Dynamic Modelling and Simulation of Non Isothermal Reactors

By

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Dissertation submitted in partial fulfillment

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CERTIFICATION OF APPROVAL

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A project dissertation submitted to the
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BACHELOR OF ENGINEERING (Hons)
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Approved by,

____

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UNIVERSITI TEKNOLOGI PETRONAS

TRONOH, PERAK

May 2013

CERTIFICATION OF ORIGINALITY

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

NG PEI YING

ABSTRACT

Reactors that operate in industrial plants are non-isothermal and thus, complex dynamic nature is expected. In order to design controllers with improved control performance, there is a need to study the dynamic behaviour of non-isothermal reactors. Dynamic modelling through mathematical modelling (which involves equations of physical and chemical laws) was conducted in this research. Polymerization reactors were the focus in this research which largely relied on the model and data taken from literature.

Polymerization reactor is difficult to control due to its complicated reaction mechanism. To study its dynamic characteristics, the Melt Index of the produced polymer is controlled by manipulating the feed rates of hydrogen, $F_{in}y_{H2,in}$. This step has yielded the understanding that the quality of the polymer materials must be regulated to obtain the desired product.

The steady state gain, K is developed from the transfer function model study. Steady state gain, K increases with the step changes in feed rates of hydrogen. The outcome of the study on K indicates the polymerization reactor has non-linear behaviour.

ACKNOWLEDGEMENTS

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ABBREVIATIONS AND NOMENCLATURES

A	area of heat transfer (m^2)
C	reaction conversion
C_p	heat capacity of monomer (kJ/kgK)
F	outlet flow rate from the reactor (kg/h)
F_{in}	inlet flow rate to the reactor (kg/h)
$\Delta H_{R,p}$	heat of polymerization (MJ/kg)
k_d	deactivation constant (l/h)
k_p	propagation constant (m^3/kg_{cat} h)

m	total mass inside the reactor (kg)
MI_i	instantaneous melt index (l/h)
MI_c	cumulative melt index (l/h)
M_w	weight average molecular weight (kg/kmol)
P_n	number average degree of polymerization
R_d	catalyst deactivation reaction rate (kg/m^3h)
R_{H2}	average hydrogen reaction rate (m^3/kg_{cat} h)
R_p	propagation reaction rate (kg/h)
t	process time (h)
T	reactor temperature (K)
T_j	jacket temperature (K)
U	heat transfer constant (MJ/h m^2 K)
V	reactor volume (m^3)
X	hydrogen molar ratio
y_c	active catalyst mass fraction (kg/kg)
y_d	deactivated catalyst concentration (kg/kg)
y_{H2}	hydrogen mass fraction (kg/kg)
y_m	monomer mass fraction in the reactor (kg/kg)
y_p	polymer mass fraction in the reactor (kg/kg)

Greek symbols

ρ	density of reaction mixture (kg/m^3)
ρ_m	monomer density (kg/m^3)

CHAPTER 1

INTRODUCTION

1.1 Background of Study

Industrial reactors that operate in process plants in general are non-isothermal. Some typical examples are reformer, catalytic reactor, hydrocracking reactor and polymerization reactor. They normally exhibit a complex dynamic behaviour. In this paper, the author focused on polymerization reactor which designed to produce propylene. There are various distinguishing characteristics of polymerization reactors – the main one being their complex dynamic behaviour. To capture the dynamic characteristic of polymerization reactors accurately, modelling and simulation studies on the dynamics of such reactors are to be conducted. In addition, this assists the design of appropriate controllers.

1.2 Objective

The main objective of this study is to investigate the dynamic behaviour of non-isothermal reactors in order to design controllers with improved control performances. Specifically, polymerization reactor has been selected as the case study.

1.3 Problem Statement

Non-isothermal reactors are widely used in process plants. Due to their non-isothermal nature, the reactors always demonstrate complex dynamic behaviour. Typically, the heat produced or consumed by the reaction is incomplete, just as the term “non-isothermal” suggests. In the design of a reactor, controllers need to be taken into consideration as well because they are important for controlling the system. The characteristic of the non-isothermal reactor need to be captured accurately to ensure correct reactor design.

Complex dynamic behaviour is one of the major characteristics of the polymerization reactor. Polymerization reactors are difficult to control due to their complicated reaction mechanisms. Besides, polymer industries do not have enough on-line measurement technology for polymer variables. The quality of the polymer materials such as the melt index need to be controlled to ensure the product properties are as desired.

1.4 Scope of Study

The scope of study based on the objectives can be simplified as follows:

i) Developing the first principle model
ii) Simulating the model
iii) Dynamic study for non-isothermal reactor
iv) Developing the transfer function mode
v) Validating the result

1.5 Feasibility of the Project within the Scope and Time Frame

Meetings between the supervisor and author have been conducted twice in a week, with the purpose of providing updates on activity progress. Based on present status, the effectiveness and efficiency of the completion progress have been thoroughly reviewed to catch up the schedule. Besides, all agreed tasks and milestones have been completed and achieved as per planning. Therefore, improvements could be done on other areas.

CHAPTER 2

LITERATURE REVIEW

2.1 Mathematical modelling

Mathematical modelling is very useful in all aspects of Chemical Engineering. An accurate model is complex. It would require more cost and effort to develop and verify it. Therefore, a balance between these factors needs to be achieved and at the same time, the model should include the crucial dynamic behaviour (Seborg et al, 2004). The physical and chemical laws, such as the laws of conservation of mass, energy and momentum are the components to develop mathematical models (Luyben, 1990).

2.2 Dynamic Model

Ordinary Differential Equation (ODE) and/or Partial Differential Equation (PDE) are normally used in dynamic models of chemical processes (Seborg et al, 2004). Time derivatives need to be included in study dynamics too (Luyben, 1990). Dynamic models are normally derived using unsteady-state conservation laws especially for process control problems. The following steps to develop a dynamic model are extracted from Seborg et al, (2004):

A Systematic Approach for Developing Dynamic Models

1. State the modelling objectives and the end use of the model. Then determine the required levels of model detail and model accuracy.
2. Draw a schematic diagram of the process and label all process variables.

3. List all of assumptions involved in developing the model. Try to be parsimonious: the model should be no more complicated than necessary to meet the modelling objectives.
4. Determine whether spatial variations of process variables are important. If so, a partial differential equation model will be required.
5. Write appropriate conservation equation (mass, component, energy, and so forth)
6. Introduce equilibrium relations and other algebraic equations (from thermodynamics, transport phenomena, chemical kinetics, equipment geometry, etc)
7. Perform a degrees of freedom analysis (Section 2.3) to ensure that the model equations can be solved.
8. Simplify the model. It is often possible to arrange the equations so that the output variables appear on the left side and the input variables appear in the right side. This model form is convenient for computer simulation and subsequent analysis.
9. Classify inputs as disturbance variables or as manipulated variables.

Researchers can proceed to solving the dynamic model once it has been developed. A variety of softwares can be used to solve the equation. Some of the popular ones include MATLAB, Mathematica, ACSL, IMSL, Mathcad and GNU Octave (Seborg et al, 2004).

2.3 Non-Isothermal Reactor

Non-isothermal reactors are widely used in process plants. Reformers, catalytic reactors, hydrocracking reactors are a few to be named. To achieve optimum rate of reaction, non-isothermal reactors are operated at various temperature conditions (Davis & Davis, 2003). Non-isothermal reactors normally operate in adiabatic and non-adiabatic conditions. According to Villa, (2007) for non-isothermal reactor in adiabatic operation, endothermic reactors require addition of heat to maintain the reactions; while for exothermic reactors, it requires the removal of heat.

2.4 Polymerization Reactor

The process of forming networks of polymer chains from monomer reaction is called polymerization (Vasanthi et al, 2012). Polymerization reactors play an important role in polymer engineering industries. The major characteristic of polymerization reactors is their complex dynamic behaviour (Soroush & Kravaris, 1992; McAuley & MacGregor, 1991). Polymerization reaction engineering contributes greatly to the modelling of the reactor. Besides, polymerization reaction engineering also helps in understanding how the reactor operating conditions affect the molecular properties (Ohshima & Tanigaki, 2000; Kiparissides, 1996). Villa, (2007) stated that polymerization reactions are strongly exothermic. Therefore, configuration of heat removal rates is required.

Other than the complex behaviour of reaction mechanisms, another common issue faced in the polymer industry is the measurement of on-line polymer quality variables due to lack of such technology (MacGregor et al., 1984; Ali et al., 2006; Hvala et al, 2011). In many cases, the final performance of the polymer materials need to be controlled (Vieira et al, 2003).

Fluidized bed reactors, as well as batch and semi-batch reactors are most commonly used in polymerization process (Hvala et al, 2011; Seki et al, 2011). In order to establish the control strategies, the inputs and the outputs variables need to be categorized. Simulated polymerization reactor models have been widely used to test the performance of a variety of control techniques. Yet, it was reported in the literature by Soroush & Kravaris (1992) that only a limited number of experimental control studies have been conducted.

CHAPTER 3

RESEARCH METHODOLOGY

3.1 Research Methodology and Project Activities

The activities listed in Figure 3.1 are the project activities that need to be executed in order for this project to meet its objectives.

The problem statement and the objective are identified after discussion between the lecturer and the author. The research is selected based on the complexity of the behaviour of non-isothermal reactor. The author then studied and gathered information from different sources which are specifically related to the case study. Many research papers show that the polymerization process exhibit dynamic behaviour due to its complicated reaction mechanism. Changes in operating conditions in a polymerization reactor will affect its products. However, this is not the same for other reactors such as catalytic reactor, urea reactor and hydrocracking reactor. Hence, polymerization reactor was chosen due to its dynamic characteristic.

The model of the polymerization reactor is developed using the first principle model and it is simulated using Matlab software (ODE45). ODE45 is a solver which helps to integrate the system of differential equation from initial time to the final time given the initial condition. ODE45 is used because it has a common function to solve an ordinary differential equation compared to ODE15s, ODE23, ODE23s, ODE23t, ODE23tb and ODE113. ODE45 helps solve non-stiff model and it is more accurate than the other types of ODE solvers. Hence, in this project, the author used ODE45 during the study.

The syntax for ODE45 is shown as follows:

```
[T,Y] = solver(odefun,tspan,y0)
[T,Y] = solver(odefun,tspan,y0,options)
[T,Y,TE,YE,IE] = solver(odefun,tspan,y0,options)
sol = solver(odefun,[t0 tf],y0...)
```

Steady state results are produced to test the program. The results are validated. The transfer function models are later on developed to obtain the steady state gain value. More details of the results are represented in the form of graphs in Chapter 5. In addition to discussion on simulation outcome, the project will be documented and reported in detail. Finally, recommendations or aspects that can be further improved in the future will also be discussed.

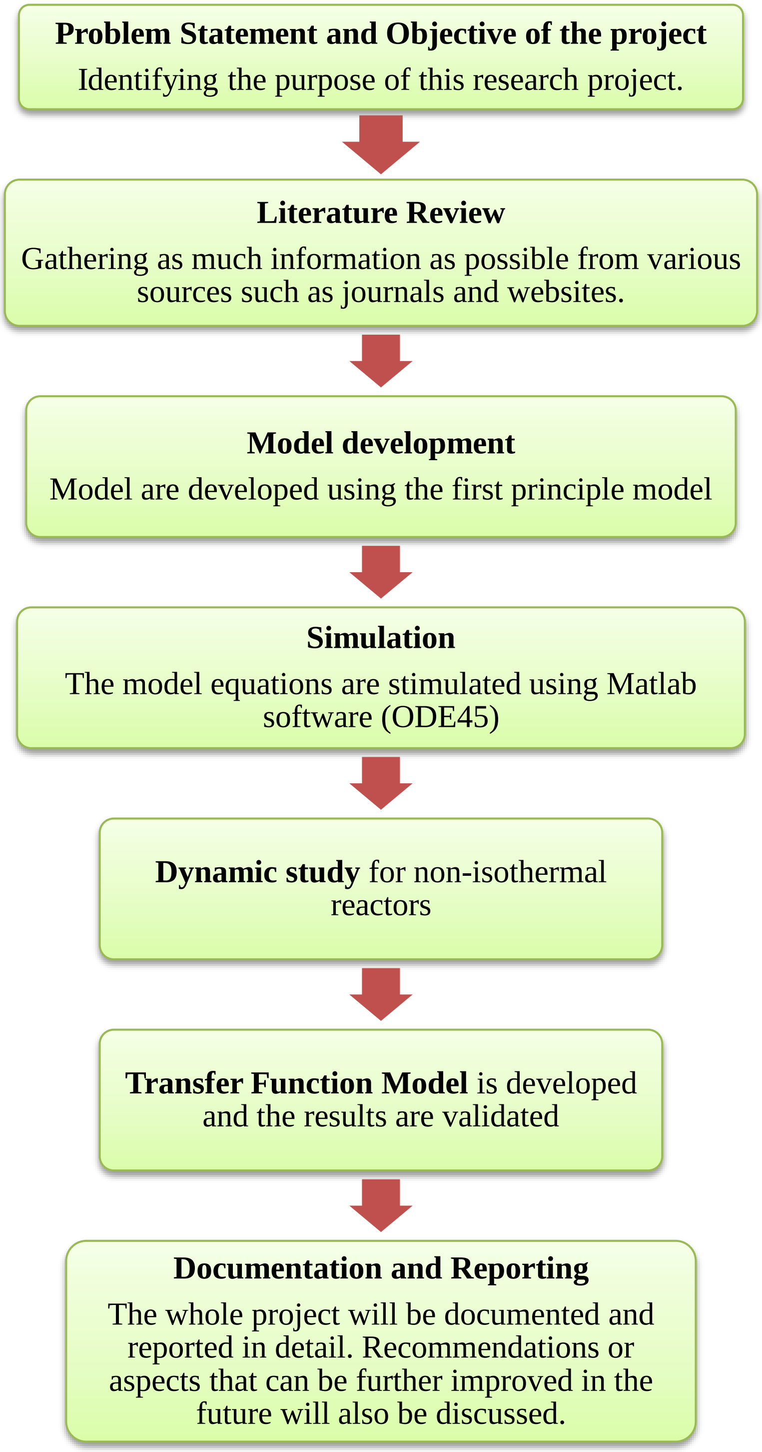


Figure 3.1: The sequence of project activities

3.2 Study Plan (Gantt-Chart)

The Gantt Chart for FYP II is outlined in Table 3.1

Table 3.1: The Gantt Chart for FYP II proposed in FYP guidelines

NO	**DETAIL** **WEEK**	**1**	**2**	**3**	**4**	**5**	**6**	**7**		**8**	**9**	**10**	**11**	**12**	**13**	**14**
1	Project Work Continues	▨	▨	▨	▨	▨	▨	▨								
2	Submission of Progress Report							●								
3	Project Work Continues									▨	▨	▨	▨	▨		
4	Pre-SEDEX											●				
5	Submission of Draft Report												●			
6	Submission of Dissertation (soft bound)													●		
7	Submission of Technical Paper													●		
8	Oral Presentation														●	
9	Submission of Project Dissertation (Hard Bound)															●

● Suggested milestone

▨ Process

The Gantt chart for FYP II is for student progress is outlined in Table 3.2

Table 3.2 Gantt Chart for FYP II

NO	**DETAIL** **WEEK**	**1**	**2**	**3**	**4**	**5**	**6**	**7**		**8**	**9**	**10**	**11**	**12**	**13**	**14**
1	Project Work Continues	▨	▨	▨	▨	▨	▨	▨		▨	▨	▨	▨	▨		
2	-Simulate the model equation	▨	▨	▨	▨	▨	▨	▨								
3	-Analyse the result of the simulation					▨	▨	▨		▨	▨					
4	-Study the dynamic of non-isothermal reactor	▨	▨	▨	▨	▨	▨	▨		▨	▨	▨	▨	▨		
5	-Identify the control system											▨	▨	▨		
6	Submission of Progress Report							●								
7	Preparing Poster for Pre-SEDEX										●					
8	Pre-SEDEX											●				
9	Preparation of Draft Report											●				
10	Submission of Draft Report												●			
11	Submission of Dissertation (soft bound)													●		
12	Submission of Technical Paper													●		
13	Oral Presentation														●	
14	Submission of Project Dissertation (Hard Bound)															●

● Suggested milestone

▨ Process

CHAPTER 4

POLYMERISATION REACTOR AND MODELLING

4.1 Polymerization Reactor

This study will be based mainly on the model and data developed by Ali et al (2006). The reactor used for polymerization is hollow shaft reactor (HSR). This type of reactor is designed for polymerizations which reacts at high viscosities and works under high pressure and temperature.

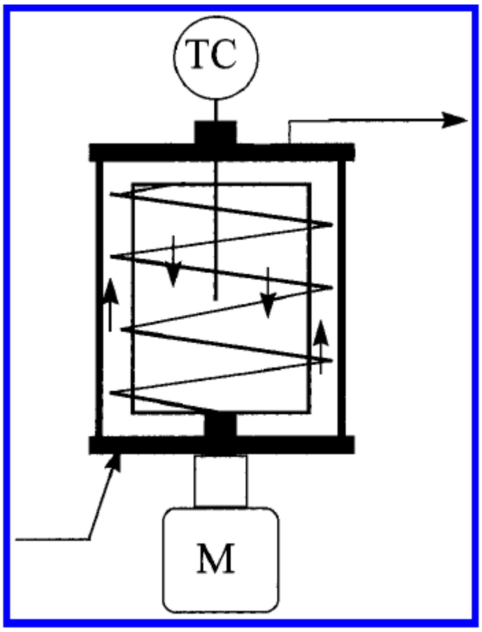


Figure 4.1: Hollow Shaft Reactor

Figure 4.1 shows the basic version of the hollow shaft reactor (HSR). It is similar to an extruder, has internal recycling of the reaction medium and it involves exothermic reaction. According to Weickert, (1998) HSR has the following characteristics: high polymerization, fast mixing, continuous stirring (CSTR) behaviour, minimum dead volume and pressure drop and maximum recycle ratio. HSR is mainly used for liquid-pool propylene polymerization with a multi-site heterogeneous Ziegler-Natta catalyst (Ali et al, 2006).

There are five inputs: mainly manipulated and disturbance variables, as well as four controlled variables in this model. The input variables (manipulated and disturbance) include:

(i) cooling water flow (F_w)
(ii) outlet liquid flow rate (F)
(iii) feed rate of monomer ($F_{in}y_{m,in}$)
(iv) feed rate of hydrogen ($F_{in}y_{H2,in}$)
(v) feed rate of catalyst ($F_{in}y_{cat,in}$).

The controlled variables are:

(i) pressure (P)
(ii) polymer melt index (MI)
(iii) reaction conversion (C)
(iv) temperature (T)

The reactor system is equipped with an automatic valve at the outlet that controls the reactor pressure by manipulating the outlet flow, F. In the initial setup, the catalyst and monomer feed rates are aimed to be constant. This means that they will not be considered when designing the control system. The control problem is then simplified to a system with manipulated inputs ($F_{in}y_{H2,in}$) and controlled variables (Melt Index).

4.2 First Principle Model

Several assumptions are made in order to develop the model of limited complexity:

- The reactions are in first order and it is irreversible.
- The reactor is ideally mixed.
- The reactor is fully filled with liquid; it contains two phases which are liquid monomer and polymer phases.
- The energy produced from mixer rotation is negligible.
- The catalyst decay through different chemical mechanisms at various types of active sites will lumped together into a single deactivation.

The overall mass balance of the reactor can be described as:

$$\frac{dm}{dt} = F_{in} - F \tag{4.1}$$

where

m: total mass inside the reactor

F: outlet mass flow rate in (kg/h)

F_{in}: 1.0 kg/h

The monomer mass fraction:

$$m\frac{dy_m}{dt} = F_{in}(y_{m,in} - y_m) - R_p \tag{4.2}$$

where

y_m: mass fraction of monomer in the outlet flow stream

R_p: propagation reaction rate

The hydrogen mass fraction:

$$m\frac{dy_{H2}}{dt} = F_{in}(y_{H2,in} - y_{H2}) - R_{H2} \qquad (4.3)$$

where

y_{H2}: mass fraction of hydrogen in kg H_2/kg inside the reactor

R_{H2}: hydrogen consumption rate

The hydrogen consumption rate, R_{H2}, can be calculated from:

$$R_{H2} = \frac{2R_p}{42.1P_n} \qquad (4.4)$$

where

2 and 42.1 are the molecular weight for hydrogen and propylene

R_p: polymerization rate

The number of average degree of polymerization, $P_n$is calculated from:

$$P_n = \frac{2}{qPD} \qquad (4.5)$$

where

PD: polydispersity of the produced polymer, for catalyst used in this study has an average value of 6.8

The polymerization termination probability q, (M.A.H, Ali et al, 2006)

$$q = d + eX; \quad X = \frac{0.02104y_{H2}}{y_m} \qquad (4.6)$$

where

X is the molar ratio of hydrogen to monomer in the reactors

The mass fraction for active catalyst, y_{c},

$$m\frac{dy_c}{dt} = F_{in}(y_{c,in} - y_c) - R_d \qquad (4.7)$$

where

R_d: deactivation reaction rate

The mass fraction for deactived catalyst, y_{d},

$$m\frac{dy_d}{dt} = F_{in}(y_{d,in} - y_d) + R_d \qquad (4.8)$$

The reaction rates are calculated using the following equations:

$$R_d = k_d m y_c \qquad (4.9)$$

$$R_p = k_d m y_c \rho_m X \qquad (4.10)$$

where

k_1: rate constants

k_d: rate constants

ρ_m: 263.7 kg/m^3

For rate constants:

$$k_1 = K_{01} + K_{02}T + K_{03}T^2 \qquad (4.11)$$

$$k_d = K_{d0}e^{-E_{a1}/RT} + K_{d1}e^{-\frac{E_{a2}}{RT}}(1 - e^{-\frac{E_{a3}}{X}}) \qquad (4.12)$$

The energy balance equation:

$$(mc_p + m_s c_{p,s})\frac{dT}{dt} = F_{in}(c_{p,in}T_{in} - c_pT) - R_p\Delta H_{R,p} - UA(T - T_{jacket}) \qquad (4.13)$$

The specific heat of the reactor contents can be calculated using the following equation:

$$c_p = y_m(a + bT + CT^2) + C_{p,p}y_p \qquad (4.14)$$

where

$C_{p,p}$: heat capacity of the polymer

The reactor outlet flow rate, F,

$$F = (\frac{F_{in}}{p_m} + R_p\left(\frac{1}{\rho_p} - \frac{1}{\rho_m}\right) - my_m\frac{dT}{dt}\frac{1}{\rho_m^2}\frac{d\rho_m}{dT})\rho \qquad (4.15)$$

where

ρ_p: polymer density

The density of the reaction mixture inside the reactor

$$\rho = \frac{\rho_m\rho_p}{y_m\rho_p + y_p\rho_m} \qquad (4.16)$$

In the studies of Mc Auley & MacGregor (1991) and Ohshima & Tanigaki (2000), several relationships are proposed to relate MI_i to X. In this research, the following relationship is used:

$$MI_i = kX^{\gamma} \qquad (4.17)$$

In the study of Chatzidoukas.C, et al, 2003, Melt Index is correlated to the polymer average molecular weight (M_w)

$$MI_c = \alpha M_w^{\beta} \qquad (4.18)$$

The differential balance for the cumulative weight average molecular weight, M_w is employed to calculate the cumulative melt index:

$$\frac{d\bar{M}_w}{dt} = \frac{1}{m_p}\left(y_{p,in}F_{in}\left(\bar{M}_{w,in} - \bar{M}_w\right) + R_p\left(M_w - \bar{M}_w\right)\right) \qquad (4.19)$$

where

m_p: the mass of polymer inside the reactor

By substituting Eq (4.18) into Eq. (4.19) with assumption of a free-polypropylene inlet stream, i.e. $y_{p,in} = 0$, the following differential equation for the cumulative melt index is produced.

$$\frac{m(1-y_m)}{\beta R_p}\frac{d}{dt}MI_c = \left(MI_i^{\frac{1}{\beta}} MI_c^{1-\left(\frac{1}{\beta}\right)} - MI_c\right) \qquad (4.20)$$

which is a first-order relationship with variable gain and time constant.

The monomer conversion is calculated from:

$$C = 1 - \frac{y_m}{y_{m,t=0}} \qquad (4.21)$$

4.3 Operating Conditions and Data

Table 4.1: Operating Conditions

Reactor Used	Hollow Shaft Reactor
Operating Temperature	57 ℃ (330K)
Operating Pressure	25 bar
Catalyst Used	Ziegler Natta Catalyst

The internal temperature of the reactor is 57 ℃ (or 330K)when the reaction takes place. It is within the typical range of 50 ℃ - 90 ℃ (Weickert, 1998). For reaction to occur, the amount of activated catalyst, $yc,_{in}$ is 0.0224 kg/kg catalyst (Samson et al, 1998).

Table 4.2 shows the thermodynamic and physical parameters for propylene polymerization.

Table 4.2 Thermodynamic and physical parameters for propylene polymerization

Parameter	**Value**
Physical Parameters	
Reactor Volume (*V*)	1.86×10^{-3} m^3
Reactor heat transfer (*A*)	0.0961 m^2
Thermodynamic parameters	
Overall heat transfer coefficient (*U*)	1.62MJ/h K m^2
Heat of propagation reaction ($\Delta H_{R,p}$)	2.03 MJ/kg
Specific heat of polypropylene ($C_{p,p}$)	2.25×10^{-3} MJ/ kg K
Density of polypropylene (ρ_p)	900 kg/m^3
Specific heat of propylene ($C_{p,m}$)	
a	2.785×10^{-3} MJ/kg K
b	-9.18×10^{-6} MJ/kg K^2
c	2.93×10^{-8} MJ/kg K^3
Density of propylene monomer (ρ_m)	263.7 kg/m^3
Parameters	
k	6818.3
γ	1.03
β	-2.34

For X <0.00144	
d	5.32×10^{-5}
e	0.115
Else	
d	1.52×10^{-4}
e	0.0405
K_0	(-204256.6, 1153.3314, -1.626207)
k_{d0}	3746 h^{-1}
k_{d1}	1.748 x 10-7 h^{-1}
E_{a1}/R	1620.8K
E_{a2}/R	5570.7K
E_{a3}	498.9

These are the initial values that use to simulate the model in steady state:

Mass (kg): 0.56

Mass fraction for monomer: 0.82

Mass fraction for hydrogen: 0.1104

Mass fraction for active catalyst: 1

Mass fraction for deactivate catalyst: 0

Temperature (K): 330

Melt Index: 15

Conversion: 0.18

Using the above data and operating conditions, the model is simulated. A number of graphs were produced. Steady-state parameters were constant with respect to time. On the other hand, the catalyst has shown deactivation through a decreasing trend in its mass fraction with respect to time. The graph is shown as below.

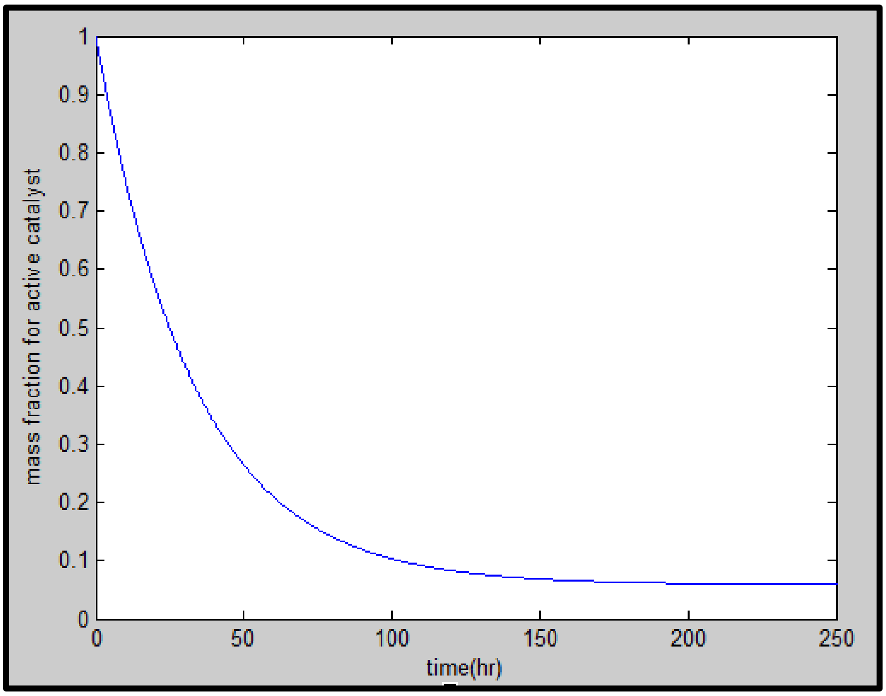


Figure 4.2 : Changes of mass fraction of active catalyst with respect to time

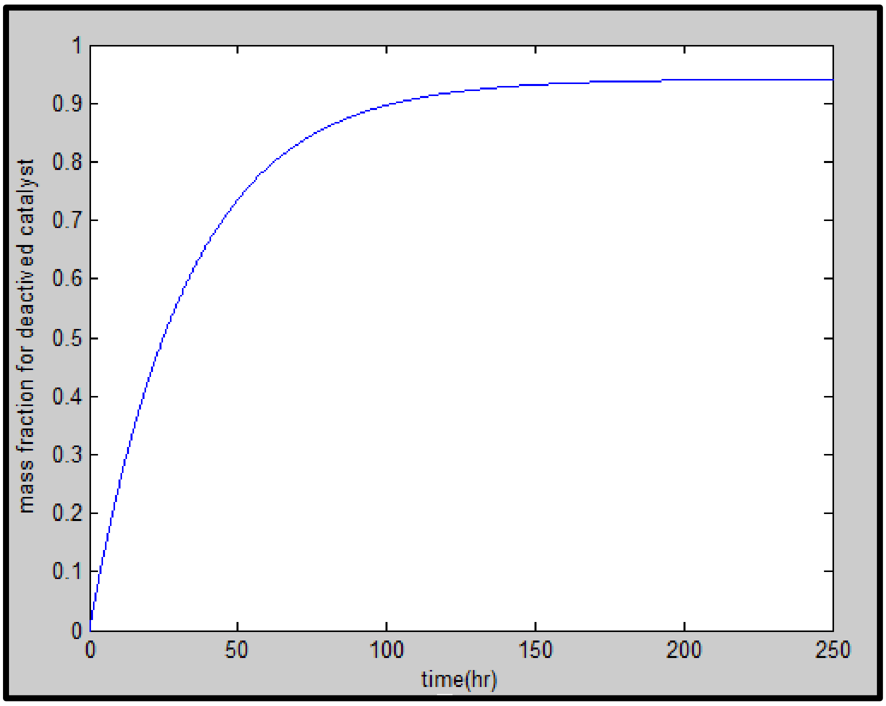
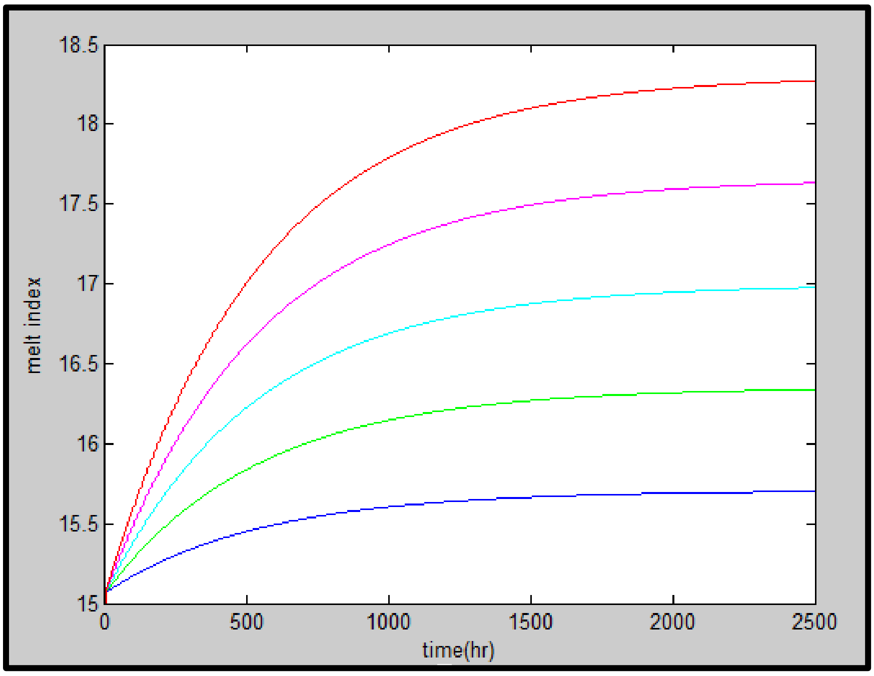


Figure 4.3 : Changes of mass fraction of deactived catalyst with respect to time

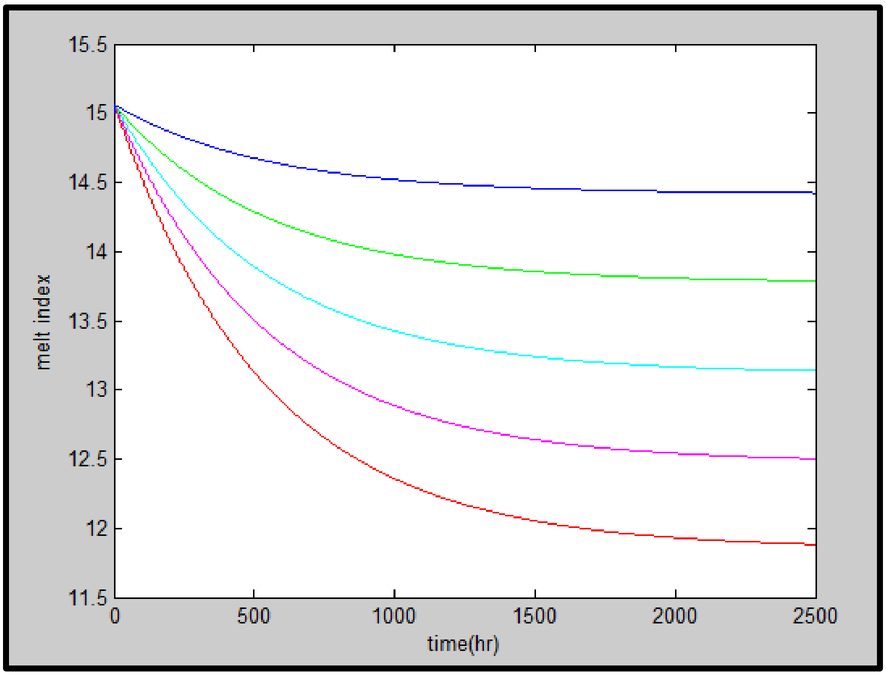
CHAPTER 5

RESULT AND DISCUSSION

Feed rate of hydrogen, $F_{in}y_{H2,in}$ was studied in this project because hydrogen will terminate the process of polymerization. The amount of hydrogen consumed in the process would affect the melt index which needed to be controlled so that it will provide the desired product. When the feed rate of hydrogen is given a value of 0.1104 kg/h, the melt index is 15. Hence, to observe the effect of hydrogen feed rate on the melt index, the steady state value of the feed rate of hydrogen (originally 0.1104) was adjusted. The value was either increased or decreased with 4% increments. The figure below shows the effect of Melt Index when the feed rate of hydrogen is changed:



. *Figure 5.1: Melt Index value when* $y_{H2,in}$ *increase by every 4%*



. Figure 5.2: Melt Index value when $y_{H2,in}$ decrease by every 4%

Figure 5.1 and 5.2 has different colour of graph lines which are used to indicate the step change in feed rate of hydrogen, $F_{in}y_{H2,in}$. Table 5.1 shows the percentages of each graph lines.

Table 5.1: Percentages of feed rate of hydrogen, $F_{in}y_{H2,in}$

━	4%
━	8%
━	12%
━	16%
━	20%

Melt Index with respect to time graph are plotted based on the step change in feed rate of hydrogen, $F_{in}y_{H2,in}$. The results showed the Melt Index value increases with the increase of percentage in the feed rate of hydrogen. Melt Index value decreases with the decrease of percentage in the feed rate of hydrogen.

After the analysis of the reactor, transfer function model is developed. Steady state gain, K is calculated. Steady state gain is the transfer function which relates the change in input to change of output at steady state conditions. It can be evaluated by setting s to zero in the transfer function. To obtain the steady-state gain, K, it can be calculated using

$$K = \frac{\Delta y}{\Delta m} \tag{5.1}$$

where

Δm = changes in the independent variable (input)

Δy = changes in the dependent variable (output)

The result is tabulated in Table 5.2 and a graph is plotted based on the steady state gain, K.

. Table 5.2: Steady State Gain, K vs $\Delta y_{H2,in}$ (%)

$\Delta y_{H2,in}$ (%)	K
-20.00	145.58
-16.00	145.81
-12.00	145.96
-8.00	146.12
-4.00	146.26
0.00	146.4
4.00	146.58
8.00	146.75
12.00	146.92
16.00	147.08
20.00	147.23

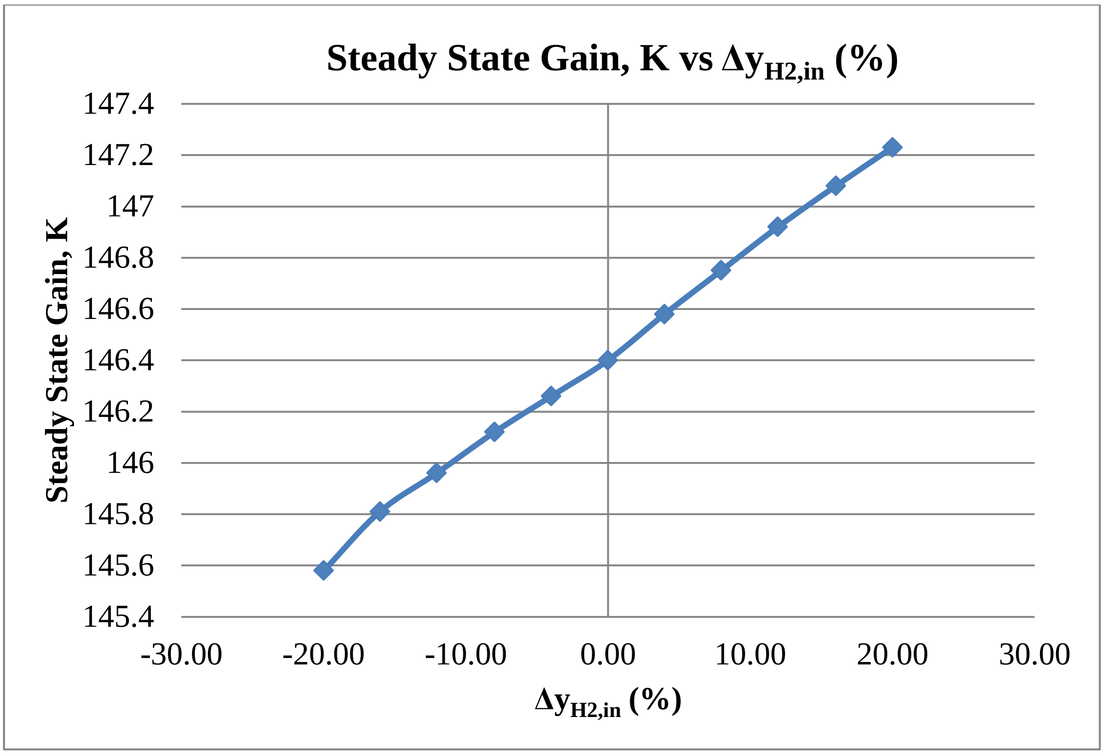


Figure 5.3: Steady State Gain, K vs $\Delta y_{H2,in}$ *(%)*

In Figure 5.3, the graph shows steady state gain, K increases with respect to the increase of feed rate of hydrogen, $F_{in}y_{H2,in}$. Steady state gain, K value changes when there are changes apply to the feed rate of hydrogen. Hence, this proves that polymerization reactor shows a non-linear behaviour in this model.

CHAPTER 6

CONCLUSION AND RECOMMENDATION

6.1 Relevancy to Objectives

These completed activities have assisted in improving the understanding of the concepts and the methods of modelling and simulating the non-isothermal reactors. For example, the author has studied the polymerization reactors which has provided a foundation or basic understanding of developing the model equations which require capturing the dynamic characteristic of the non-isothermal reactors. Throughout the study, the polymerization reactors showed controlling difficulties due to its complicated reaction mechanism. Furthermore, the quality of the polymer materials such as melt index are needed to be controlled to ensure the product properties are as desired. If the quality of the product is not been controlled, the output of the polymer might not be as desired.

Besides, the journal papers studied presented various methodologies used to study the dynamic response of the non-isothermal reactors. After polymerization reactors was selected as the main approach, further research was focused on how to capture the dynamic characteristics of the polymerization reactor starting from developing the first model equations until developing the transfer function model. Transfer function model has helped in providing a better insight for the analysis to produce the best results.

6.2 Recommendations

For future continuation, the research should be focused on designing the appropriate control system by choosing the control strategies which is suitable and relevant to this project. In addition, the assumptions of the model can be changed by reading more journals papers or doing research on the particular subject. The summary of journal papers should be maintained. The document or file should be handed on to the next researcher who wishes to expand on this topic. It would provide a lot of relevant background information, collected in one place. Moreover, future students or researchers can attempt modelling other types of reactors. Hence, the parameters of the model will also change indirectly. This way, the next researcher or student would have some form of advantages in the early stage of their research.

Furthermore, in this research, the catalyst and monomer feed rates were assumed to be constant and were not used in designing the control system. However, for future study, these features can be included in designing so that the result will be more accurate. Comparison can be done between the results of this simpler model with that of the more complex one to evaluate how accurate it has become.

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