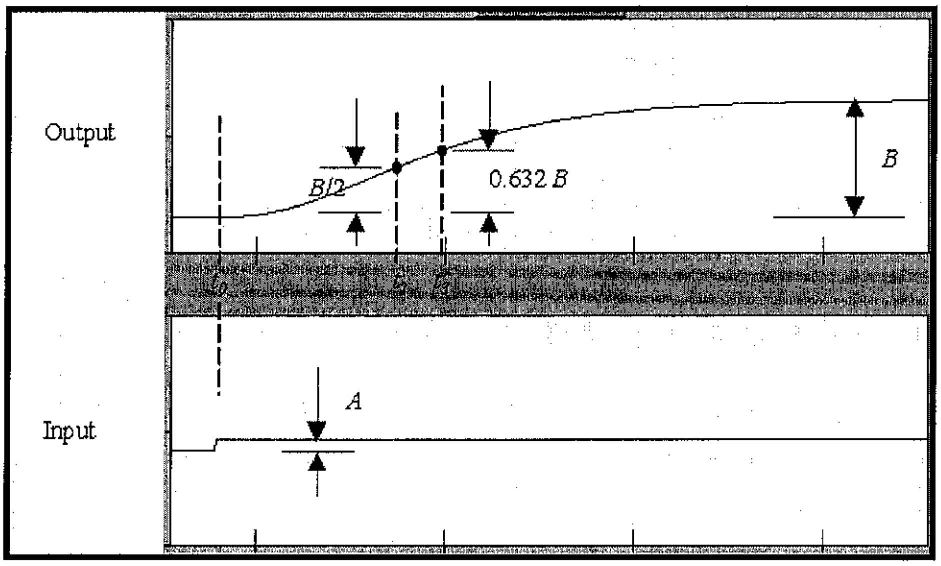
1. Under Manual mode, wait until the process is at steady state.
2. Next, introduce a step change in the input.
3. Based on the output, obtain an approximate first order process with a time constant t delayed by t_{DEL} units from when the input step was introduced.

The values of t and t_{DEL} can be obtained by first recording the following time instances:

t_0 = time when input step was initiated

t_2 = time when half point occurs

t_3 = time when 63.2% point occurs



Graph (iv) Step graph and t determination

4. From the measurements based on the step test: t_0, t_2, t_3, A and B, evaluate the following process parameters:

$$t_1 = (t_2 - \ln(2)\, t_3)/(1 - \ln(2))$$

$$\tau = t_3 - t_1$$

$$\tau_{\mathrm{DEL}} = t_1 - t_0$$

$$K = B/A$$

5. Based on the parameters K, τ and τ_{DEL}, the following formulas prescribe the controller parameters K_c, t_I and t_D:

	K_c	t_I	t_D
P	$\frac{1}{K\cdot r}\cdot\left(1+\frac{r}{3}\right)$		
PI	$\frac{1}{K\cdot r}\cdot\left(0.9+\frac{r}{12}\right)$	$\tau_{\mathrm{DEL}}\cdot\frac{30+3\cdot r}{9+20\cdot r}$	
PID	$\frac{1}{K\cdot r}\cdot\left(\frac{4}{3}+\frac{r}{4}\right)$	$\tau_{\mathrm{DEL}}\cdot\frac{32+6\cdot r}{13+8\cdot r}$	$\tau_{\mathrm{DEL}}\cdot\frac{4}{11+2\cdot r}$

where $r = \frac{\tau_{\mathrm{DEL}}}{\tau}$

4.2. TOOLS USED

Matlab and HYSIS are the software used in order to complete this simulation. The simulation is done using the Matlab software. Meanwhile HYSIS program is used to gather information regarding chemical physical properties.

There are many more ways to get information regarding chemical properties; using HYSIS is one of it. As long as the properties can be obtained, it could be used in the simulation regardless from where it is gained.

4.2.1. MATLAB SIMULATION SOFTWARE

MATLAB is a high-performance language for technical computing. It integrates computation, visualization, and programming in an easy-to-use environment where problems and solutions are expressed in familiar mathematical notation. Typical uses include:

- Math and computation
- Algorithm development
- Modeling, simulation, and prototyping
- Data analysis, exploration, and visualization
- Scientific and engineering graphics
- Application development, including graphical user interface building

MATLAB is an interactive system whose basic data element is an array that does not require dimensioning. This allows you to solve many technical computing problems, especially those with matrix and vector formulations, in a fraction of the time it would take to write a program in a scalar non-interactive language such as C or Fortran.

MATLAB has evolved over a period of years with input from many users. In university environments, it is the standard instructional tool for introductory and advanced courses in mathematics, engineering, and science. In industry, MATLAB is the tool of choice for high-productivity research, development, and analysis.

MATLAB features a family of application-specific solutions called toolboxes. Very important to most users of MATLAB, toolboxes allow you to learn and apply specialized technology. Toolboxes are comprehensive collections of MATLAB functions (M-files) that extend the MATLAB environment to solve particular classes of problems. Areas in which toolboxes are available include signal processing, control systems, neural networks, fuzzy logic, wavelets, simulation, and many others.

4.2.2. HYSIS SIMULATION SOFTWARE

HYSYS provides an intuitive and interactive approach toward process modeling, simulation and optimization.

This software helps to create detailed high-fidelity plant simulations for analyzing and optimizing your plant's operation. Through the completely interactive HYSYS interface, you have access to a fine level of equipment geometry, performance detail as well as the ability to completely customize your simulation using its OLE extensibility capability.

In HYSYS, all necessary information pertaining to pure component flash and physical property calculations is contained within the Fluid Package. This approach allows to define all the required information inside a single entity. There are four key advantages to this approach:

- All associated information is defined in a single location, allowing for easy creation and modification of the information.

- Fluid Packages can be exported and imported as completely defined packages for use in any simulation.

- Fluid Packages can be cloned, which simplifies the task of making small changes to a complex Fluid Package.

- Multiple Fluid Packages can be used in the same simulation.

CHAPTER 5

RESULTS AND DISCUSSION

5. RESULTS & DISCUSSION

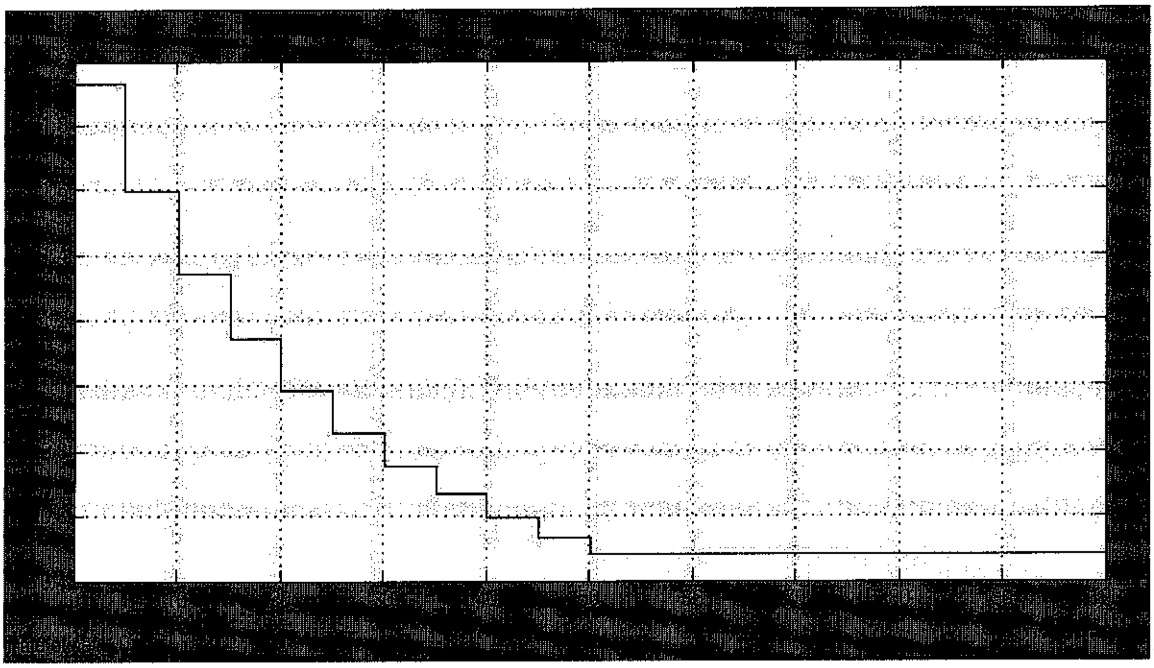
To study the corresponding results of the responses, the simulation will be tested. The simulation should be compared by varying the values of height of inlet flow and valve opening of inlets and outlets.

Putting this simulation into a test, sulfuric acid will be used as the solution to be diluted with water. The properties of the sulfuric acid are obtained through using HYSIS software.

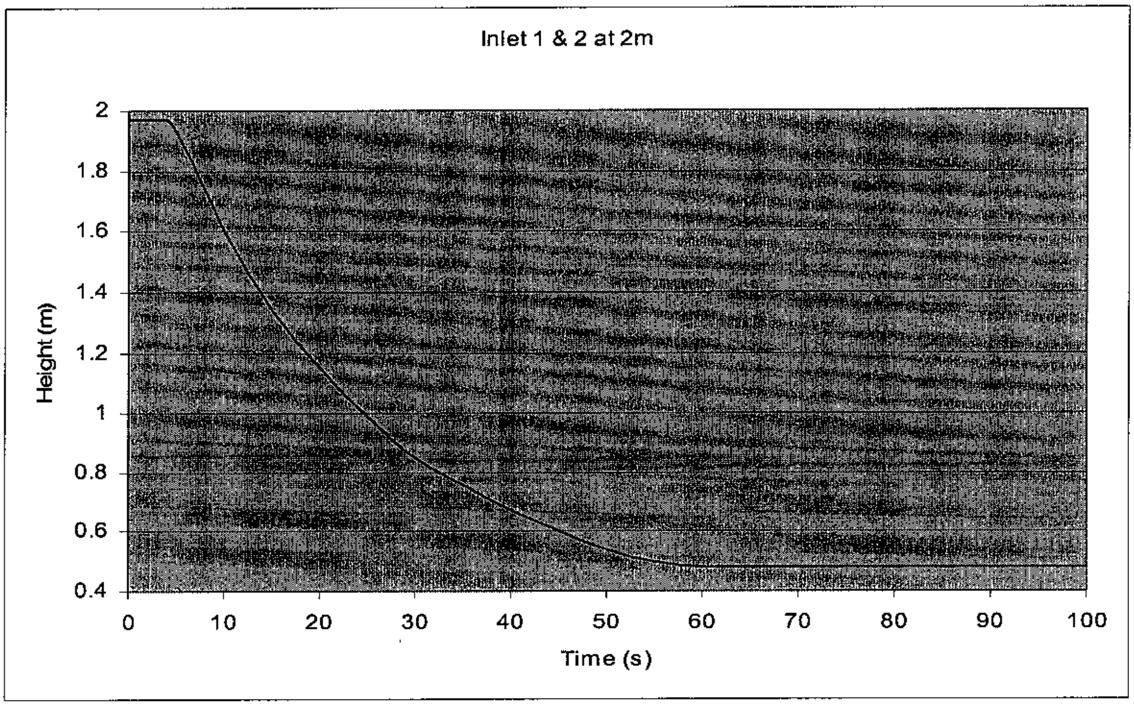
The cross-sectional tank area will be taken in a small scale as in the laboratory's mixing tank of 0.7855 m^2 and the height of inlet flow from the bottom of the tank would be at varied at 1m to 2 m of both inlets.

Meanwhile, the control valve value for both 1 and 2 are calculated based on the equation $f_1(t) = C_{v1}\, v\rho_1(t) \sqrt{(\Delta P_1 / G_1)}$ and $f_2(t) = C_{v2}\, v\rho_2(t) \sqrt{(\Delta P_2/G_2)}$

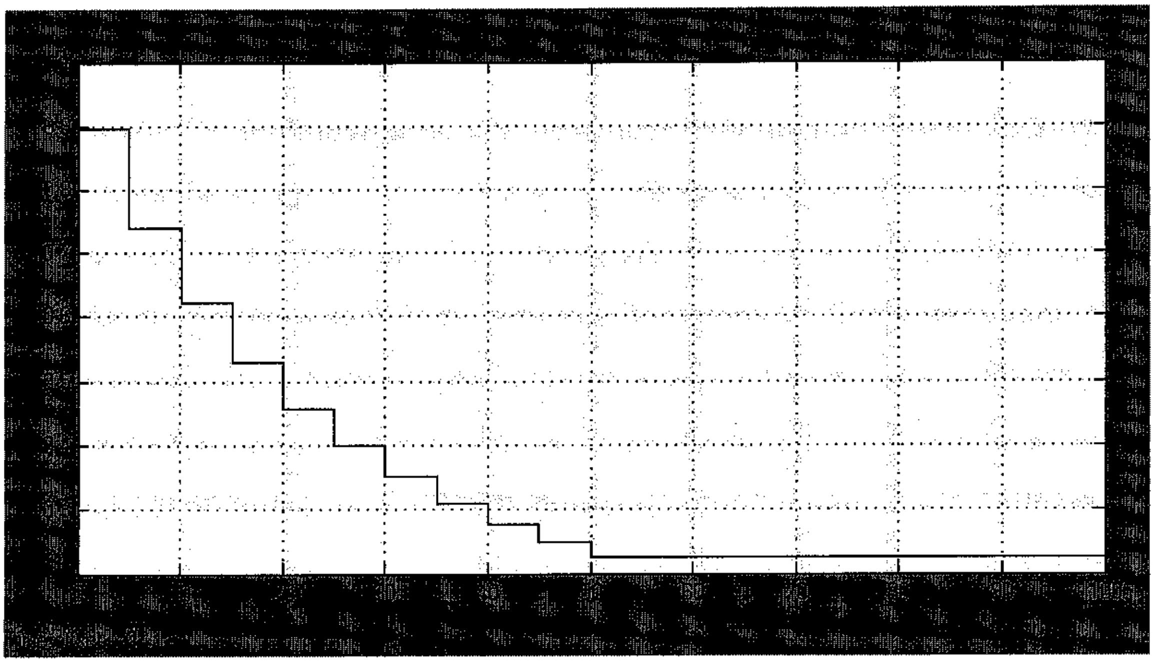
5.1. FINDINGS



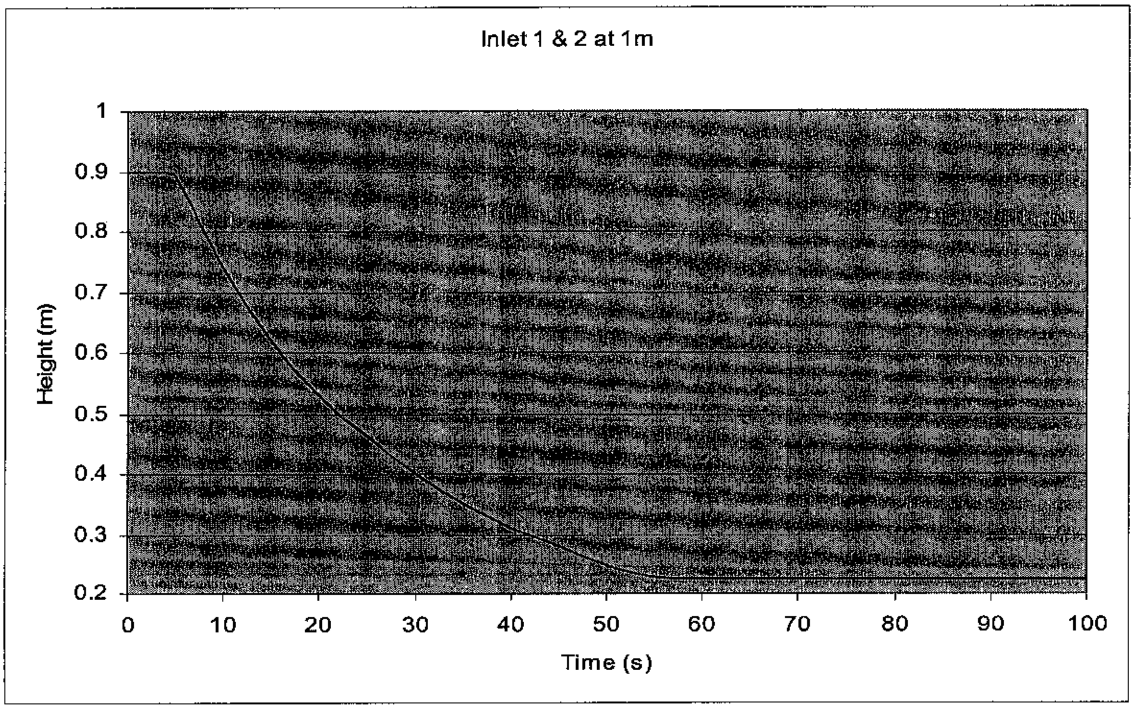
Graph 1 Height Inlet 1 & 2 at 2m



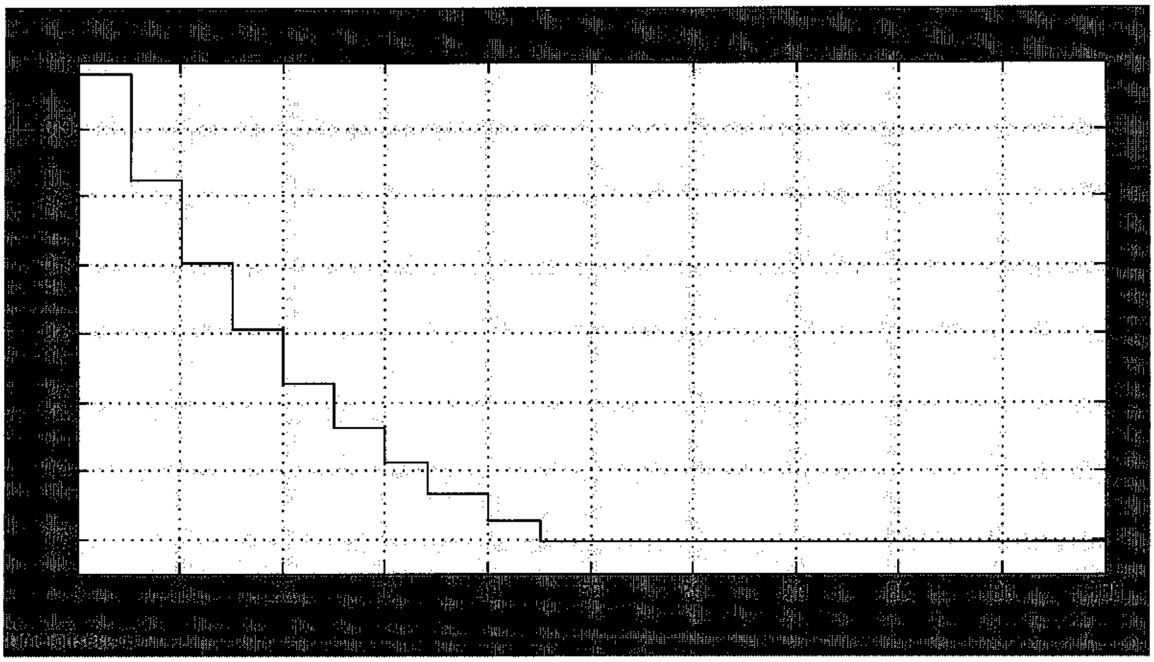
Graph (a) = Graph 1



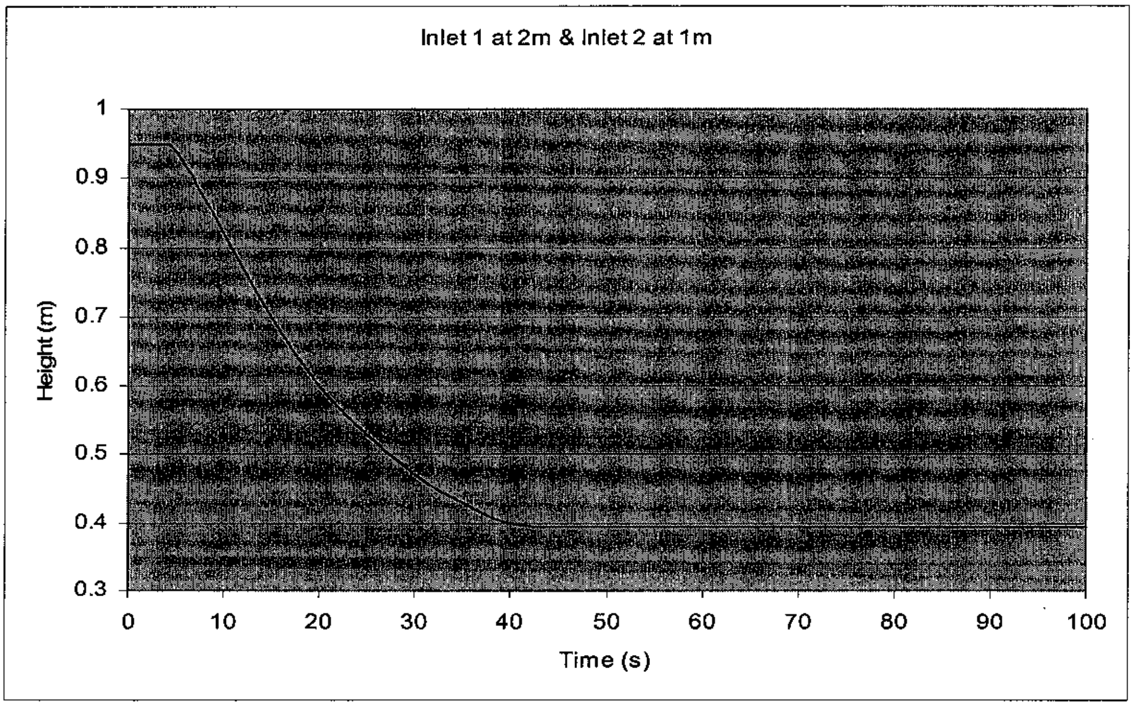
Graph 2 Height Inlet 1 & 2 at 1m



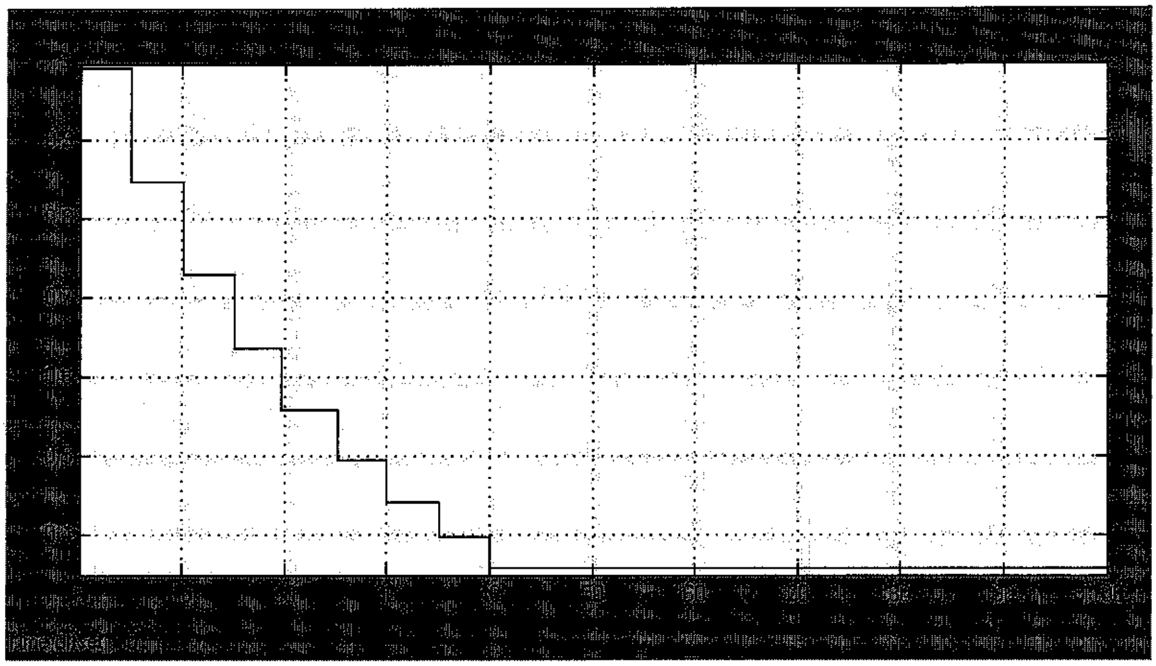
Graph (b) = Graph 2



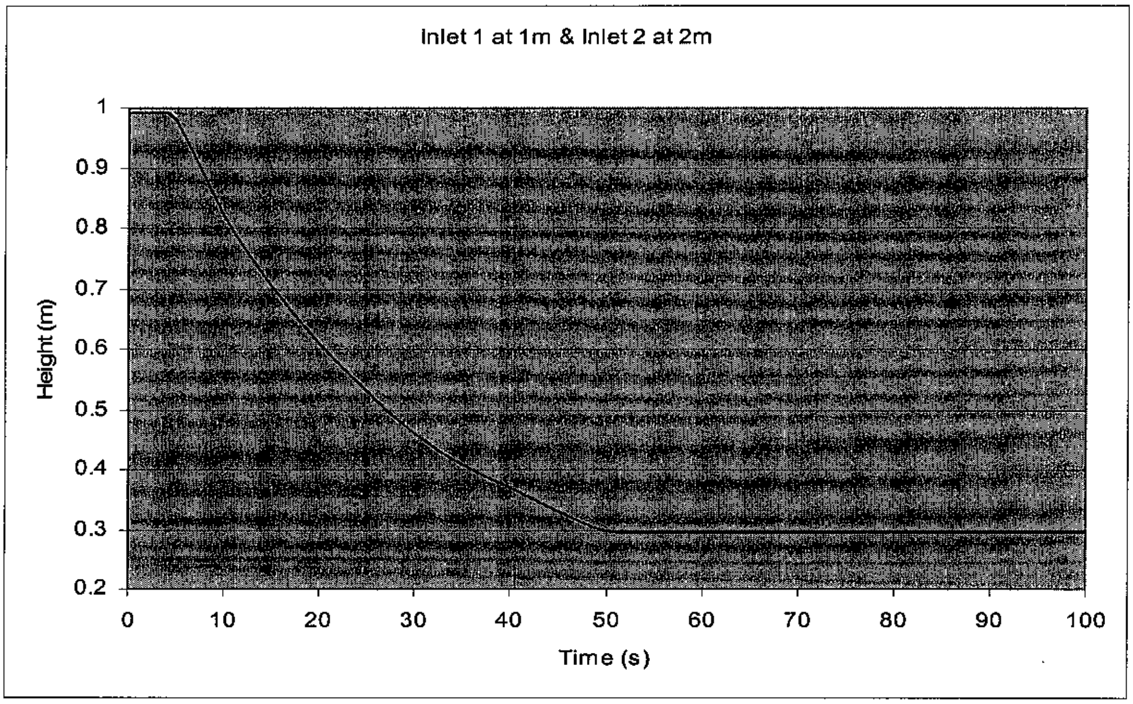
Graph 3 Height 2m inlet 1 & 1m inlet 2



Graph (c) = Graph 3



Graph 4 Height 1m inlet 1 & 2m inlet 2



Graph (d) = Graph 4

Looking into all graphs 1, 2, 3 and 4 it shows a sampled-data graphs. Similarly, the graphs show that the level inside the tank decreases before it settles down on a constant value. Meanwhile, graph (a), (b), (c) and (d) is the graph representing the sampled-data graphs which have been re-plotted.

Basically, the graph obtained through decreasing the outlet valve opening within average range between half opening (50%) to full opening (100%) by increment of 5% each.

5.2. DISCUSSION

In order to find the values of time constant, gain value and the time delay value, it can be calculated by simple equations. Where time delay can be find from graph by finding the best slope line. Meanwhile, gain value can be calculated by Δy (output)/ Δx (input) and lastly, time constant can be find by using the multiplying 63.2% of Δy.

The results obtained from calculated gain value, time constant and time delay are as follows: -

Graph	**a**	**b**	**c**	**d**
K	-0.98	-1.35	-1.39	-1.54
τ	19	19.5	15	19
τ_D	1	1	1	1

Based from these above values, the proportional, integral and also the derivative value can be determined. The values than can be used to initiate the PID controller so that the process can be controlled. There a re several ways to find the PID values, and among of the methods that will be used are the Cohen Coon method, ITAE method, IAE method, Quarter Decay Ratio and Ziegler Nichols method.

The calculated values of proportional, integral and also derivative are as shown below.

For graph (a): -

Cohen Coon

k	-0.98
τ	19
t_0	1

controller	P	PI	PID
Kc	-19.7279	-17.5340	-26.1054
τ_I		3.0000	2.4078
t_D			0.3602

IAE

controller	PI	PID
Kc	-9.7600	-14.3166
τ_I	18.9432	25.9153
t_D		0.4483

Decay Ratio

controller	P	PI	PID
K'c	-19.3878	-17.4490	-23.2653
τ'_I		3.3300	2.0000
t'_D			0.5000

Kc	-19.388	-17.449	-29.082
τ_I		3.3300	2.5000
t_D			0.4

ITAE

controller	PI	PID
Kc	-8.8718	-24.8583
τ_I	18.6035	24.1036
t_D		0.3794

For graph (b): -

Cohen Coon

k	-1.35
τ	19.5
t_0	1

controller	P	PI	PID
Kc	-14.6914	-13.0617	-19.4444
τ_I		3.0077	2.4092
t_D			0.3603

IAE

controller	PI	PID
Kc	-7.2453	-10.6301
τ_I	19.4332	26.5909
t_D		0.4493

Decay Ratio

controller	P	PI	PID
K'c	-14.4444	-13.0000	-17.3333
τ'_1		3.3300	2.0000
t'_D			0.5000

Kc	-14.444	-13	-21.667
τ_1		3.3300	2.5000
t_D			0.4

ITAE

controller	PI	PID
Kc	-6.5953	-18.4505
τ_1	19.0889	24.7317
t_D		0.3801

For graph (c): -

Cohen Coon

k	-1.39
τ	15
t_0	1

controller	P	PI	PID
Kc	-11.0312	-9.7722	-14.5683
τ_1		2.9226	2.3941
t_D			0.3593

IAE

controller	PI	PID
Kc	-5.6140	-8.2194
τ_1	15.0230	20.5105
t_D		0.4393

Decay Ratio

controller	P	PI	PID
K'c	-10.7914	-9.7122	-12.9496
τ'_1		3.3300	2.0000
t'_D			0.5000

Kc	-10.791	-9.7122	-16.187
τ_1		3.3300	2.5000
t_D			0.4

ITAE

controller	PI	PID
Kc	-5.0371	-14.3188
τ_1	14.7203	19.0791
t_D		0.3731

For graph (d): -

Cohen Coon

k	-1.54
τ	19
t_0	1

controller	P	PI	PID
Kc	-12.5541	-11.1580	-16.6126
τ_I		3.0000	2.4078
t_D			0.3602

IAE

controller	PI	PID
Kc	-6.2109	-9.1106
τ_I	18.9432	25.9153
t_D		0.4483

Decay Ratio

controller	P	PI	PID
K'c	-12.3377	-11.1039	-14.8052
τ'_I		3.3300	2.0000
t'_D			0.5000

Kc	-12.338	-11.104	-18.506
τ_I		3.3300	2.5000
t_D			0.4

ITAE

controller	PI	PID
Kc	-5.6457	-15.8189
τ_I	18.6035	24.1036
t_D		0.3794

Using this calculated PID values, the process control can be done. The obtained graph results of applied calculated PID values are as shown in the appendix for P and PI. However, the simulation could not cater for any control tuning using PID. This may be due to internal reasons itself. This means the simulation itself.

The simulation itself could be said not sufficient enough as the results obtained for P and PI are all nearly similar. It is hard to be differentiated. But if observed carefully there are some differences between them. Especially, when comparing the differences between when using ITAE or IAE with using Decay Ratio or Cohen Coon. It seems that the rate to settle is much faster by using ITAE or IAE instead of using Cohen Coon or Decay Ratio.

As for explaining why the graphs for P, either using Decay Ratio or Cohen Coon method, a straight line is obtained is still unknown. The expected graph that should be obtained is a graph that exist a offset between the set point line with the 'should be' line.

Lastly, explaining why the simulation cannot cater for any PID control is because of the same reason. Either there exists errors in the simulation itself or the value used for calculation is wrong or any possible reason that may be acceptable that causes this simulation to fail.

If the theory of process control really does applied to this research project, the resulting graph would be a graph of oscillating line settling to the set point after applying the PID controller. However it seems that, this simulation developed is not applying the theory.

The most concerning part for the failure of this simulation is maybe due to errors in the simulink itself. Further detail checking is required to identify the problem which led to this unsuccessful simulation.

Theoretically, based on controlling manually and automatically using the PID control, the use of PID controller has many benefits regardless of easy to be operated. The process becomes smoother compared to manual process control.

This is because the PID controller has its very own function. Those functions are the reasons which help the process to be smoother and reluctantly optimize the process itself to the limit.

The Proportional control acts as offset eliminator. Proportional band, PB is equal to 100% / K_c, where K_c is the controller gain. Or in other words K_c = 1/ PB. As K_c increases, the offset will reduce however, it would begin to oscillate.

Meanwhile the purpose of Integral control is also to eliminate offset. The integral mode will repeat the proportional mode until the error is zero. However, this integral mode will cause oscillatory which lead to instability.

That is where derivative control will do its job. Derivative control will tend to stabilize the controlled process. The control will help improve dynamic by decreasing the settling time. It could also be used to counteract the destabilizing tendency of the integral mode.

CHAPTER 6

CONCLUSSION AND RECOMMENDATIONS

6. CONCLUSION & RECOMMENDATIONS

6.1. CONCLUSION

This research project is a 1 semester project. At the end of this research, we would be able to have a simplified dynamic model and simulation of a first order reaction of a mixing process.

At this point of time, the progress has come to the completion of the dynamic modeling and the simulation itself. However, the resulting of the simulation was not meet to expectation. There is still some more modification need to be done, for the successful of the simulation. For this time being, the simulation is not ready to be used in manual mode or manual tuning for application in the real world. Not as long as the problems occurred for the simulation is resolved.

This research project has not completely finished yet. However basically the objectives have been achieved where: -

- A mathematical model has been developed where the model is actually the reference of a mixing process.

- The characterization response has been studied where eventually the gain value, time constant and also the time delay has been obtained.

6.2. RECOMMENDATION

- It is recommended that to develop this simulation may requires more time in order to obtained better simulation.

- This simulation may be used for industrial purposes. In order to improve the simulation to a higher performance level, a team work may be needed to rectify any problems occur.

- The simulation can be more simplified with tabulated data regarding the valve characteristics values for easier use in the future.

- Further detailed checking of the simulation is needed to rectify the problem or any other problem that may occur in future.

- The next person to continue this research is needed to make close contact with the previous person in charge of the research and also the supervisors for information exchange as this project is quite tedious to be completed and also needed extra attention to the specific information especially regarding the simulation itself.

CHAPTER 8

REFERENCE

The formats of references for the sources are as below:

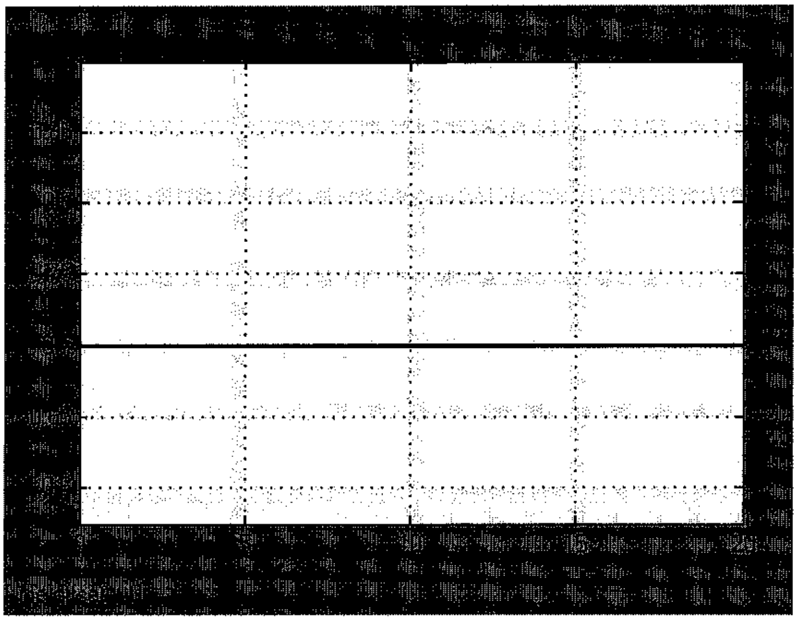
1. Dale E. Seborg, Thomas F Edgar, Duncan A. Mellichamp, 1989, Process Dynamics and Control, (105), John Wiley & Sons

2. Carlos A. Smith, Armando B. Corripio, 1997, Principles and Practice of Automatic Process Control, Second Edition, (128), John Wiley & Sons

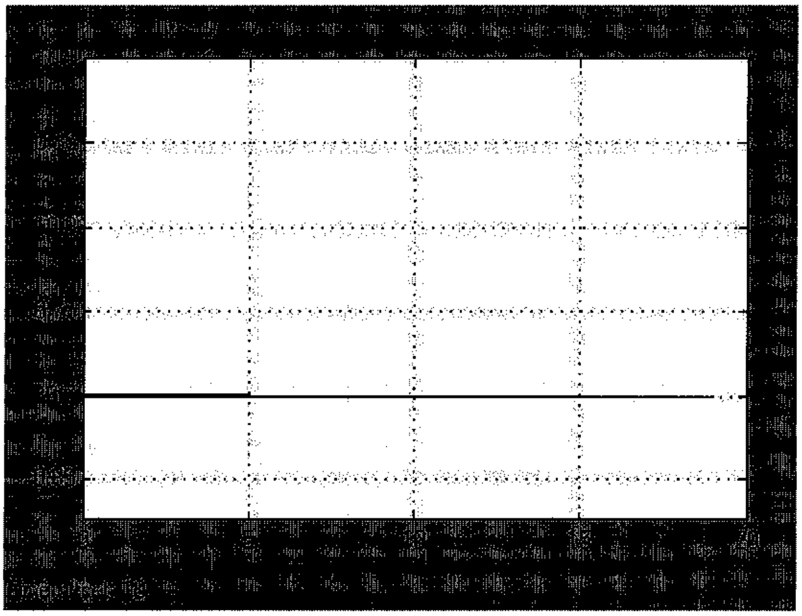
3. http://www.sciencedirect.com/science_Chemical_Engineering_Science_Mixing_of_viscous_liquid_mixtures

APPENDICES

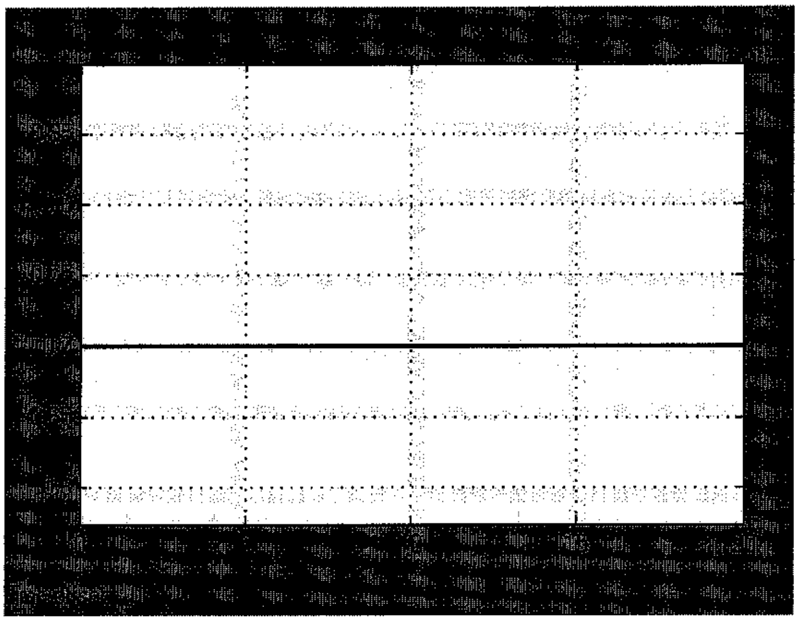
Graphs for P



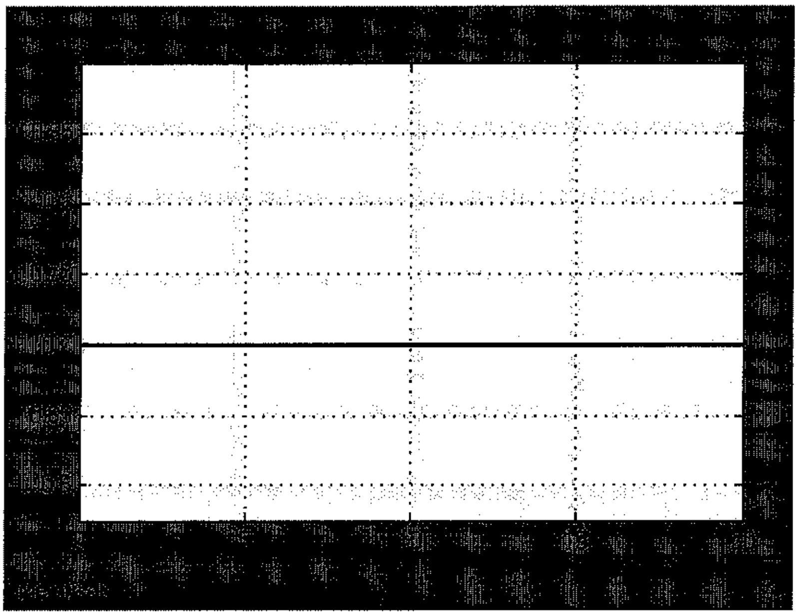
Cohen Coon (graph a)



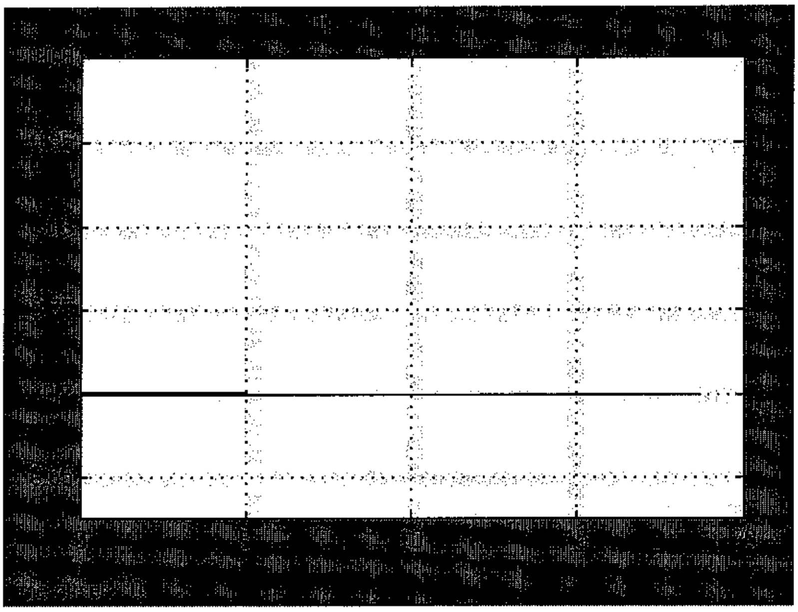
Cohen Coon (graph b)



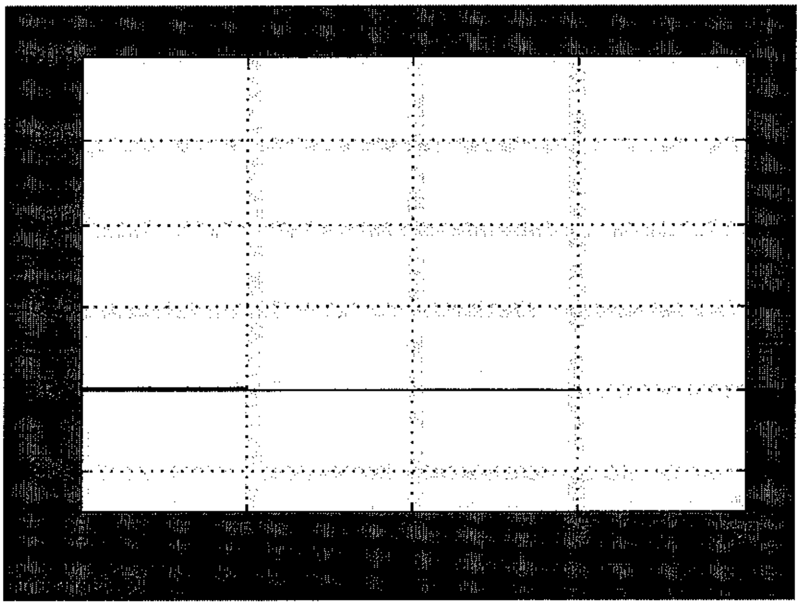
Cohen Coon (graph c)



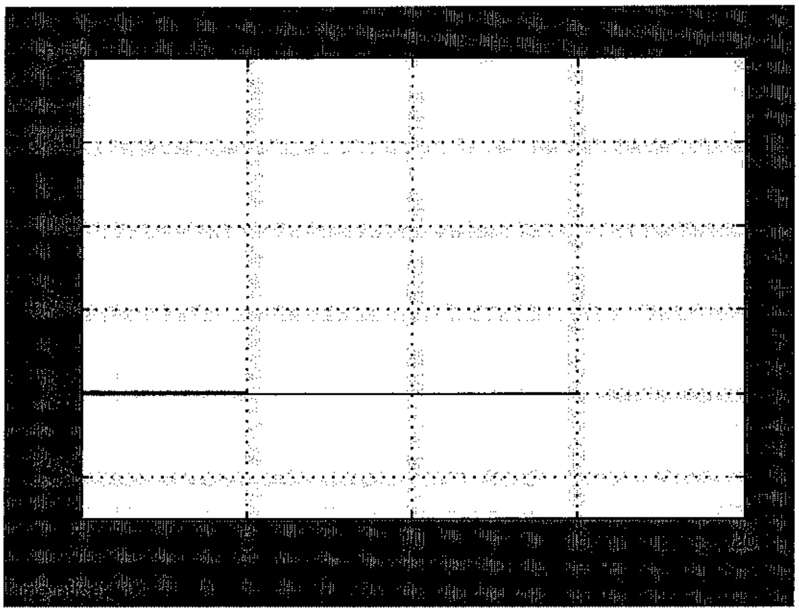
Cohen Coon (graph d)



Decay Ratio (graph a)



Decay Ratio (b)



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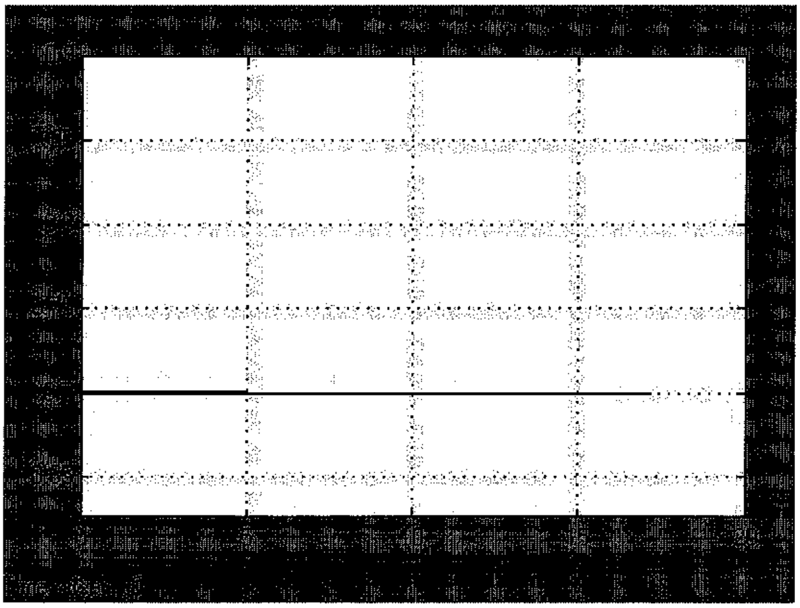
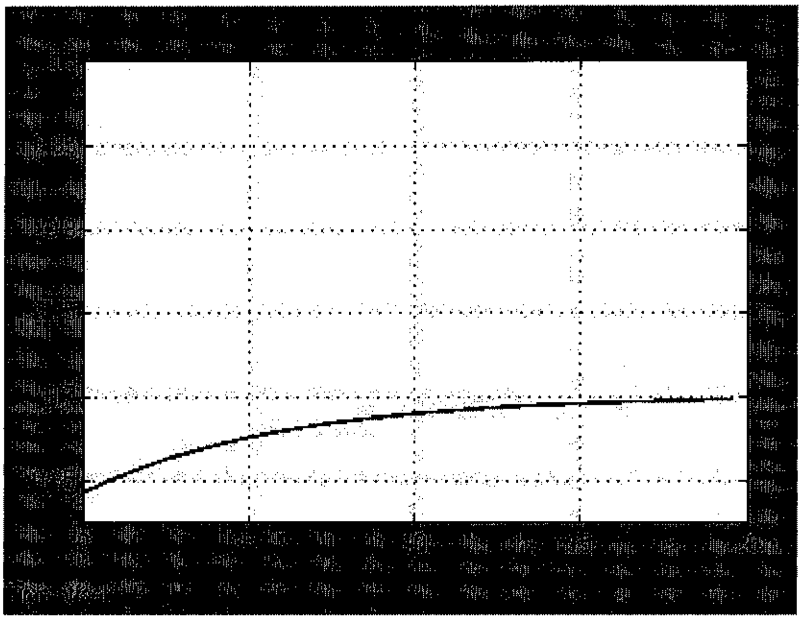
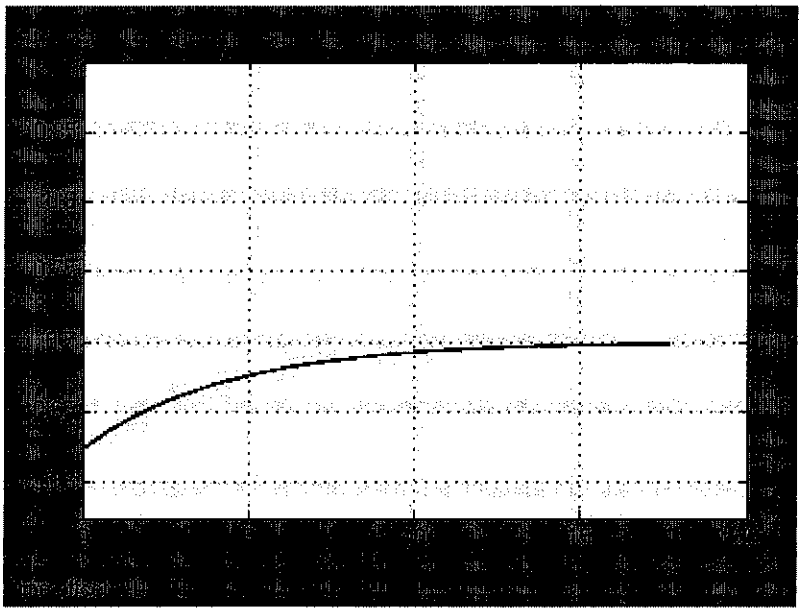


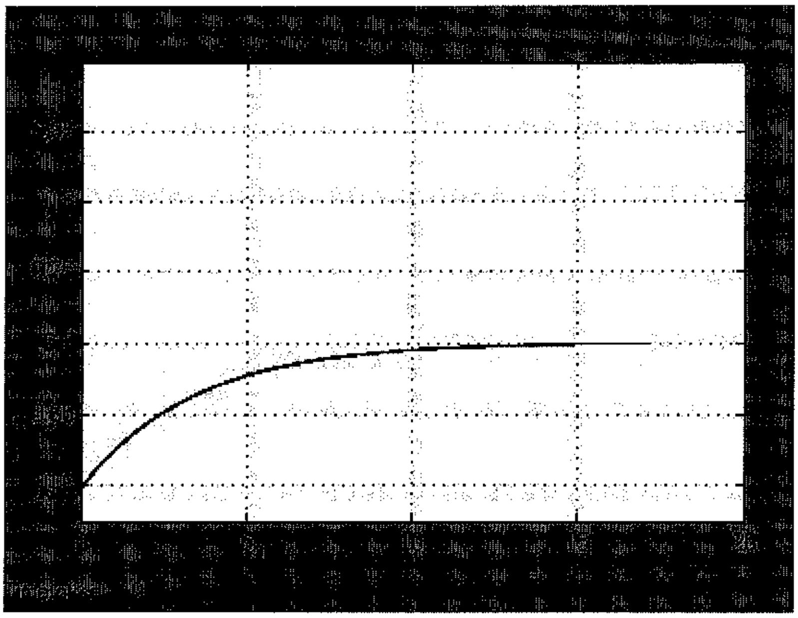
Decay Ratio (graph d)

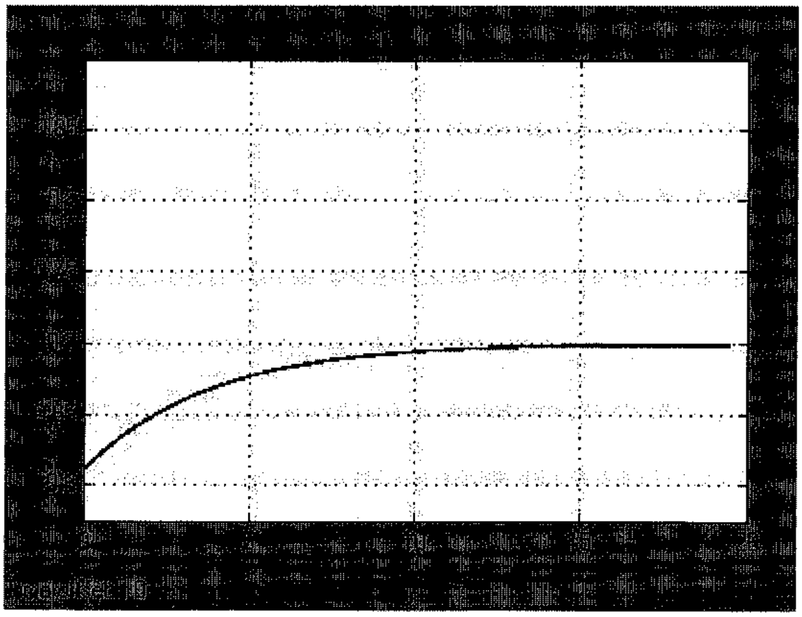
Graphs for PI

Cohen Coon graph a, b, c and d

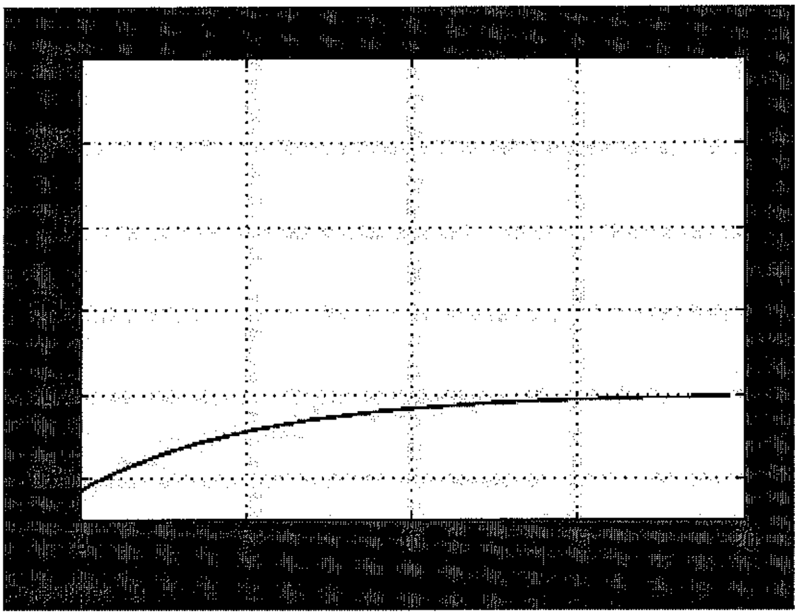


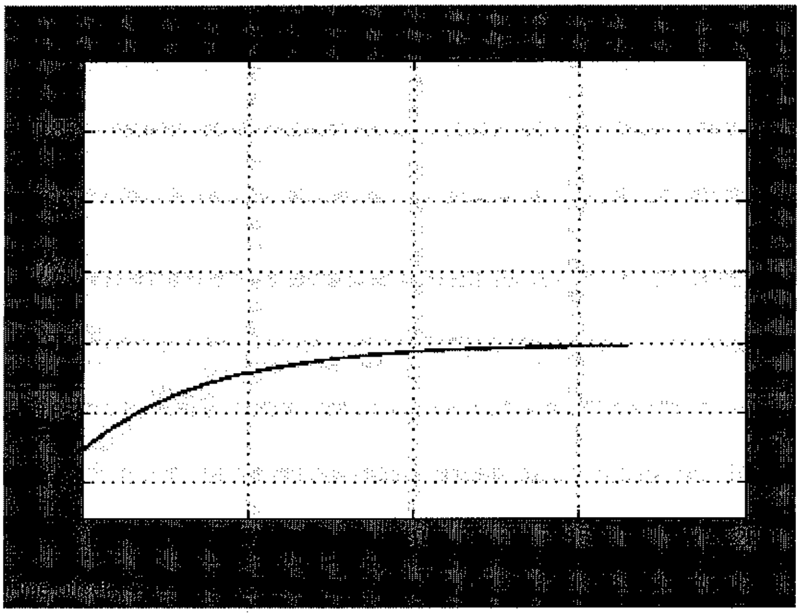


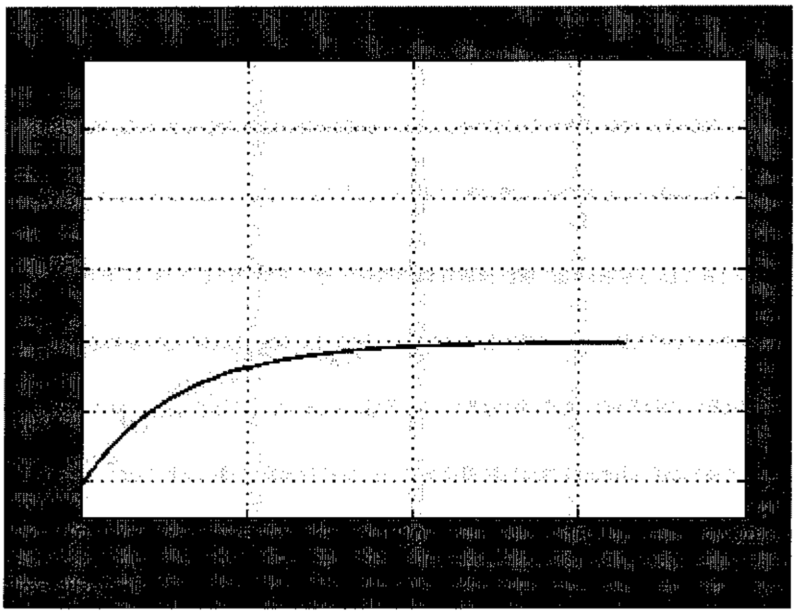


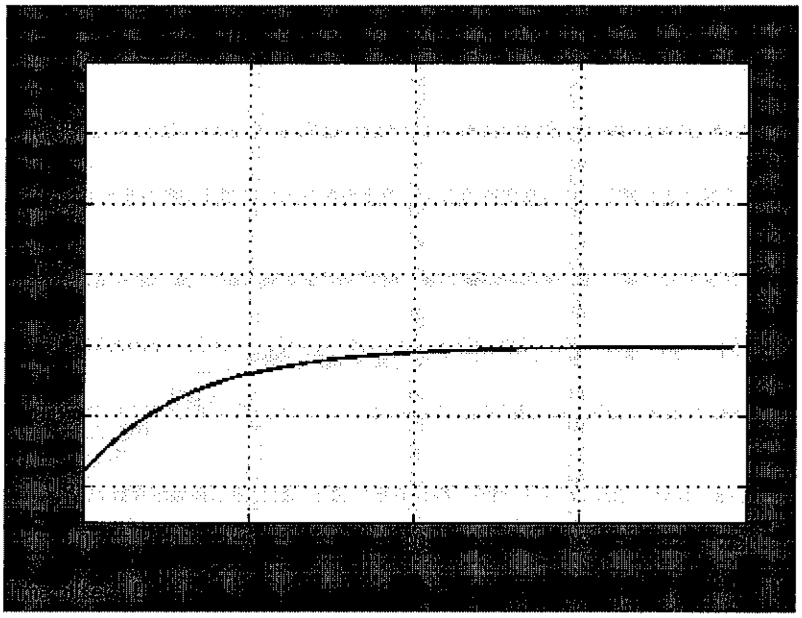


Decay Ratio for graph a, b, c and d

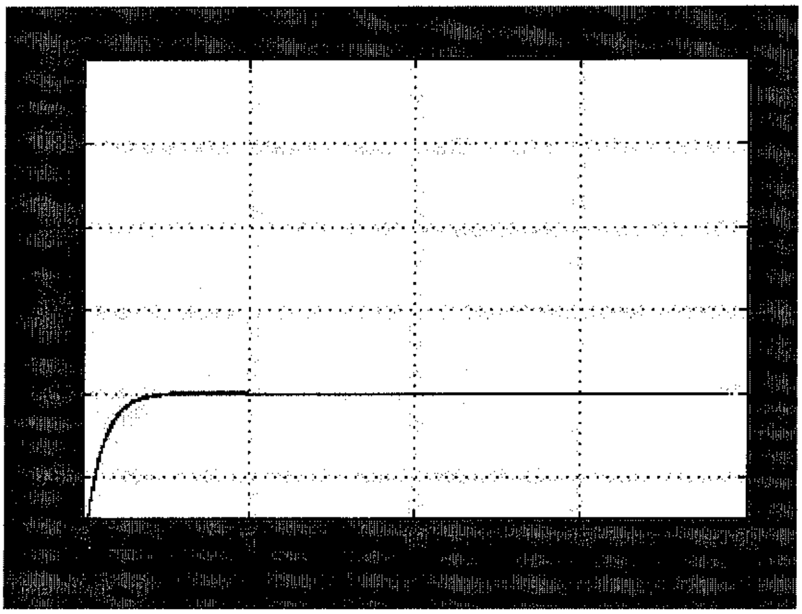


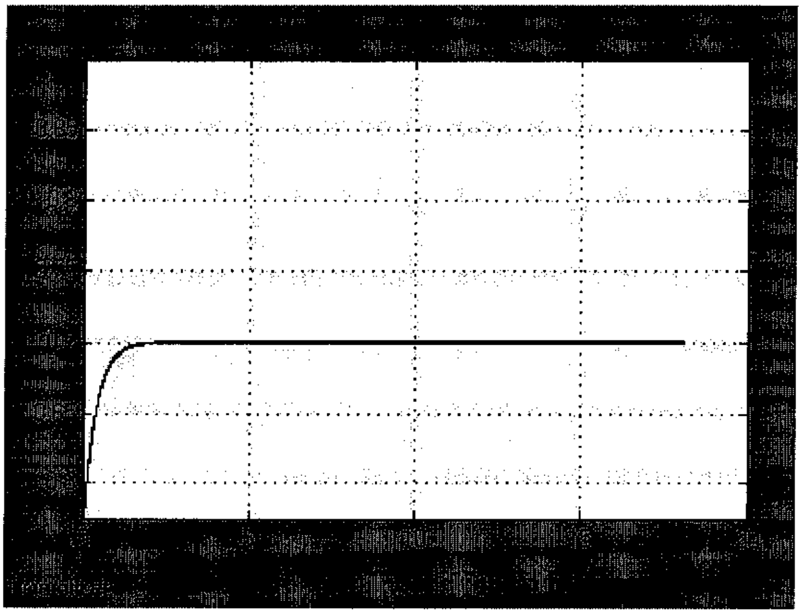


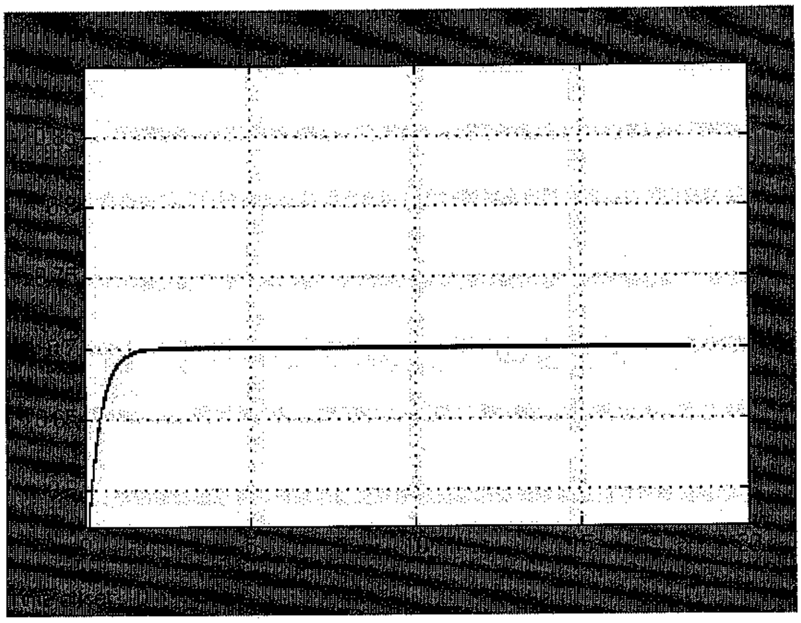


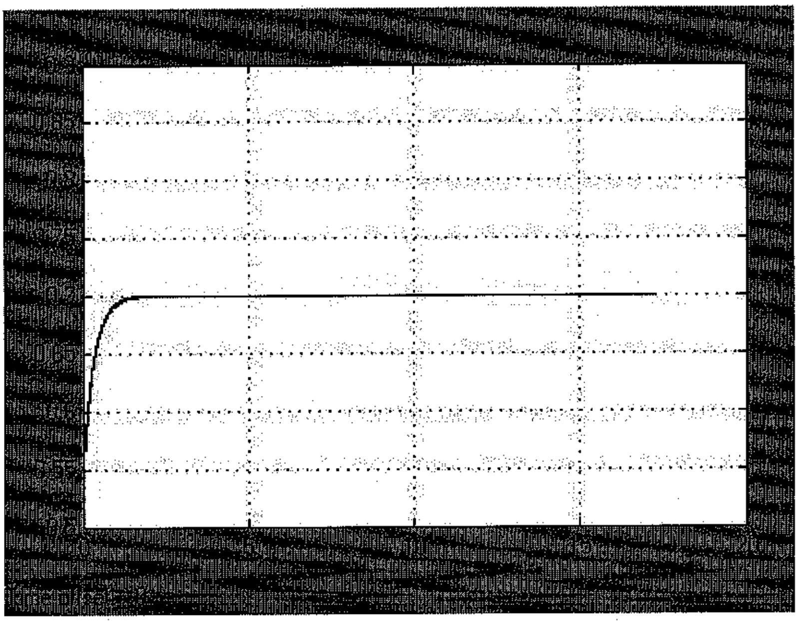


IAE for graph a, b, c and d









ITAE for graphs a, b, c and d