CONCEPTUAL DESIGN OF 5 KG/HR PRODUCTION OF PENTAERYTHRITOL TETRADODECANOATE (PETD)

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CONCEPTUAL DESIGN OF 5 KG/HR PRODUCTION OF PENTAERYTHRITOL TETRADODECANOATE (PETD)

JEDIDIAH JOHNNY

A thesis submitted in fulfillment of the requirements for the award of the degree
of Bachelor of Chemical Engineering

Faculty of Chemical & Natural Resources Engineering

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I declare that this thesis entitled *“Conceptual Design of 5 kg/hr Production of Pentaerythritol Tetradodecanoate (PETD)”* is the result of my own research except as cited in the references. The thesis has not been accepted for any degree and is not concurrently submitted in candidature of any other degree.

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Special Dedication to my…

Beloved parents;
Johnny Lagang Tapan
Julie ak Edward

Beloved sister;
Jacobina Johnny

Encouraging friends;
Shahril Mohamad
Azrul Azmi Yaziz
Mohd Farridd Termizi

For Their Love, Support, Advices, Help and Best Wishes.

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ABSTRACT

Conceptual design is becoming a common method used in the industries to estimate and design the optimum condition for their production, by concerning the time and money constraint. The objective of this study is to synthesis the process flowsheet for the optimum production of Pentaerythritol Tetradodecanoate (PETD) at 5 kg/hour. This study covers on the production cost estimation. The analytical methods of finding the properties were done using Thermogravimetry Analysis (TGA), Differential Scanning Calorimeter (DSC) and Calorimeter Bomb. To validate the conceptual design, rigorous steady state simulations are performed. Extensive simulation using ASPEN Plus software was performed and a scheme that can address the requirement is proposed. This study shows the usage of concepts to model the optimum design of reaction, separation and the utilities of PETD production. The framework which used to develop the flowsheet scheme is general enough for further investigation by extending its application to other problem.

ABSTRAK

Reka bentuk konsep telah menjadi satu kaedah lazim yang digunakan oleh industri untuk menganggar dan mereka bentuk keadaan optimum bagi pengeluaran mereka dengan mengambil kira kekangan masa dan kewangan. Tujuan bagi kajian ini ialah untuk mensintesis rajah alir proses yang optimum bagi penghasilan “Pentaerythritol Tetradodecanoate (PETD)” pada kadar 5 kg/jam. Kajian ini meliputi anggaran kos pengeluaran. Kaedah analitikal untuk mencari sifat-sifat kimia dilakukan dengan menggunakan “Thermogravimetry Analysis (TGA)”, “Differential Scanning Calorimeter (DSC)” and Kalorimeter Bom. Untuk mengesahkan reka bentuk ini, satu simulasi keadaan stabil yang menghampiri proses sebenar dilakukan. Simulasi dilakukan menggunakan perisian ASPEN Plus dan satu skema untuk menepati keperluan telah dicadangkan. Kajian ini menunjukkan penggunaan konsep untuk pemodelan keadaan reka bentuk optimum bagi tindak balas, pemisahan dan utiliti dalam penghasilan PETD. Struktur yang digunakan untuk menghasilkan rajah alir adalah sangat lazim untuk kajian seterusnya dengan aplikasi kepada masalah yang lain.

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CHAPTER 1

INTRODUCTION

1.0 Introduction

Over the past number of years, industry has needed to become more effective in bringing new products to the market. In terms of product design, the effect has been that manufacturers must have extremely efficient product development process [17]. In chemical engineering, we might try to generate new ideas to produce something new or to improve the production with new technologies. These new ideas will be translated into real equipment and processes for producing those new materials or for significantly upgrading the value off those existing products.

While conceptual design is regarded as the most demanding phase of design on the designer [14], it also offers the greatest scope for improvements in the design of the product [12]. The design should be done carefully because it affects the accuracy of the estimation cost for designing and operating. All this is called a process synthesis of producing new product where the goal is to find the best process flow sheet and estimating the optimum design condition [1]. It is widely acknowledge that up to 80 per cent of a product's total cost is dictated by decisions made during the conceptual phase of design [14].

For the conceptual design of Pentaerythritol Tetradodecanoate (PETD) production, it is synthesis process of a plant that can produce PETD at optimum rate. This will consider the cost factor as the parameter. The design will be developed by using order-of-magnitude, means that limiting our attention to the major piece of process equipment and then add up the minor piece equipment. At the end of the project, the best design for the production of PETD will be chosen from the most profitable with a low operating cost and considering all the other factors, including safety and environment control.

1.1 Problem Statement

Traditionally, the design process involves the draftspersons and the design engineers, who, once they have completed their jobs, usually present the blueprints (layouts) of the product to the manufacturing or production division. Product performance failure is usually due to a lack of analysis [18].

The conventional design process may take a lot of time and become costly to be done. From the manual design procedure until the realization of the production, some of the design may not be effective and run as what people want. The manual design procedures that take place is by creating a lot of alternatives, and doing a lot of experiments just for one processes. The process will use a lot of the cost because of damages on the equipments, raw materials, and energy used. Most errors in design, as opposed to those made during production, are due to use of a flawed conceptual design [16].

In this research, the design process that is studied is the conceptual design of Pentaerythritol Tetradodecanoate(PETD) production. Problem that occurs is how to produce the product wanted at an optimum output in terms of purity, production rate, energy consumption and process minimization. Besides, less than 1% of ideas for new designs ever become commercialized [1].

1.2 Objective

The objective of doing this project is to find the process flow diagram and estimate the optimum design to produce 5 kilogram per hour of Pentaerythritol Tetradodecanoate (PETD).

1.3 Scope of Study

This project will cover on the study of the process parameter (ie. chemical and phase equilibrium, entrainer selection, kinetic design and optimization) of the esterification reaction that will affect the operation cost of the plant from the feed of raw material until the final product. The scope of this research is to:

i. Run an analysis of PETD by using Calorimeter Bomb to find the enthalpy of combustion.
ii. Find the properties of PETD by using Thermogravity Analysis (TGA) & Differential Scanning Calorimeter (DSC).
iii. Study on the operation cost which involves the number of equipments and materials used in process.
iv. Run the process simulation by using ASPEN PLUS software.

CHAPTER 2

LITERATURE REVIEW

2.1 Conceptual Design

Generally, concept gives the meaning of a principle or an idea. It also is an abstract, notion or unit that serves to designate a category of entities, events or relations [5]. Conceptual design also has been defined as that phase of design which takes a statement of a design problem and generates broad solution to it in the form of, what are generally referred to as, ‘schemes’ [12]. Conceptual design is also the process by which the design is initiated, carried to the point of creating a number of possible solutions, narrowed down to single best concepts. It is sometimes called the feasible study [13].

Before this, designs were done empirically. There was no concept practised on designation process. Empirically means that the designation is only based on try and error. A chemist might discover a new reaction to make an existing product or a new catalyst for an existing, commercial reaction, and designers want to translate these discoveries to a new process. Thus, designers start with only knowledge of reaction conditions that they obtain from the chemist, as well as some information about raw materials and product obtained from marketing organization. A lot of these process alternatives to be done to archive the same goal which can be up to 10^4 until 10^9 processes [1].

2.2 Definition of Terms

2.2.1 Batch Process

Batch process refers to a discontinuous process involving the bulk movement of material through sequential manufacturing steps. Mass, temperature, concentration, and other properties of a system vary with time. Addition of raw material and withdrawal of product do not typically occur simultaneously in a batch process.

2.2.2 Continuous Process

Continuous process means a process where the inputs and outputs flow continuously throughout the duration of the process. Continuous processes are typically steady-state.

2.2.3 Order-of-magnitude Estimate

For a beginner designer, it is useful to have a systematic approach for developing order-of-magnitude estimates. Order-of-magnitude estimates usually made before the facility is designed, and must therefore rely on the cost data of similar facilities built in the past [1]. The Order of Magnitude estimate in is completed when only minimal information is available. The proposed use and size of the planned structure should be known and ay be the only requirement. The “units” can be very general and need not be well defined. The probable accuracy of the design may exceed ±40%.

2.2.4 Rules of Thumb

Originally rules of thumb or also know as heuristics evaluations were developed by experienced designers. It is desirable to recover more than 99% of valuable components in column [1].

Heuristic Evaluation is a method of design evaluation. Based on a heuristic evaluation, the expert should also be able to provide alternative design solutions to address potentially major problems for users. The basic approach requires that a domain expert (someone very familiar with product area) review the product design using a set of heuristics (guiding principles e.g. provide appropriate feedback) with the purpose of identifying design decisions (e.g. layout, labeling, etc) that may lead to use errors [8].

2.3 Description of Material

The materials being used for this study are mercury in Pentaerythritol Tetradodecanoate (PETD), Lauric Acid and Pentaerythritol.

2.3.1 Raw Material

Below are some descriptions of the raw materials used in the production of PETD:

Table 2.1: Raw material properties *(Taken from MSDS of material)*

Description	**Materials**	
	Pentaerythritol	**Dodecanoic Acid**
Commercial name	-	Lauric Acid
CAS number	115-77-5	143-07-7
Molecular formula	$C_5H_{12}O_4$	$C_{11}H_{22}COOH$

Melting point (K)	533.15	317.15
Boiling point (K)	Decomposes	Decomposes
Molecule weight (g/mole)	136.15	200.32
Physical state and appearance	Solid	Solid
Price (USD/kg)	59.00	68.64
Purity	100%	98%

2.3.2 Product

PETD is formed by esterification process between the alcohol group which is the Pentaerythritol and the carboxylic acid which is Lauric Acid or also known as Dodecanoic Acid. The reaction occurs as shown in equation 1:

$$C_5H_8(OH)_4 + 4C_{11}H_{22}COOH \rightleftharpoons C_5H_8(C_{11}H_{22}COOH)_4 + 4H_2O \qquad [1]$$

The non-catalytic reaction occurred at the range 150°C to 230°C. The product was then dried by using water extraction prior to be crystallized at the ambient temperature. The powder was finally obtained by crushing the crystal. The standard material of Pentaerythritol Tetradodecanoate (PETD) is obtained from Kaneka Chemical (M) Sdn. Bhd. The chemicals are those laboratory grades and used without any further purification. Below are some descriptions of the product:

Table 2.2: Physical properties of PETD *(Taken from Kaneka Sdn. Bhd.)*

Properties	**Description**
Molecular formula	$C_5H_8(C_{11}H_{22}COOH)_4$
Physical state	Crystalline solid (powder)
Colour	White
Specific gravity	-

Boiling point	-
Melting point	-
Molecular weight	865.372 g/mole

2.4 Chemical Properties of Pentaerythritol Tetradodecanoic (PETD)

The analysis of Pentaerythritol Tetradodecanoate (PETD) is done based quantitative analysis which can be further split into different areas of study. For quantitative analysis, the material can be analyzed for the amount of an element, or for the amount of an element in a specific chemical species.

2.4.1 Thermal Stability

The thermal stability of a pure organic compound is roughly spoken a combination of the thermodynamic and the kinetic stability of a molecule. The addition of other compounds or impurities can effect higher or lower stabilities, in most cases as a consequence of kinetic effects: the added compound (or impurities that could not be removed during the synthesis-procedure) can prevent or open reaction pathways leading to the effects of opposite directions: an advanced stability or an elevated decomposition.

The key parameters for a general view on thermal stabilities with regard to technical applications are:

i. maximum operating temperature, below which degradation and thus production and evolution of volatile degradants are negligible,
ii. the rate of degradation at a specific temperature,
iii. the identification of the decomposition products.

Thermal stability of the Pentaerythritol Tetradodecanoate should be in excess of processing or use temperatures. The thermal stability range can be determined after analyzing the graph of weight percentage remaining versus time.

2.4.2 Melting Point

A melting point is the temperature at which a solid becomes a liquid at normal atmospheric pressure [9]. Determining the melting point of a compound is one way to test if the substance is pure. A pure substance generally has a melting range (the difference between the temperature where the sample starts to melt and the temperature where melting is complete) of one or two degrees. Impurities tend to depress and broaden the melting range so the purified sample should have a higher and smaller melting range than the original, impure sample.

2.4.3 Product Purity

Purchasers of raw products became more demanding about the quality and purity of the product they were purchasing. This means that information about purity and quality of the product flows downstream and that information coming from consumer demand flows upstream [22]. Quality standards are enforced by private commitment to industry standards, as the product value is greater given higher purity levels. Standards enforcement is crucial, as products that do not conform to the desired quality level will not be accepted. Tolerance levels vary from product to product and also depend on the preferences of the final consumer. Testing and tolerance levels are important to ensure that the purity and the high quality levels of the product are maintained. Through purity and product control, it enhances the demand of product hence giving ideal competition to gain customer.

2.4.4 Heat Capacity

Heat capacity is mathematically defined as the ratio of a small amount of heat δQ added to the body, to the corresponding small increase in its temperature dT:

$$C = \left(\frac{\partial Q}{dT}\right)_{cond.} = T\left(\frac{dS}{dT}\right)_{cond.}$$

Where δQ is the infinitesimal amount of heat added, and dT is the subsequent rise in temperature.

The heat capacity at constant volume is

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V$$

$$dU = C_V dT$$

$$\Delta U = \int_{T_1}^{T_2} C_V dT$$

And the heat capacity at constant pressure is

$$C_P = \left(\frac{\partial H}{\partial T}\right)_P$$

$$dH = C_P dT$$

$$\Delta H = \int_{T_1}^{T_2} C_P dT$$

2.4.5 Enthalpy

Enthalpy, H can be defined as the sum of the internal energy of the system plus the product of the pressure of the gas in the system and its volume:

$$H_{sys} = E_{sys} + PV$$

After a series of rearrangements, and if pressure is kept constant, we can arrive at the following equation:

$$\Delta H_{sys} = q \qquad \text{(at constant pressure)}$$

where ΔH is the H_{final} minus H_{initial} and q is heat

The enthalpy is defined by $H = U + PV$. The increment of enthalpy is

$$dH = TdS + VdP$$

2.4.6 Heat of Combustion

Since the calorimeter is isolated from the rest of the universe, we can define the reactants (sample and oxygen) to be the system and the rest of the calorimeter (bomb and water) to be the surroundings. The change in internal energy of the reactants upon combustion can be calculated from

$$\begin{aligned}
dU_{tot} &= dU_{sys} + dU_{surr} = 0 \\
dU_{sys} &= -dU_{surr} \\
dU_{sys} &= -\left[\left(\frac{\partial U}{\partial T}\right)_V dT + \left(\frac{\partial U}{\partial T}\right)_T dV\right]
\end{aligned}$$

Since the process if constant volume, dV=0. Thus, recognizing the definition of heat capacity C_v yields

$$dU_{sys} = -C_V dT$$

Assuming C_v to be independent of T over small temperature ranges, this expression can be integrated to give

$$\Delta U = -C_V \Delta T$$

where C_v is the heat capacity of the surroundings, *i.e.*, the water and the bomb.

By definition of enthalpy

$$\Delta H = \Delta U + \Delta(pV)$$

Since there is very little expansion work done by condensed phases, $\Delta(pV) \approx 0$ for solids and liquids. Assuming the gas to be ideal yields

$$\Delta H = \Delta U + RT\Delta n_{gas}$$

Recall that $\Delta U = q_{\mathrm{v}}$ is the heat flow under constant volume conditions, whereas $\Delta H = q_{\mathrm{p}}$is the heat flow under constant pressure conditions. The difference between these two situations is that pV work can be done under constant pressure conditions, whereas no pV work is done under constant volume conditions.

Consider the case where $\Delta n_{\mathrm{gas}} > 0$. *i.e.*, the system expands during the reaction. The same amount of energy is released by the reaction under both sets of conditions. However, some of the energy is released in the form of work at constant pressure; thus, the heat released will be less than at constant volume. Mathematically,

$$\begin{aligned} \text{heat released} &< \text{energy released} \\ -\Delta H &< -\Delta U \\ \Delta H &> \Delta U \end{aligned}$$

In the case where $\Delta n_{\mathrm{gas}} < 0$, *i.e.*, the system contracts during the reaction, the surroundings do work on the system. Thus, this work is available for energy release from the system back to the surroundings in the form of heat. Mathematically,

$$\begin{aligned} \text{heat released} &> \text{energy released} \\ -\Delta H &> -\Delta U \\ \Delta H &< \Delta U \end{aligned}$$

Enthalpy of a reaction or energy change of a reaction ΔH, is the amount of energy or heat absorbed in a reaction. If the energy is required, ΔH is positive, and if energy is released, the ΔH, is negative.

2.5 Simulation

Process simulation allows us to predict the behaviour of a process using basic engineering relationships such as mass and energy balances, and phase and chemical equilibrium. The simulation process will help to realize the design and the production process that comes out will be almost the same with the real process. Doing it this way can help to avoid loss because we don’t have to construct the real plant and test it on the real plant. This software can be used to change the specification interactively, such as, flowsheet configuration; operating condition; and feed composition in terms of running new cases and analyze process alternatives [3]. Hence the usage of this method can help on creating the process flowsheet.

CHAPTER 3

METHODOLOGY

3.1 Design of Process Flowsheet

Flowsheets are intended to represent and explain processes [2]. For this research, the process flowsheet is simplified and focusing towards the main processes in the production. The flowsheet is being produced using order-of-magnitude and rules of thumbs to simplify the process material balances, the equipment design equation, and the cost calculation. Selection of major adjustment shall be made depend on the major equipment used in the process (ie. reactor, evaporator, etc.) that can affect most of the total plant cost.

Early designs are based on costing procedures for the most expensive equipment items used. Then, improvement made on the estimation-material and energy-balance calculation to increase the accuracy of the real cost that are needed for the plant. The designs are then added with some small equipment which doesn't give a big impact on total on total plant cost (ie. Pumps, valve, etc.). These shortcut calculations often are sufficiently accurate to eliminate the 90% or so, of the alternatives that do not correspond to profitable operation [1]. Below is the hierarchy of decisions process:

i. Batch versus continuous
ii. Input-output structure of the flowsheet
iii. Recycle structure of the flowsheet
iv. General structure of the separation system
    a. Vapor recovery system

   - b. Liquid recovery system
- v. Heat-exchanger network

3.1.1 Batch versus Continuous

In this project, the first design procedure is to decide the type of operation for the PETD production. The process preferred is a batch operation. This type of operation is chosen because of cost and market demand for the product. The demand for the material is still at low level where the quantity that will be produced depends on the industrial needs.

Malone and Irribarren suggest that the best approach to design a batch is to design a continuous process first. With this approach it is simpler to screen the process alternatives and to determine the best process flowsheet [1]. So the procedure of the flowsheet design in this project will apply on the continuous process.

3.1.2 Input-Output Structure

The input and output data in the production is selected. The structure will be based on a continuous process flow. The input connected to the reactor and the reactor effluent will directly connected to a distillation column for separation process. The equilibrium reactor affords a mixture of reaction products near its equilibrium composition.

Considering the fact that conversion of this of this equilibrium reaction is near 67% [19], a reaction distillation column for increasing the conversion and separation was used. The advantage of esterification pre-reactor is based on the fact that the greatest part of reaction component can react before reaction distillation column and the throughput of reaction system increases [20]. For the output rate of the product from the distillation column should be 5 kg/hour.

3.1.3 Recycle Structure of the Flowsheet

There are decisions to be made in terms of recycle structure needed in the process flowsheet. If sets of reaction take place at different temperatures of pressure, different reactor systems are needed for this reaction. For this process, the production reaction which is said to be an esterification reaction involving the mixture of lauric acid and pentaerythritol substrates occurred at the range $150^{o}C$ to $300^{o}C$. Because the reaction occurs to be only one reaction, and both take place at the same temperature and pressure without catalyst, only one reactor required. The excess of reactant is also a factor for a certain reaction to improve its selectivity. However, the production of Pentaerythritol Tetradodecanoate (PETD) does not need an excess reactant to yield a higher selectivity. So, there will be no recycle flow for PETD production. To increase the selectivity, the process continuously will separate the main product from the by product using distillation column.

3.1.4 Separation System

The reaction occurs at high temperature and it will produce water vapour effluent. Hence the separation system needed for this process is a vapour-liquid separation system. The reactor can be used as a phase splitter or put a flash drum after the reactor [1]. But since the major effluent from the reactor is in liquid phase, we assume that the liquid separation system is more applicable. The system chosen for the separation is a distillation column.

3.1.4.1 Relative Volatility

For quick estimates, a relative volatility can be estimated as follows [21]:

Overall balance: $F = V + L$

Component balance: $Fz_i = Vy_i + Lx_i$

The equilibrium vaporization constant K is defined for a compound by

$$y_i = K_i x_i$$

Where:

y_i = Mole fraction of component i in the vapour phase

x_i = Mole fraction of component i in the liquid phase

To calculate a distillation, the relative volatility, **α** is needed where it is defined as

$$\boldsymbol{\alpha} = K_i/K_j$$

where i and j represent two components to be separated as obey Raoult's Law.

3.1.4.2 Minimum reflux

The Underwood Method will provide a quick estimation of minimum reflux requirements. It is a good method when distillate and bottoms composition are specified [21]. The following are the Underwood equations:

For bubble point liquid feed:

$$R_m = \frac{1}{\alpha - 1}\left[\frac{x_{LD}}{x_{LF}} - \frac{\alpha(1 - x_{LD})}{(1 - x_{LF})}\right]$$

For dew point vapour feed:

$$R_m = \frac{1}{\alpha - 1}\left[\frac{\alpha x_{LD}}{x_{LF}} - \frac{(1 - x_{LD})}{(1 - x_{LF})} - 1\right]$$

Where:

α_i = Relative volatility of component i versus the heavy key component

x_{LD} = Mole fraction of light distillate component

x_{LF} = Mole fraction of light feed component

3.1.4.3 Minimum stages

The Fenske Method gives a quick estimate for the minimum theoretical stages [21]. The minimum number of tray from Fenske-Underwood equation:

$$N_m = \frac{\log\left[\frac{(x/[1-x])_O}{(x/[1-x])_B}\right]}{\log \alpha}$$

When O refers to overhead; B to bottoms; x is mole fraction.

3.1.5 Heat-Exchanger Network

Energy conservation has always been important in process design. Thus, it was common to practice to install feed-effluent exchangers around reactors and distillation columns. The starting point for an energy integration analysis is the calculation of the minimum heating and cooling requirements for a heat-exchanger network. The calculation of the heat required is by doing first-law analysis [1]:

$$Q_i = FC_{Pi}\Delta T$$

Then the second law analysis is to determine the heat flow of streams that is the heat energy may only flow into direction of hot to cold. The heat integration flow used to drive the cold stream using hot stream available or so on to minimize cost of utilities. However, as a starting point, the heat transfer in each interval has to be considered separately. The calculation is as shown below:

$$Q_i = \left[\sum (FC_p)_{hot,i} - \sum (FC_p)_{cold,i}\right] \Delta T_i$$

Where:

i = the number of stream.

Q = heat
F = flowrate
C_p = heat capacity at constant pressure
ΔT = temperature change

3.2 Analytical Method

Conceptual designs often focus on attempts to make new materials, so that in many cases physical property data are not available in the literature [1]. As for this design process needs, the analysis of Pentaerythritol Tetradodecanoate (PETD) is to be done. For this material, the analysis study will be done in three ways which are Thermogravimetric Analysis (TGA), Differential Scanning Calorimeter (DSC) and Bomb Calorimeter.

3.2.1 Analysis Using Thermogravimetric Analyzer

The TGA instrument used is Q500 from TA Instruments. The thermal change detector for this instrument is a thermocouple. The range of weight sample used is below 1000mg using platinum pan [6]. Method that will be used in this analysis is Dynamic Hi-Resolution TGA. For this method heating rate is continuously varied in response to actual rate of weight loss. For the first run, the start temperature setting will be 20°C. Gas change from N_2 to O_2 will be set at 700°C and the final temperature will be at 900°C. Ramp value is set to 50°C per minute for each analysis. For the next run, the gas change will be depending on the first run result where the result will be shown in weight percentage versus temperature graph plotted. The adjustment to be made is to decompose the carbon left on the pan.

3.2.2 Analysis Using Differential Scanning Calorimeter

The DSC used in analyzing the sample is Q1000 from TA Instruments. For this study, the pan used for sample preparation is aluminum standard pan with and upper limit of 600°C with range of sample mass from 1 mg until 50 mg [7]. The temperature range for the analyzing process is from -50°C until 200°C by using MDSC experiments. The MDSC experiments will separates the total heat flow of DSC into two parts based on the heat flow that does and does not respond to a changing heating rate. MDSC applies a changing heating rate on top of a linear heating rate in order to measure the heat flow that responds to the changing heating rate.

3.2.3 Analysis Using Bomb Calorimeter

Bomb calorimetry is used to determine the enthalpy of combustion, H_g or also known as heat of combustion. Since combustion reactions are usually exothermic (give off heat), H_g is typically negative. The bomb calorimeter consists primarily of the sample, oxygen, the stainless steel bomb, and water. Heat of combustion can be calculated using a formula of [4]:

$$H_g = \frac{tW - e_1 - e_2 - e_3}{m}$$

Where:

t = temperature rise/different

W = 2409.26 cal/°C

e_1 = correction in calories for heat of formation of nitric acid (HNO_3)

e_2 = correction in calories for heat of formation of sulphuric acid

e_3 = correction in calories for heat of combustion of fuse wire

= 2.3 x centimetres of fuse wire consumed in firing

m = mass

3.3 Cost Study

For this research, the cost study focus on the cost production only, covers the cost of equipments and the raw material needs only. The calculation step chosen for the equipment or unit cost is based on Guthrie's correlations. Guthrie's correlations provide more information than most other cost correlation although they are simple to use as other procedures [1]. The value of CEPCI index is 468.2 for 2005 [28] and value of M&S for 4th quarter of 2005 is 1274.8 [27].

3.4 Simulation assumption

The simulation for this project is a process of running the production of Pentaerythritol Tetradodecanoate (PETD) using computer software which is ASPEN Plus® 12.1. Therefore, a set of assumption was applied to simplify the calculation. A model of a continuous isothermal equilibrium reactor is used for the esterification process. The model added up with a distillation column for the separation process. The assumption made was made based on fact that the mathematical model supposed both vapour-liquid and chemical equilibrium in all theoretical stages of the reaction zone and the separation sections [11]. Pressure drop was neglected in the column and the column runs under atmospheric pressure where liquid and vapour phases were ideally mixed. The basic parameters of the apparatus are summarized in Table 3.1.

Table 3.1: Process simulation parameters

Mathematical Model	Parameter	Dimension	Value
Equilibrium reactor	Feed rate	kg/hr	7.2432
	Operation Temperature	°C	180
	Molar ratio Pentaerythritol/Lauric Acid	-	0.25

Distillation Column	Number of stages	-	3
	Reflux Ratio	-	0.9038
	Operation Temperature	°C	180
	Numerical Method	-	Peng-robinson

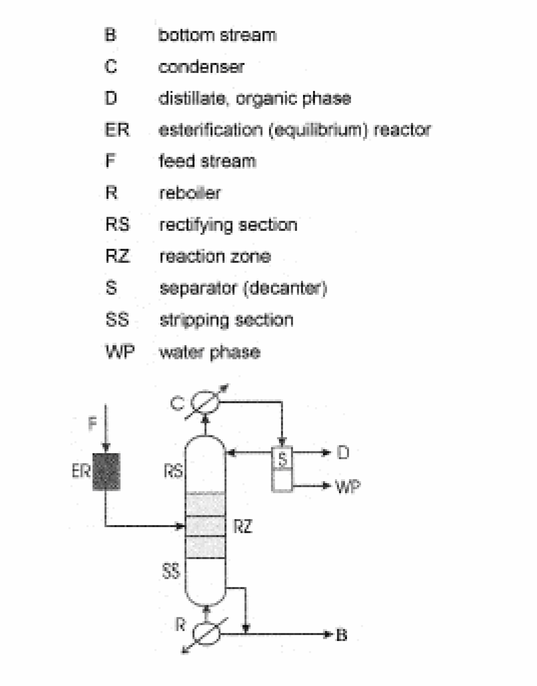

Figure 3.1: Flow sheet of the equilibrium reactor and the distillation column for production of PETD

CHAPTER 4

RESULT AND DISCUSSION

4.1 Process Flow Diagram

The process flow diagram is finalized as shown in figure 4.1. The feed rate for the process is 7.2432 kg per hour which it considers the conversion rate of 0.67 in the reactor.

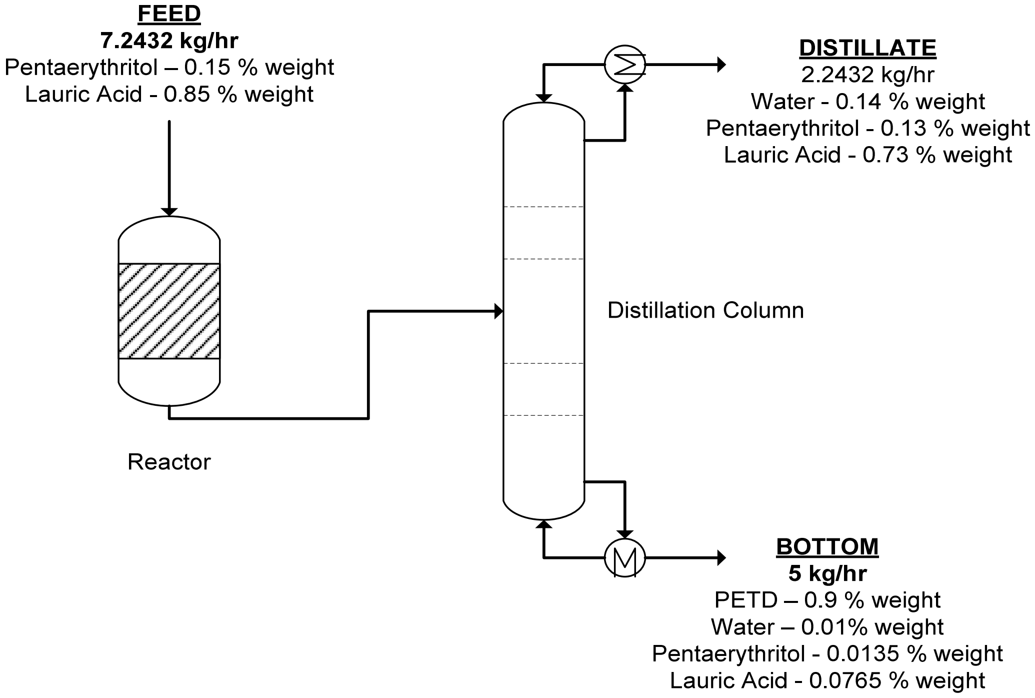

Figure 4.1: Process Flow Diagram (PFD)

4.2 Analytical Result

4.2.1 Thermogravimetric Analysis (TGA)

From analysis done by the TGA experiments, the data of purity and the decomposition point are obtained from the Pentaerythritol Tetradodecanoate (PETD) standard sample provided by Kaneka Chemical (M) Sdn. Bhd. Below are the results of the analysis:

Table 4.1: Percentage of PETD and decomposition point

No. of experiment	**PETD**		**Residue**		**Decomposition Point (°C)**
	Weight (mg)	**%**	**Weight (mg)**	**%**	
1	18.12	94.19	1.084	5.364	368.6
2	21.34	81.55	4.806	18.36	351.87
3	31.02	94.52	1.738	5.296	381.2
4	25.11	78.83	6.722	21.1	341.59
5	23.69	94.21	1.405	5.589	374.16
Average	**23.856**	**88.66**	**3.151**	**11.1418**	**363.484**

Based on average value calculated, the production should reach the minimum value of 88.66% of purity in the PETD. This is to make sure that product produced can meet the quality or standard for the industries or the customers demand.

From figure 4.2, there are 2 lines plotted differently from the other trend. This happens because the material is in powder form where during the analysis, the sample taken randomly from the storage of the powder. Even though the trends are deviated, it is used for the calculation because it affects the overall purity in the sample.

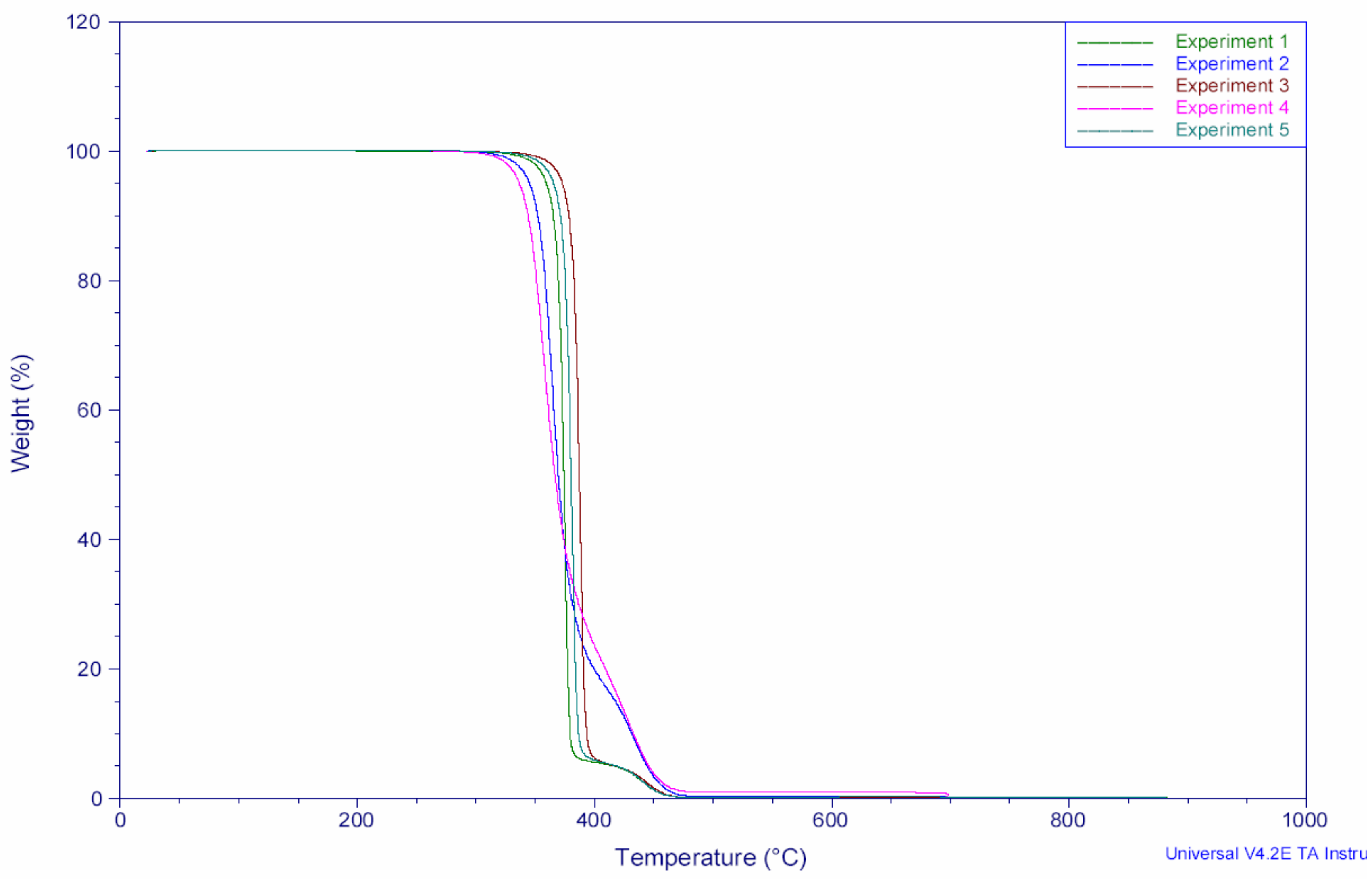

Figure 4.2: Weight Percentage versus Temperature

4.2.2 Differential Scanning Calorimetry (DSC)

From analysis done by the DSC experiments, melting point of the PETD standard samples are at the average of 52°C. From the Universal Analysis software, graph of heat flow versus temperature are plotted to determine the heat of fusion of the samples. The average value of heat of fusion, 1446.66 J/g is extrapolated at onset temperature between 44.03°C – 46.48°C. Below are the results of the analysis:

Table 4.2: Observation of melting

Experiment	**Extrapolated Onset Temperature (°C)**	**Heat of fusion (J/g)**	**Width@half height (°C)**	**Melting Point (°C)**
1	45.69	160.1	9.16	53.14
2	45.6	107.8	10.57	52.98
3	46.48	144.8	9.53	51.98
4	43.54	159.2	10.59	50.67
5	44.03	161.4	10.77	51
Average	**45.068**	**146.66**	**10.124**	**51.954**

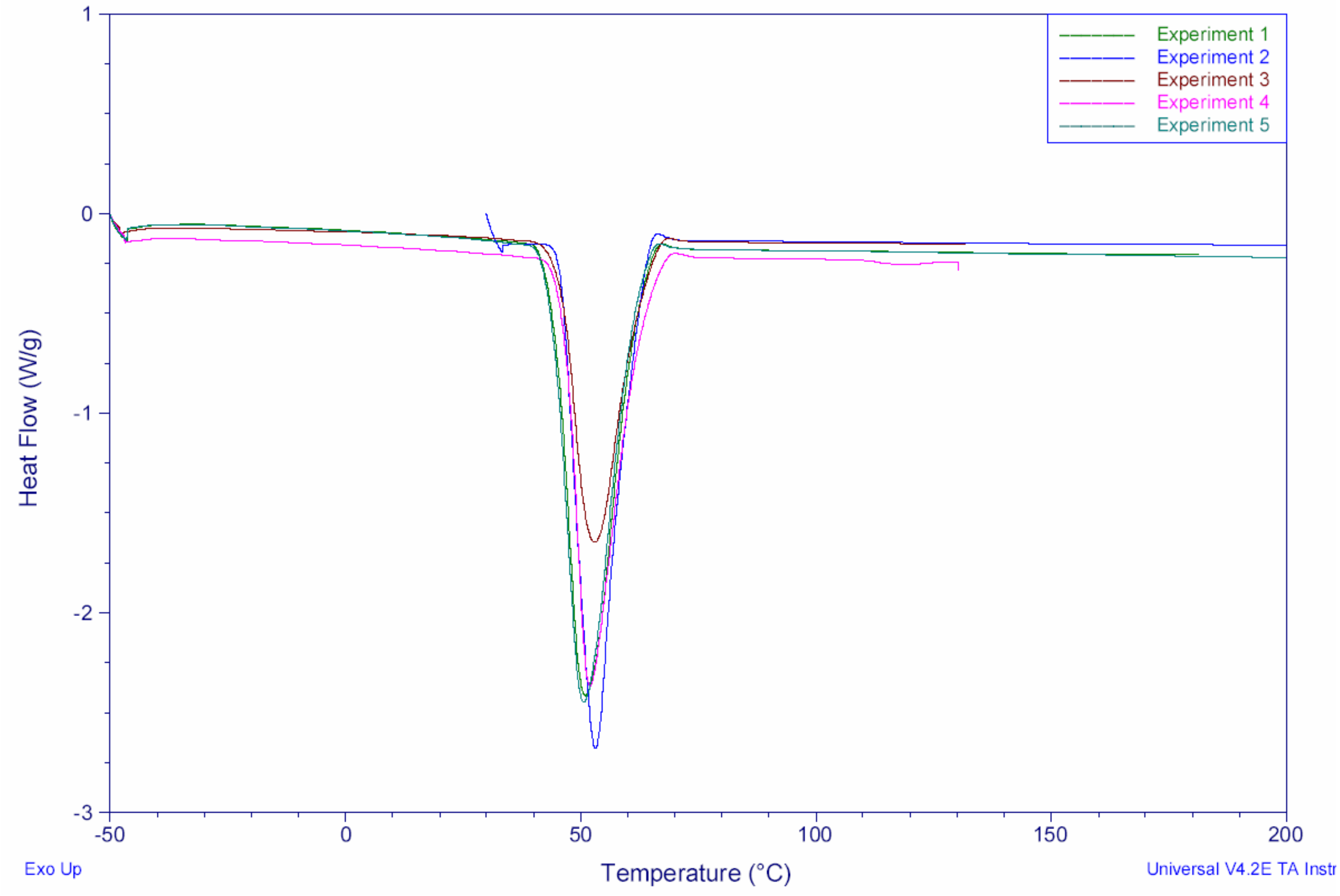

Figure 4.3: Heat Flow versus Temperature

4.2.3 Calorimeter Bomb

From the calorimeter bomb analysis, we obtain the data in terms of temperature rise versus time. From calculation done based on the temperature rise data, the value of heat of combustion for Pentaerythritol Tetradodecanoate (PETD) is -9521.8359 cal/g. Since that the value of the combustion is negative, it shows that the combustion released heat.

Table 4.3: Temperature Rise in Calorimeter Bomb

Time (min)	**Experiment 1 (°C)**	**Experiment 2 (°C)**	**Experiment 3 (°C)**
1	28.6	29.6	30
2	28.6	29.6	30.2
3	28.6	29.6	30.2
4	28.6	29.6	30.2
5	28.6	29.6	30.2
6	31.6	31.8	32.5
7	34.1	34.2	35
8	34.7	34.8	35.9
9	34.9	35.1	36.2
10	35	35.2	36.3
11	35	35.2	36.3

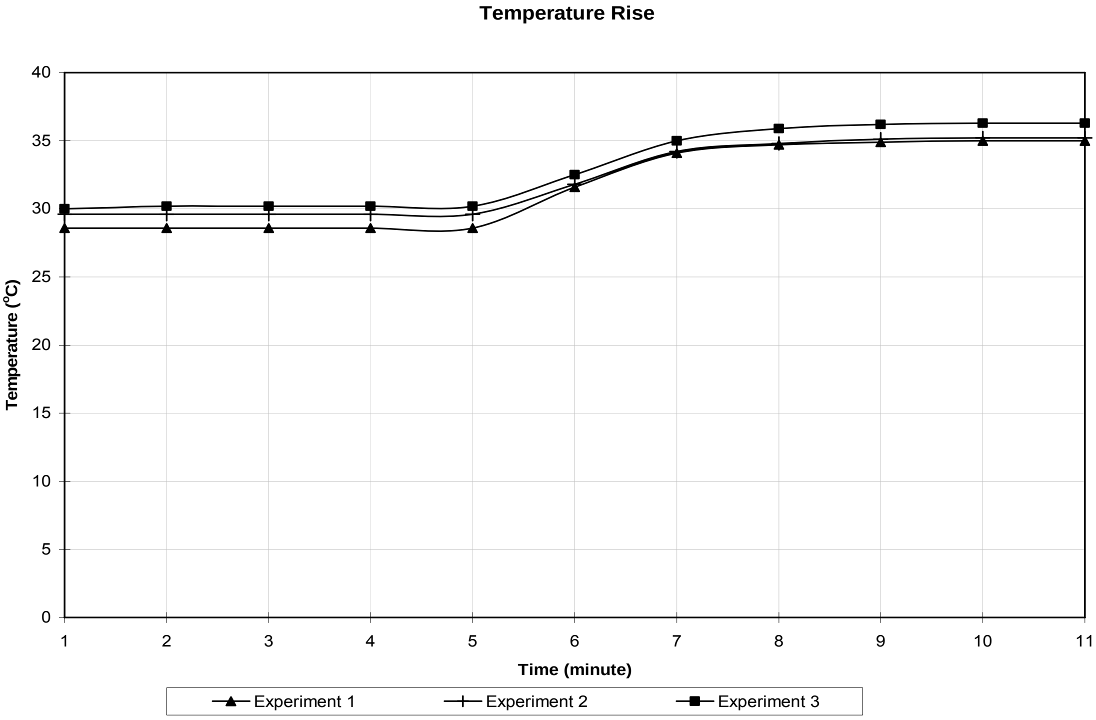

Figure 4.4: Temperature rise profile

4.3 Hierarchy of Decision

4.3.1 Level 0: Input Information

1. Reaction information

(a) Reactions:

Pentaerythritol + 4 Lauric Acid $\rightleftharpoons$ PETD + 4 Water

(b) Reaction conditions:

Reactor inlet temperature = 180°C

Reactor pressure = 1 atm

(c) Condition: Liquid Phase

(d) Catalyst: No

2. Production rate = 5 kg/hr

$= 5.778 \times 10^{-3}$ kmol/hr

3. Product purity:

$x_B \geq 0.8866$

4. Raw materials: Pentaerythritol 100% and Lauric Acid 98%

5. Constraints: No

4.3.2 Level 1: Batch versus Continuous

Choose a continuous process.

4.3.3 Level 2: Input-Output Structure

1. Purify feed streams: Do not purify the Pentaerythritol and Lauric Acid because the purity is very high. So, there is no need to add up a separation system for the feed streams
2. Reversible by-products: There is only one reaction occurs to produce PETD and the reversible reaction does not produce a by –product. So, the process does not consider any recycle loop.
3. Recycle and purge: Since a reactant (Pentaerythritol and Lauric Acid) boil higher than propylene, we don’t need a gas recycle and purge stream.

Table 4.4: Component destination

Component	NBP, °C	Destination
PETD	1368.54	Primary product
Water	100	Waste

Lauric Acid	225	Waste
Pentaerythritol	276	Waste

4. Number of product streams: The component boiling points and destinations are given in Table 4.1. The water, lauric acid and pentaerythritol are lumped as one product streams and PETD are in one product stream. Thus the flowsheet is given in Figure 4.1.

5. Material balances and stream costs: Let

P_{PETD} = 5778 mol/hr

X = 0.75

Y_{PH} = 0.4

Table 4.5: Stream cost

Material	**Value**
PETD*	C_{PETD} = \$100.00/kg = \$86.54/mol
Pentaerythritol	C_A = \$59.00/kg = \$8.03/mol
Lauric Acid	C_B = \$68.64/kg = \$13.75/mol

4.3.4 Level 3: Recycle Structure of the Flowsheet

1. Only one reactor is required since there is only one reaction take place at same temperature and pressure.
2. No recycle streams.
3. No gas-recycle compressor required.

4.3.5 Level 4: Separation System

1. Vapor recovery system: No
2. Liquid recovery system: Distillation column

i. Temperature = 180 °C
ii. Pressure=1 atm
iii. Stages = 3 (minimum)
iv. Reflux Ratio = 0.903788422

4.3.6 Level 5: Heat Exchanger Network

No heat integration.

4.4 ASPEN Plus Simulation

In this study, the esterification reactor was calculated with the aid of build-in equilibrium models. The final product of Pentaerythritol Tetradodecanoate (PETD) achieved at the bottom product of the distillation column, which has the flowrate of 5 kg/hr. The PETD purity is at 89% of total product weight.

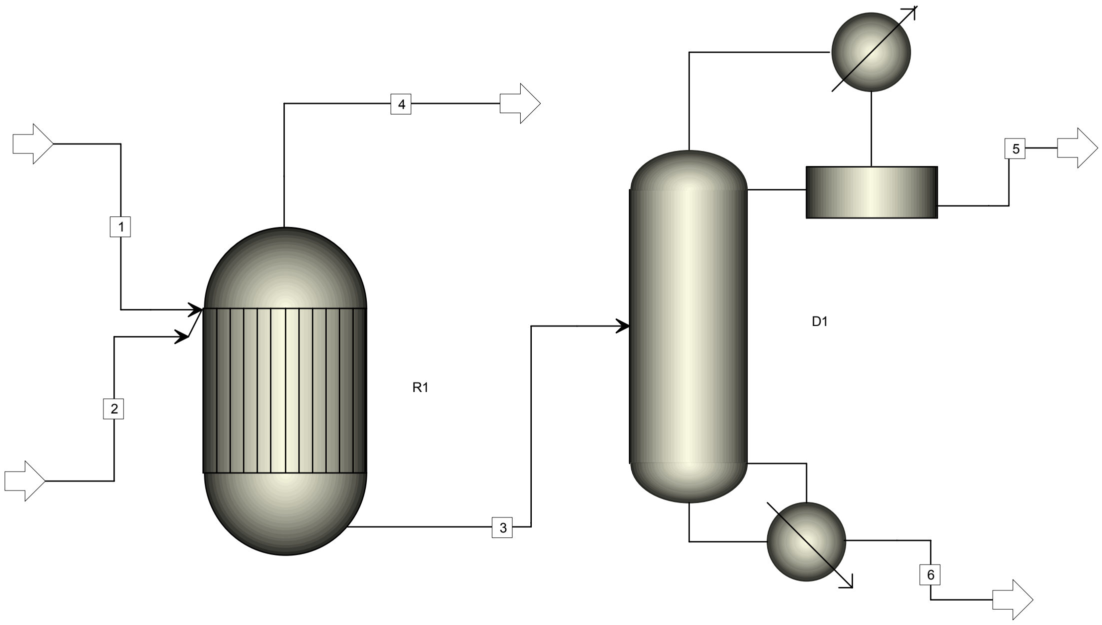

Figure 4.5: Simulation Flowsheet Diagram

Table 4.6: Stream Result

Reactive Distillation							
Stream ID		1	2	3	4	5	6
Temperature	C	100.0	100.0	180.0		90.0	91.1
Pressure	bar	1.013	1.013	1.013	1.013	1.013	1.013
Vapor Frac		0.000	0.000	0.000		0.000	0.000
Mole Flow	kmol/hr	0.008	0.031	0.039	0.000	0.030	0.009
Mass Flow	kg/hr	1.086	6.157	7.243	0.000	2.243	5.000
Volume Flow	cum/hr	< 0.001	0.007	0.044	0.000	0.003	0.055
Enthalpy	MMkcal/hr	-0.002	-0.005	-0.006		-0.003	-0.003
Mole Flow	kmol/hr						
N-DOD-01			0.031	0.010		0.007	0.003
PENTA-01		0.008		0.003		0.002	0.001
PETD				0.005		< 0.001	0.005
WATER				0.021		0.020	0.001

4.5 Chemical properties estimation

The estimation of properties are made base on Peng-Robinson models obtained by using ASPEN Plus simulation engine calculation. Properties estimated are as below:

Table 4.7: PETD Pure Component Properties

Property Name	Parameter	Estimated value	Units	Method
Normal Boiling Point	TB	1641.69	K	JOBACK
Critical Temperature	TC	3637.97253	K	JOBACK
Critical Pressure	PC	254613.021	N/sqm	JOBACK
Critical Volume	VC	3.0965	cum/kmol	JOBACK
Critical Compres.Fac	ZC	0.02606543		DEFINITI
Ideal Gas Cp at 300 K		1285584.19	J/kmol-K	BENSON

At 500 K		1914847.61	J/kmol-K	BENSON
At 1000 K		2811838.96	J/kmol-K	BENSON
Std. Ht.of Formation	DHFORM	-2.42E+09	J/kmol	BENSON
Std.Free Energy Form	DGFORM	-843260000	J/kmol	JOBACK
Vapor Pressure at TB		101233.515	N/sqm	RIEDEL
At 0.9*TC		194970.433	N/sqm	RIEDEL
At TC		254613.021	N/sqm	RIEDEL
Acentric Factor	OMEGA	-0.6586047		DEFINITI
Liquid Mol Vol at TB	VB	17.569871	cum/kmol	GUNN-YAM
PARACHOR	PARC	2246.2		PARACHOR

4.6 Production Cost

The cost study only covers the main equipment which is the reaction unit and the separation unit. The currency used for the calculation is based on the dollar of United States of America (USD). The total of the grass-roof capital (GRC) in this study is USD 3528.87. The total capital investment (TCI) which is the total amount invested to buy all the basic need to start the production and it is estimated about USD 9972.60. The overall total manufacturing cost is estimated around USD 1,362,388.13 per year or USD 34.40 per kg of Pentaerythritol Tetradodecanoate (PETD) produced. The total of general expenses is estimated around USD 173,553.85 per year or USD 4.38/kg PETD. Lastly, the total production cost that has been estimated is around USD 4,337,342.31 per year or also equal to USD 109.53 per kg of PETD.

Since there is no source of product unit price found, the calculations are limited until the total cost of production. Selling price of the PETD actually can be estimated from the total production cost. Usually the selling price should be higher than the total production cost to gain profit at the end.

CHAPTER 5

CONCLUSION AND RECOMMENDATIONS

5.1 Conclusion

From this research, it can be conclude that the process flow sheet produced in this project is one of the alternatives available in the production of Pentaerythritol Tetradodecanoate (PETD).

From the rigorous analysis, apparently some of the properties of PETD were found. Hence, it gives the basic information and limited specification of the PETD since it is a new compound to be produced.

Meanwhile, the cost study is a way to estimate the economic side of the production as well as doing the optimization process. The value of cost of production is USD 109.53 per kg of product produced. However, the unavailability of the product unit cost becomes a factor that prevents the optimization of the process in terms of doing the review of profit value per unit of the overall production.

Moreover, the ASPEN Plus simulation software is a great addition in designing process in order to achieve the optimum design of a production. It can yield and estimate some of the unknown parameters that are needed in the manual calculation. At the end of the project, the conceptual design of PETD production yields 5 kg/hr PETD with 89% purity. Impurities are water 1%, Pentaerythritol 2% and Lauric Acid 8%.

5.2 Recommendations

- The process flow sheet can be used as a reference to construct the pilot plant of the production of 5 kg/hr of Pentaerythritol Tetradodecanoate (PETD)
- Further study should be done on the findings of the other properties of the material through experimental procedures.
- A study of scaling up the plant to a larger capacity should be done in case of a higher need of the market.

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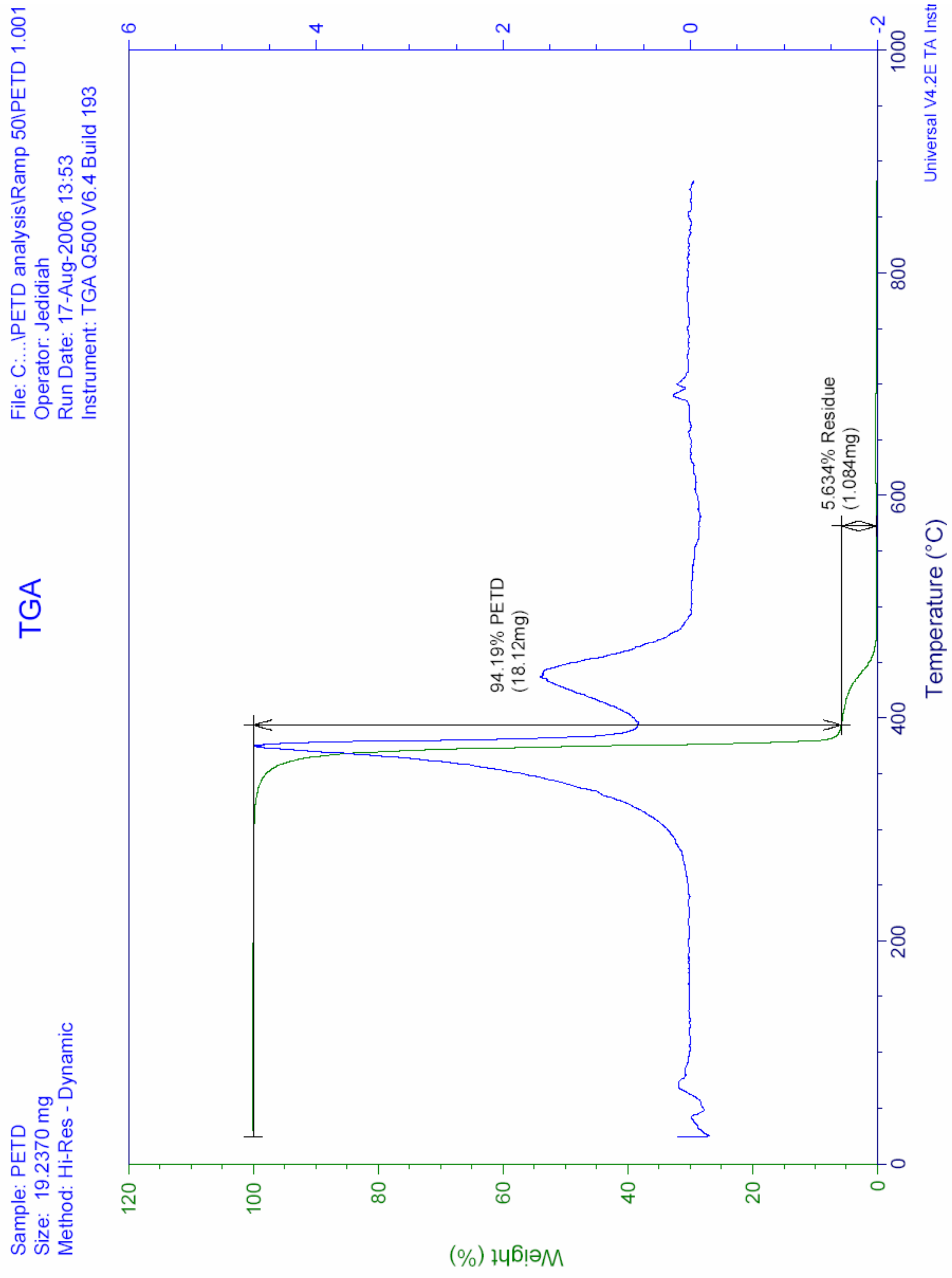
APPENDIX A

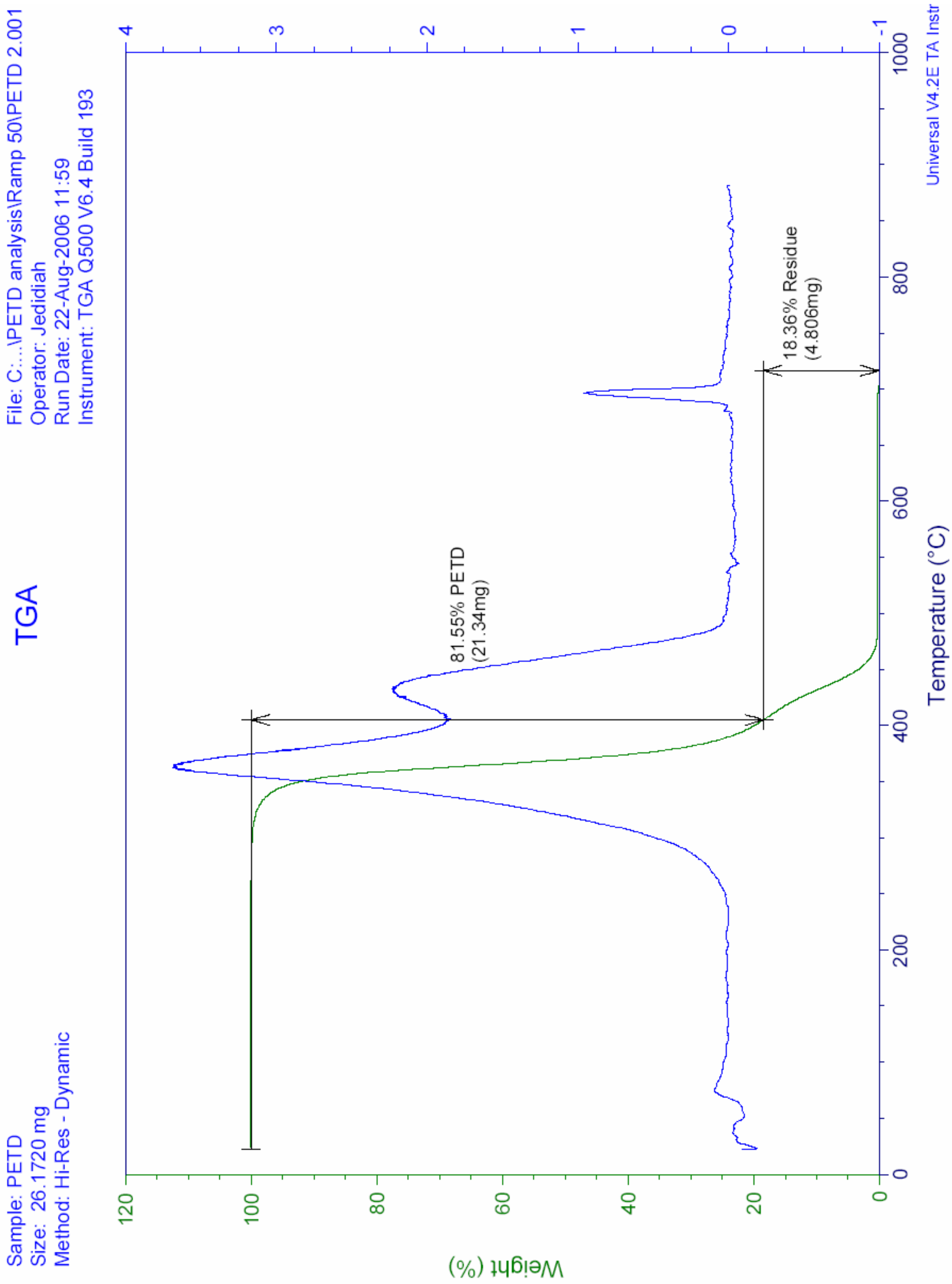
ANALYSIS

Appendix A.1: Plot of TGA analysis

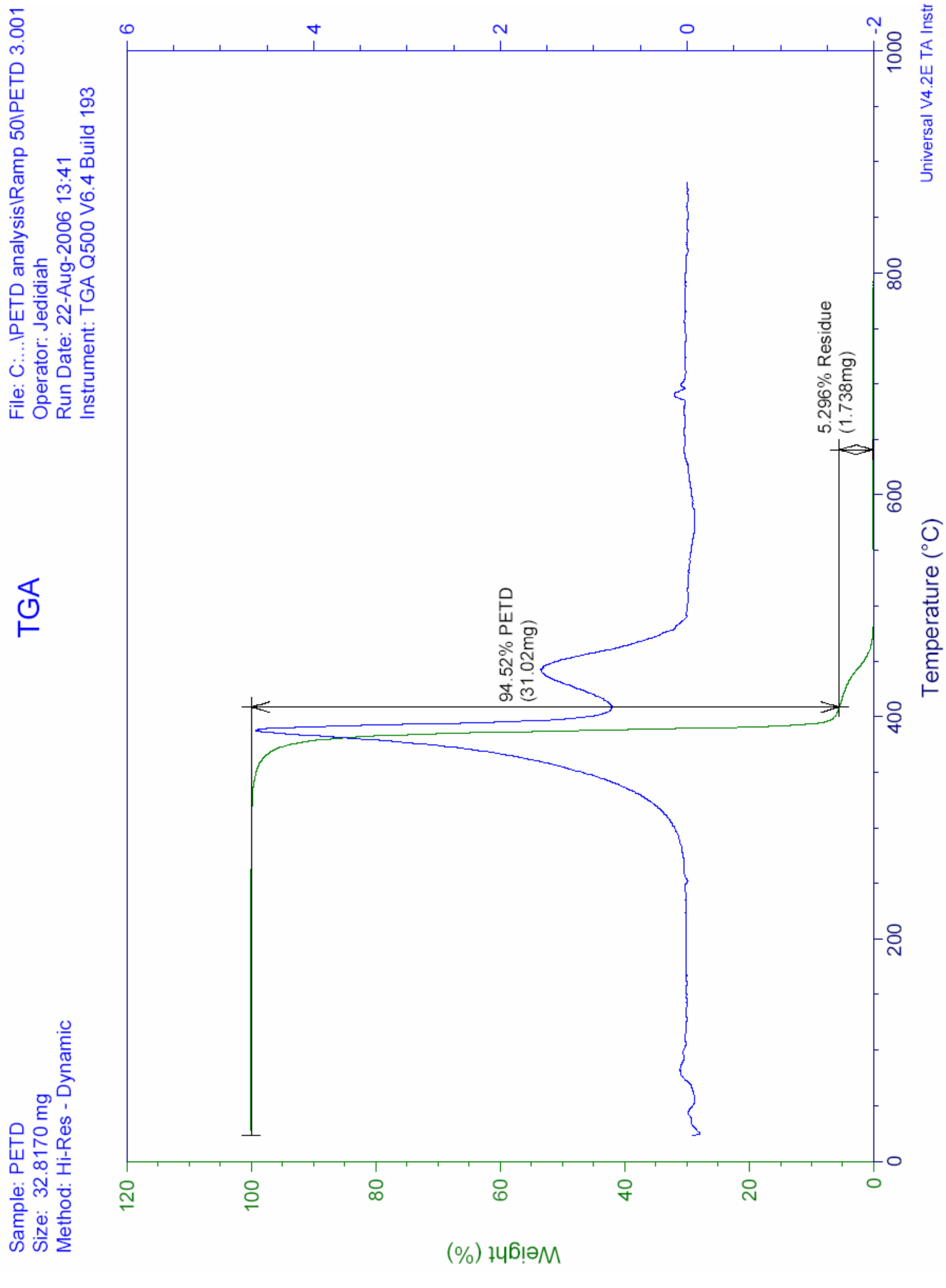
(i) TGA experiment 1



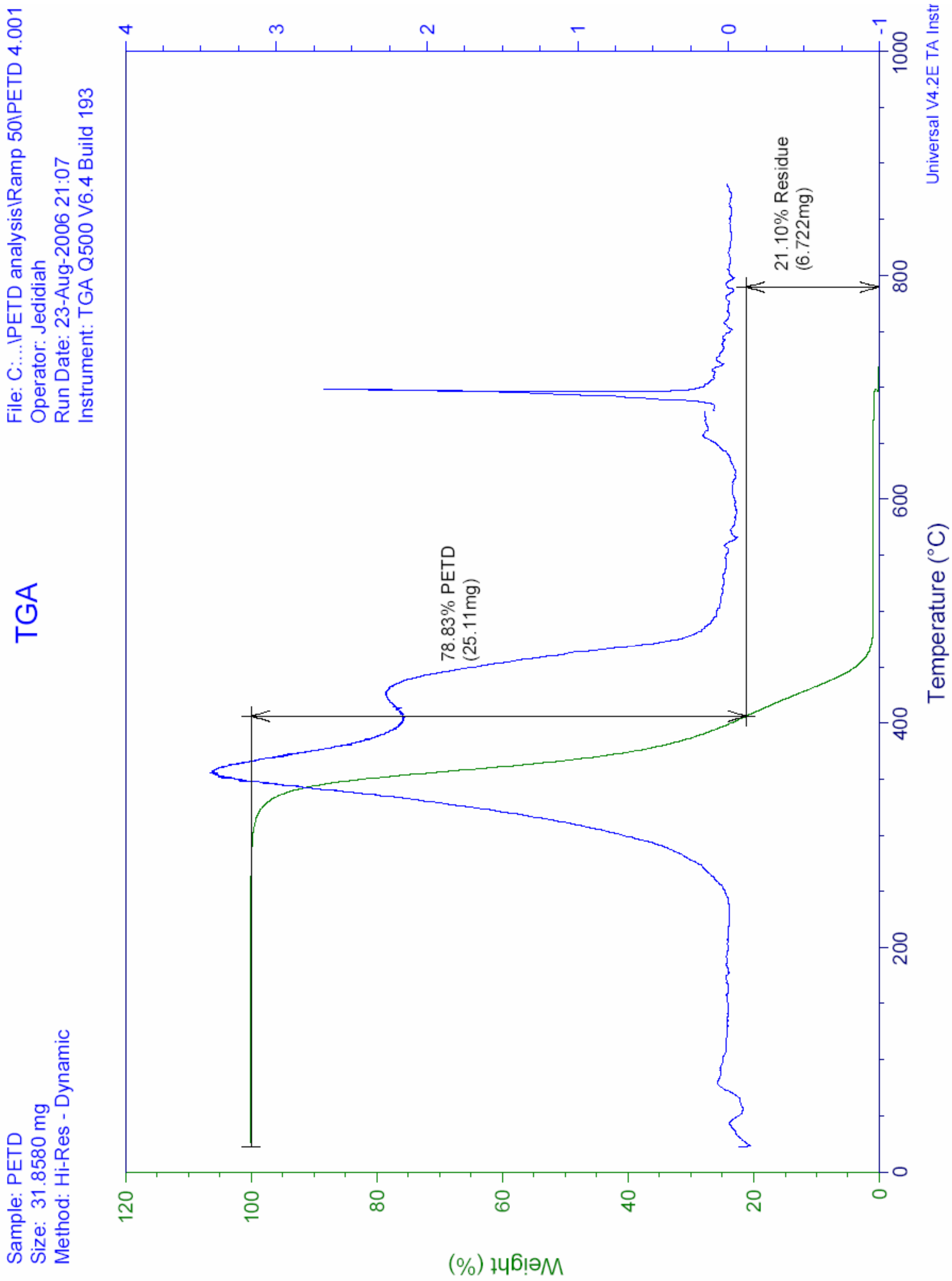
(ii) TGA experiment 2



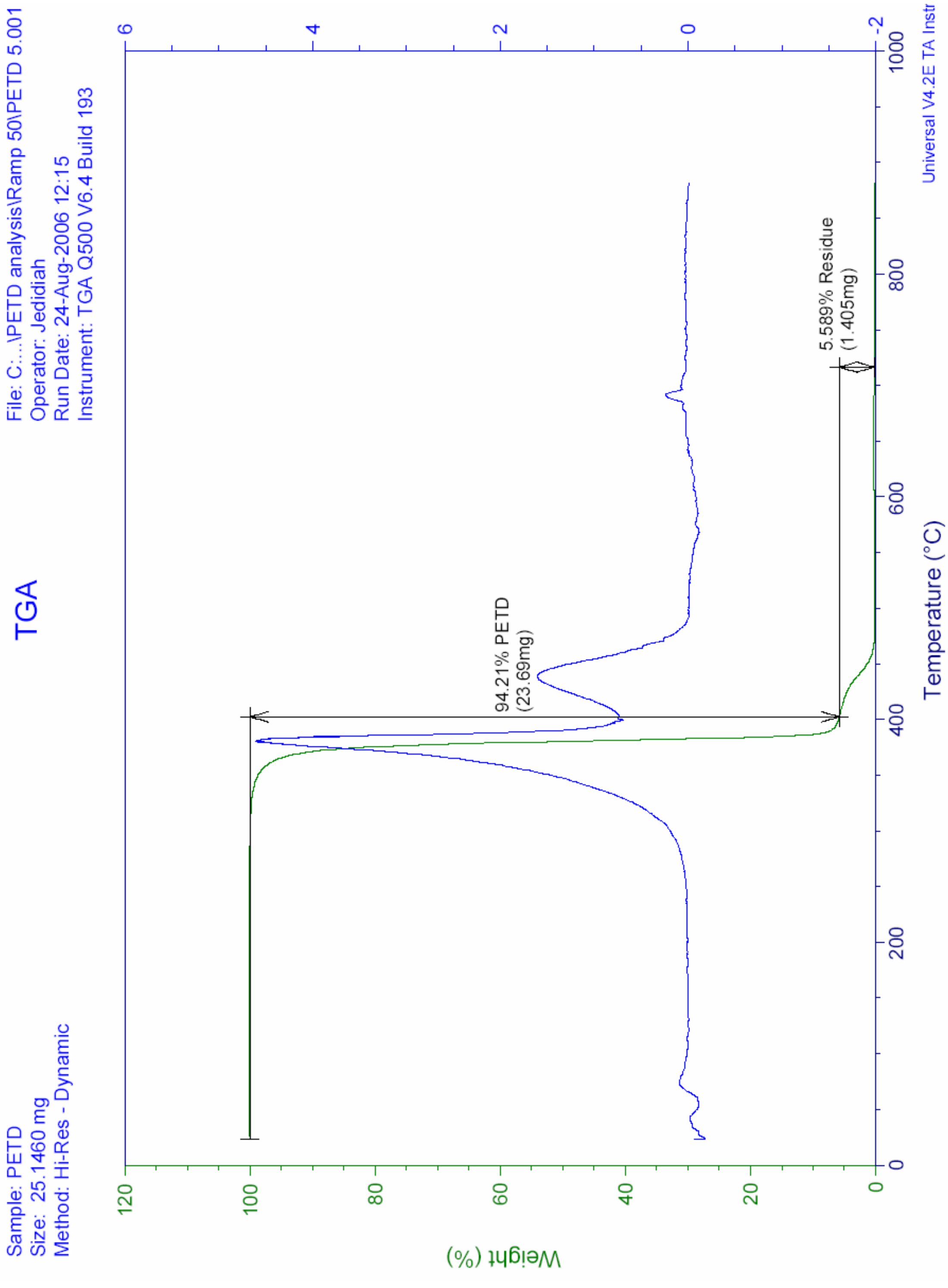
(iii) TGA experiment 3



(iv) TGA experiment 4

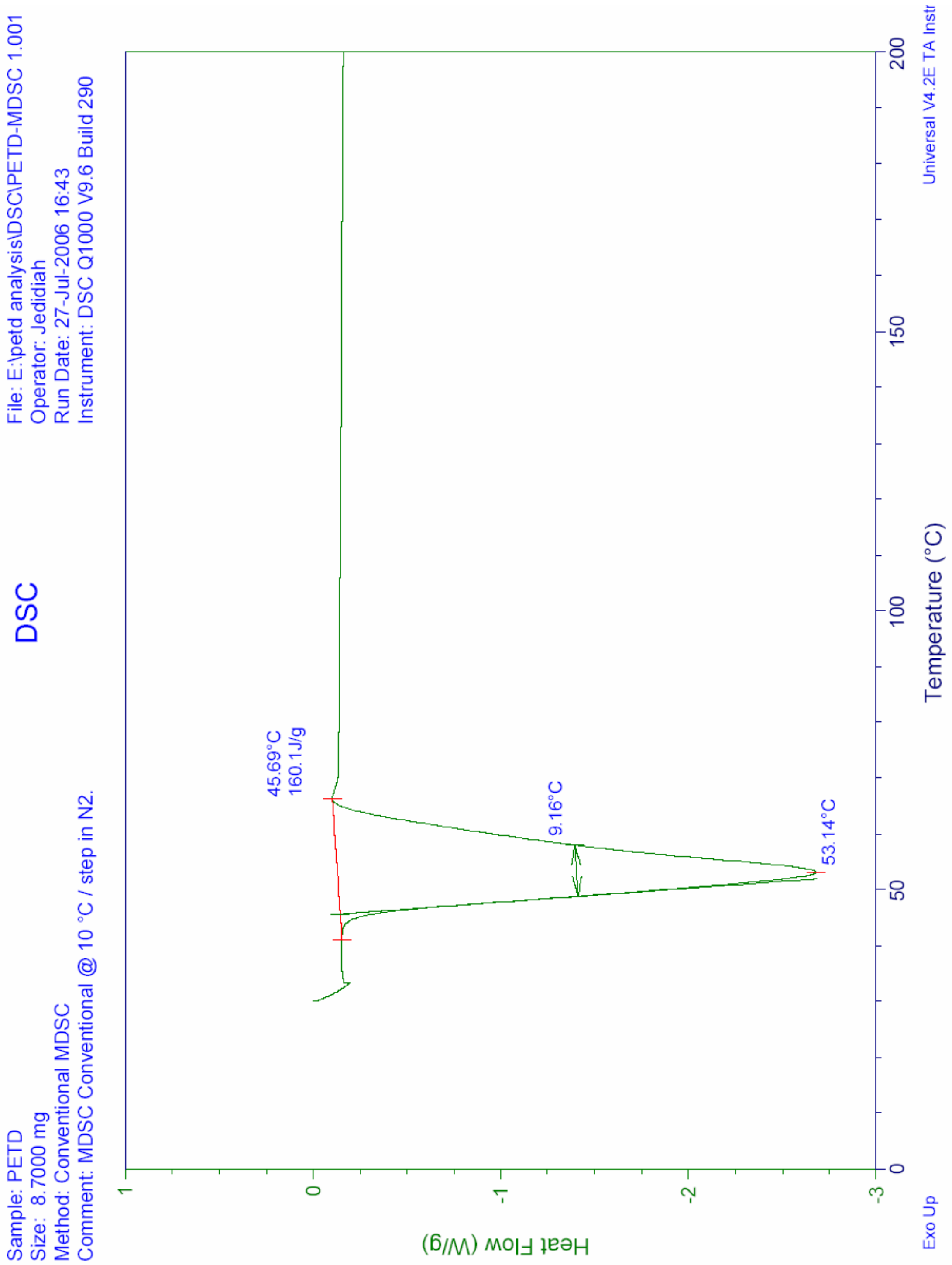


(v) TGA experiment 5

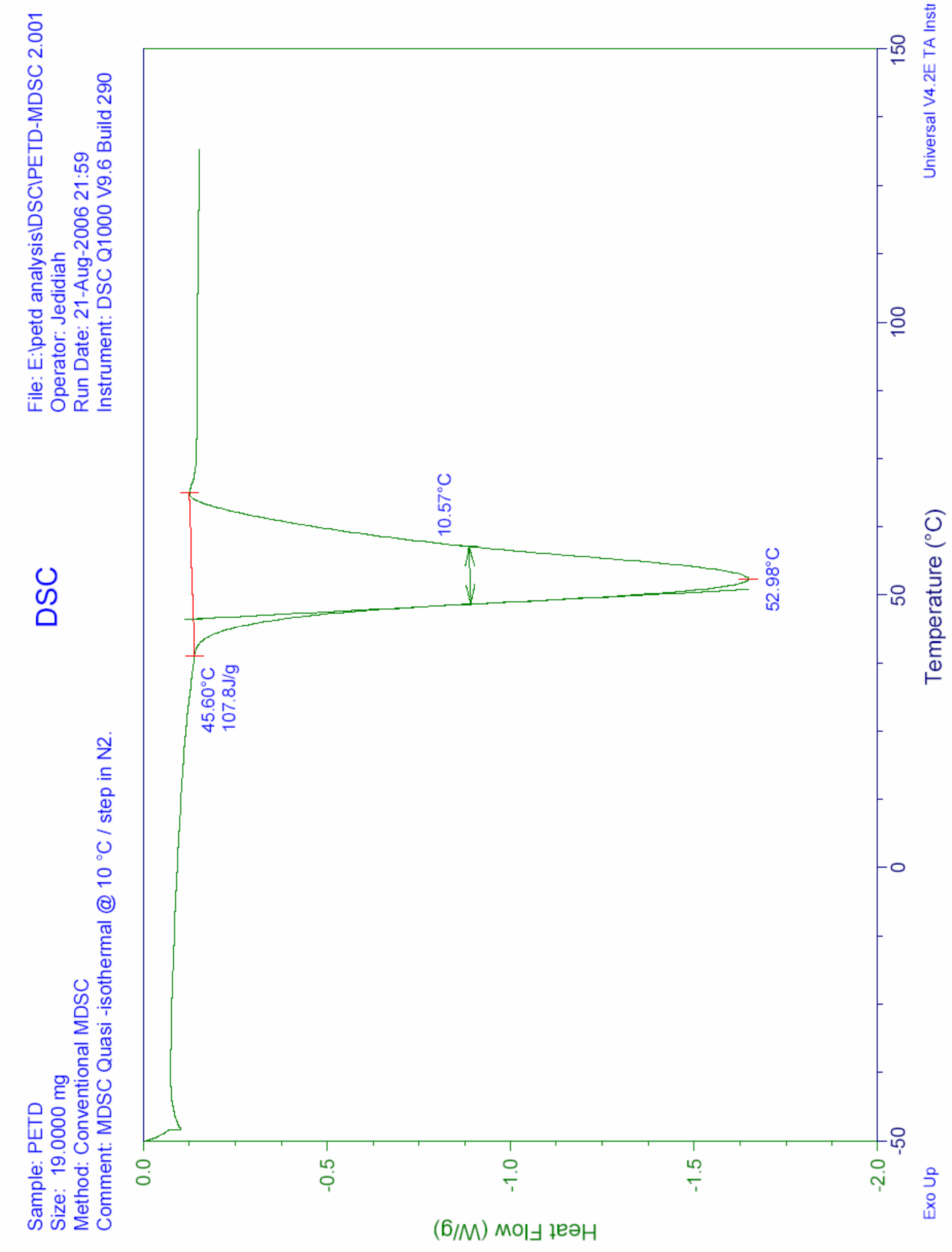


Appendix A.2: Plot of DSC analysis

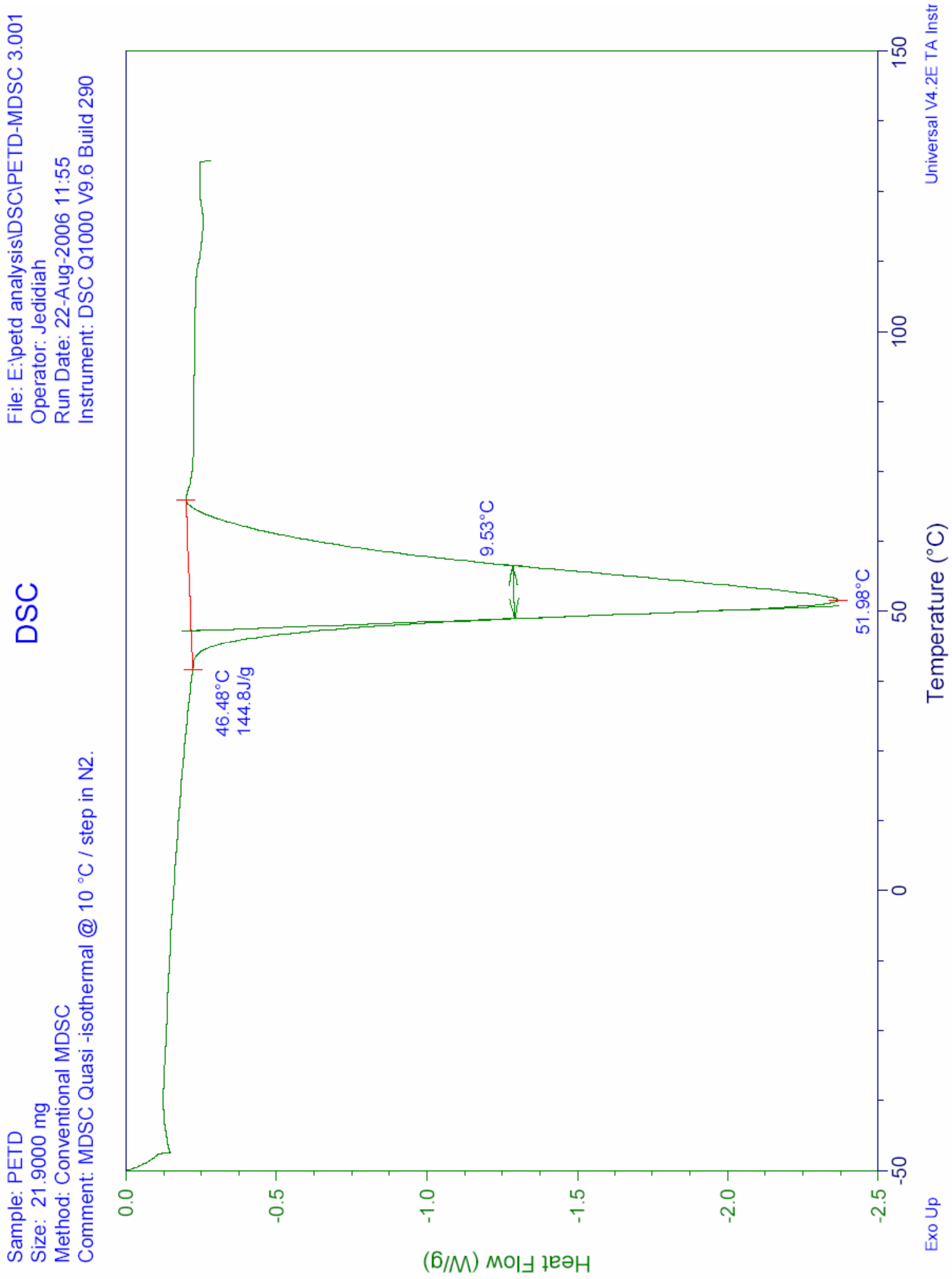
(i) DSC experiment 1



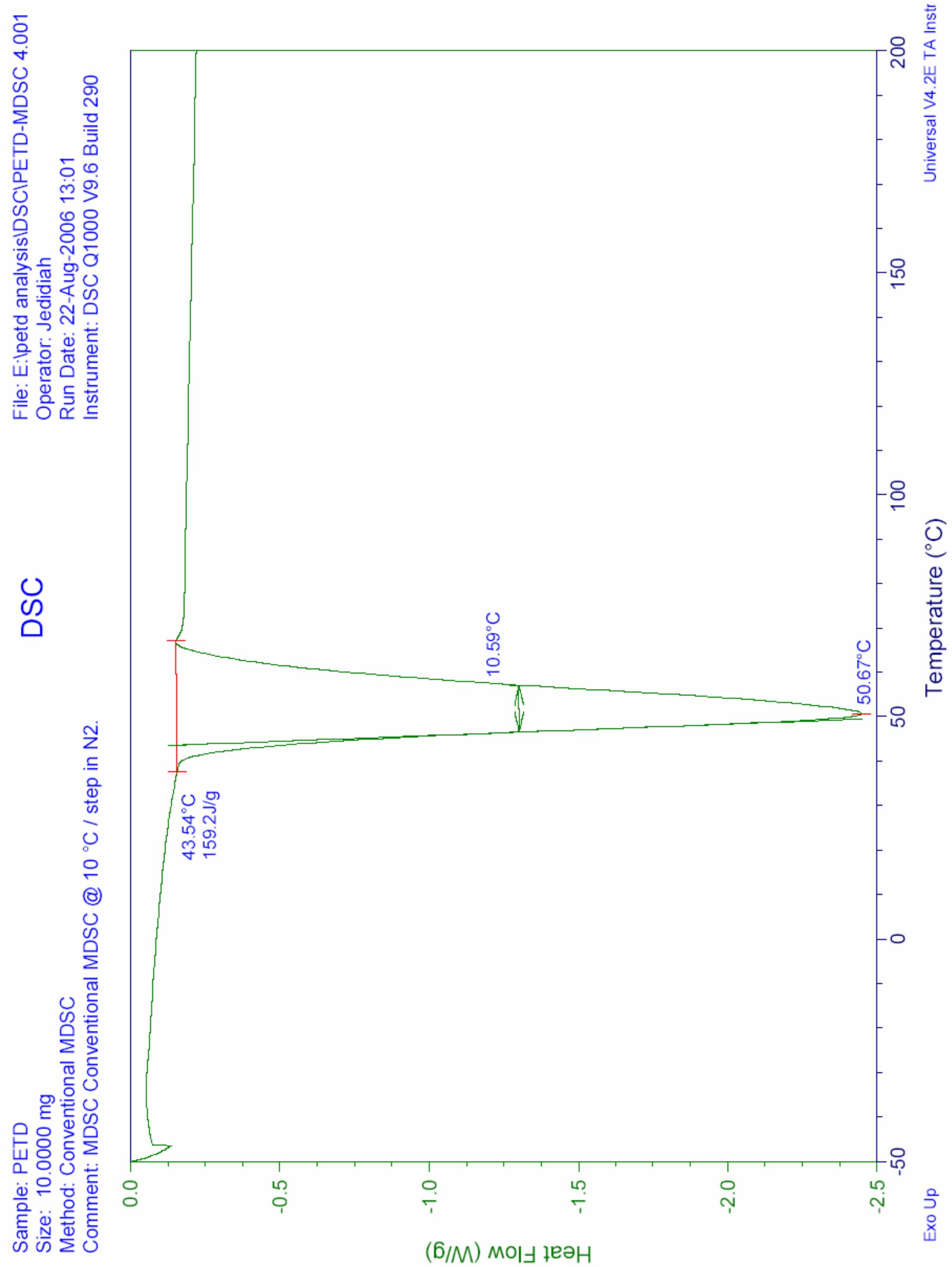
(ii) DSC experiment 2



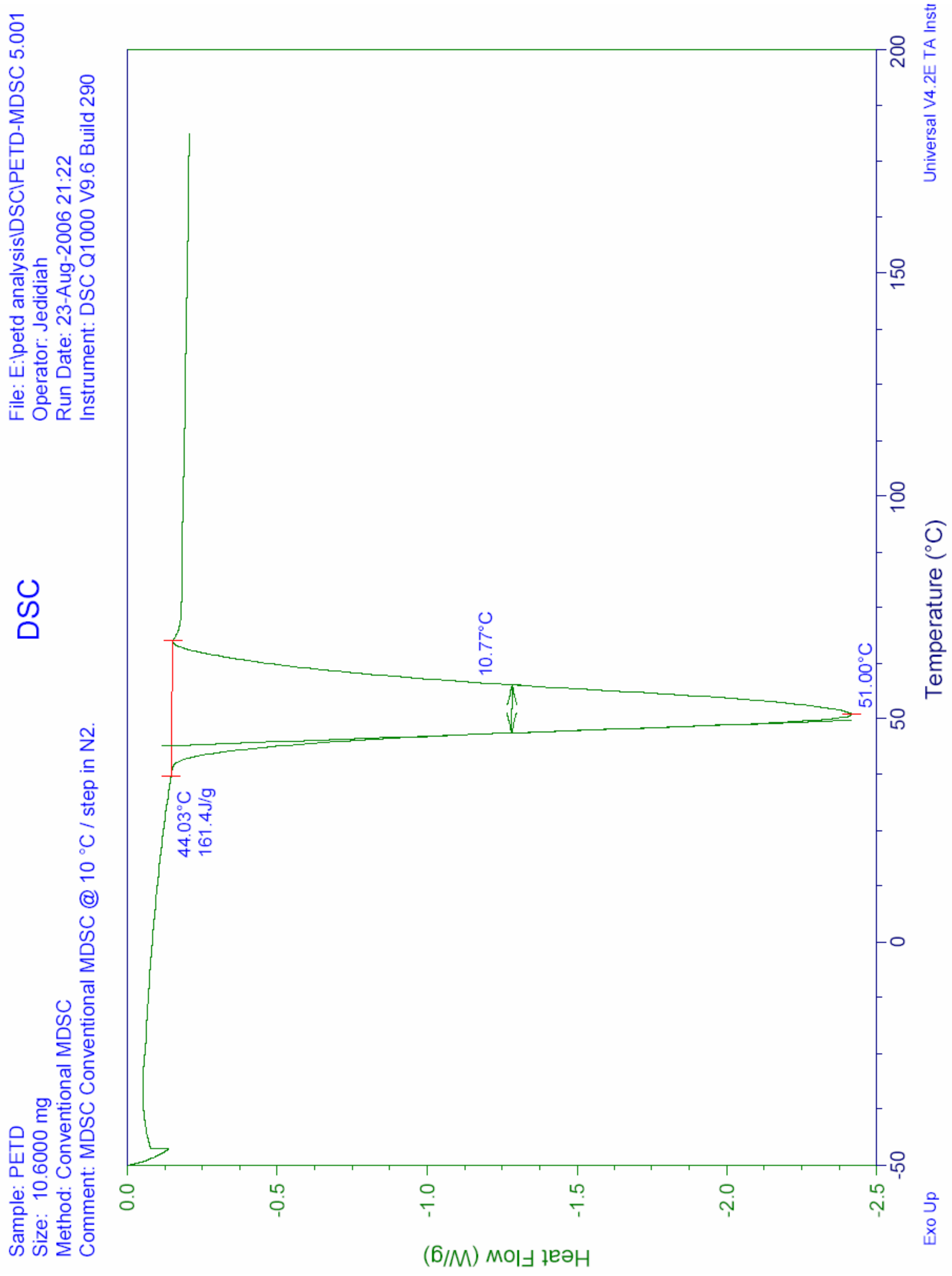
(iii) DSC experiment 3



(iv) DSC experiment 4



(v) DSC experiment 5



APPENDIX B

CALCULATION

Appendix B.1: Sizing and costing for reactor

Reactor Sizing

component	**F(kg/hr)**	**ρL(kg/m3)**	τ	**V(m3)**
Pentaerythritol	1.086	1396	0.083333	0.00013
Lauric Acid	6.157	867.9	0.083333	0.001182
Total				0.001312

Assumption L = 4D

πD3 = 0.001312
D^3 = 0.000418
D = 0.074744 m
= 0.24522 ft

L = 0.298976 m
= 0.980881 ft

- Installed cost = $\left(\frac{1274.8}{280}\right)\left(101.9\times0.24522^{1.066}\times0.980881^{0.802}\right)\left(2.18+1+3.67\right)$

= $ 698.91

Appendix B.2: Sizing and costing for distillation column

Column Calculation:

Determining Tray Numbers And Reflux Ratio

Light key component = Water
Heavy key component = PETD

Overhead light key recovery, ξ_{lk} = 90 %
Overhead heavy key recovery, ξ_{hk} = 5 %

Relative volatility, $\alpha_{lk/hk}$ = **29.4052917**

$\beta_{lk} = \xi_{lk}$ = 90 %
$\beta_{hk} = 1-\xi_{hk}$ = 95 %

Theoretical Number of Stages

$N_i = 12.3/[(\alpha_{lk/hk}-1)^{2/3}(1-\beta_i)^{1/6}]$
N_{water} = 1.939272962
N_{PETD} = 2.176760302
N_{total} = 2.129262834

Reflux Ratio

$R_i = 13.8/[(\alpha_{lk/hk}-1)^{0.9}(1-\beta_i)^{0.1}]$

R_{water} = 0.854711915
R_{PETD} = 0.916057549
R_{tota}l= 0.903788422

Determining the Column Height

Assume efficiency, ɥ = **0.8**

$N_{actual} = N_{total}$/ɥ = **2.661578542**

Assume a two-foot (0.6m) tray spacing;

Tray stack = (N-1)(0.6m), (m)	0.506449
Extra feed space, (m)	1.5
Disengagement space, (m)	3
Skirt height, (m)	1.5
Column Height (m)	**6.506449**
Column Height (ft)	**21.34636**

Determining the Column Diameter

Component	Feed(kmol/hr)	Distillate(kmol/hr)	Bottom(kmol/hr)	Mwi
PETD	0.005200076	0	0.005200076	865.372
Water	0.020800303	0.018024885	0.002775419	18.0153
Total	**0.026000379**	**0.018024885**	**0.007975494**	

D = 0.018024885
L = 0.016290682
V = 0.034315567

Calculation for bottom section

Pressure= 101.325 kPa
Temperature = 364.25 K

Top liquid density, ρ_l = 547235.5 g/m^3

From ideal gas law,
Top gas density, $\rho_g = PM/RT$ = 602.7657 g/m^3

L' = L*Mw = 4.353995 kg/s

V' = (V+F)*Mw = 3.935704 kg/s

Liquid vapor flow factor, $F_{LV} = (L'/V')*(\rho_g/\rho_l)$ = 0.929962

K_1= 0.0075 (From figure 11.27, RK Sinnott, Chem. Eng. Design 4th Ed., Elsevier.)

$u_f = K_1\sqrt{[(\rho_l-\rho_g)/\rho_g)]}$ = 0.225858 m/s

$D_c = [4V'/(0.8\pi\varepsilon\rho_g u_f)]$^0.5 = **0.247669 m = 0.812551 ft**

* Assume sieve trays,ε= 0.75

- Installed cost $_{\text{column}} = \left(\frac{1274.8}{280}\right)\left(4.7 \times 0.81551^{1.55} \times 21.34636\right) \times \left(2.2 + 0 + 1.7\right)$

  = $ 1298.63

Condenser calculation:

Duty, Q = 1.3361351 kW

T_{out} = 330.15 K

T_{in} = 300.15 K

The Overall Heat Transfer Coefficient can be estimated from Table 4.2 (pg. 114, Westerberg) as well as in Perry’s Chemical Handbook. We select U = (250) (5.678) = 1419.5 W/m^2K.

ΔT_{lm} = 63°C

A $= \frac{Q_C}{U\Delta T_{lm}}$

A $= 0.01494\ \text{m}^2$

$= 0.1608\ \text{ft}^2$

- Installed cost $_{\text{condenser}}$ $= \left(\frac{1274.8}{280}\right)\left(101.3 \times 0.1608^{0.65}\right) \times 2.29$

  = $ 321.99

Reboiler calculation:

Duty, Q = 0.10685468 kW

T_{out} = 503.15 K

T_{in} = 523.15 K

The Overall Heat Transfer Coefficient can be estimated from Table 4.2 (pg. 114, Westerberg) as well as in Perry's Chemical Handbook. We select U = (50) (5.678) = 283.9 W/m^{2}K.

ΔT_{lm} = 158.9°C

A $= \frac{Q_R}{U\Delta T_{lm}}$

A $= 0.002369\ \text{m}^2$

$= 0.0255\ \text{ft}^2$

- Installed cost $_{\text{reboiler}}$ $= \left(\frac{1274.8}{280}\right)\left(101.3 \times 0.0255^{0.65}\right) \times 4.16$

  = $ 415.08

- Distillation column total installed cost = $ 1298.63 + $ 321.99 + $ 415.08

  = $ 2035.70

APPENDIX C

SIMULATION RESULT

Appendix C.1: Reactor simulation result

Summary

Outlet temperature:	180	C
Outlet pressure:	1.01325	bar
Heat duty:	1.19236357	kW
Net heat duty:	1.19236357	kW

Mass and energy balance

Total		In	Out	Generated	Rel. diff
mole flow	kmol/hr	0.03871436	0.03871436	6.10E-18	-2.17E-17
mass flow	kg/hr	7.2432	7.2432		1.44E-07
enthalpy	kcal/hr	-6822.9115	-5797.6487		-0.1502676

Kinetic of reaction

No.	Name	k	n	E	To
1	ESTER	1.00E-35	1.00E-35	0	-273.15

Appendix C.2: Distillation column simulation result

Summary

Condenser			**Reboiler**		
Temperature:	-263.15	C	Temperature:	91.1005341	C
Heat duty:	-1.3361351	kW	Heat duty:	-1.07E-01	kW
Subcooled duty:	0.86579035	kW	Bottom rate:	0.00906197	kmol/hr
Distillate rate:	0.02965238	kmol/hr	Boilup rate:	3.87E-07	kmol/hr
Reflux rate:	0.02679948	kmol/hr	Boilup ratio:	4.27E-05	
Reflux ratio:	0.90378842				

Mass and energy balance

Total		In	Out	Rel. diff
Mole flow:	kmol/hr	0.03871436	0.03871436	0
Mass flow:	kg/hr	7.2432	7.2432	-6.49E-10
Enthalpy:	MMkcal/hr	-0.0057976	-0.0062939	0.07885799

Split fraction

Component	Stream	
	5	6
N-DOD-01	0.72213953	0.27786047
PENTA-01	0.80893162	0.19106838
PETD	0.03077555	0.96922444
WATER	0.96487968	0.03512031

TPFQ summary

Stage	Temperature C	Pressure bar	Heat duty kW	Liquid flow kmol/hr	Vapor flow kmol/hr	Liquid feed kmol/hr
1	-263.15	1.01325	-1.3361351	0.02679948	0	0
2	91.0155522	1.01325	0	0.00906236	0.05645186	0
3	91.1005341	1.01325	-1.07E-01	0.00906197	3.87E-07	0

Stage	Vapor feed kmol/hr	Mixed feed kmol/hr	Liquid product kmol/hr	Vapor product kmol/hr	Liquid enthalpy kcal/mol	Vapor enthalpy kcal/mol
1	0	0	0.02965238	0	-111.75969	-616.40565
2	0	0.0387144	0	0	-372.00129	-91.407384
3	0	0	0.00906197	0	-371.99387	-91.44859

Composition

	Vapor				**Liquid**			
Stage	N-DOD-01	PENTA-01	PETD	WATER	N-DOD-01	PENTA-01	PETD	WATER
1	0	0	1	9.98E-35	0.241926	0.075842	0.005	0.67684
2	0.241926	0.0758417	0.0054	0.676836	0.304593	0.058617	0.556	0.08064
3	0.242243	0.0759227	0.00541	0.676428	0.304596	0.058617	0.556	0.08061

K-values

Stage	N-DOD-01	PENTA-01	PETD	WATER
1	0	0	1.00E+20	1.00E-35
2	0.794223	1.29380461	0.00970412	8.39390268
3	0.7950429	1.29498398	0.00971619	8.39521079

Appendix C.3: Utilities simulation result

Summary

Utility type:	WATER		STEAM	
Costing rate:	0.00845215	$/hr	0.0004246	$/hr
Mass flow:	38.4188682	kg/hr	0.21251485	kg/hr
Duty:	1.33613505	kW	0.10685468	kW
Heating/Cooling value:	-125.20114	kJ/kg	1810.11745	kJ/kg
Purchase price:	0.00022	$/kg	0.001998	$/kg
Inlet temperature:	27	C	250	C
Outlet temperature:	57	C	230	C
Inlet pressure:	1	bar	39.73	bar
Outlet pressure:	1	bar	27.97	bar
Inlet vapor fraction:	0		1	
Outlet vapor fraction:	0		0	

APPENDIX D

COSTING

Appendix D.1: Cost evaluation

Equipment	**Actual Bare Cost Module**
Reactor	348.67
Distillation Column	2035.7
TOTAL Bare Cost Module	2384.37
Contigency and fees	429.1866
Total Module Cost	2813.5566
Auxiliary Facilities	715.311
GRASS-ROOF CAPITAL	**3528.8676**

Specification	**Range (%)**	**Cost (RM)**
DIRECT COST		
Onsite		
Purchased Equipment Installation	30 % GRC	1058.66028
Instrumentation and Control (installed)	15 % GRC	529.33014
Piping (installed)	40 % GRC	1411.54704
Electrical and Material (installed)	8 % GRC	282.309408
Offsite		
Building	10 % GRC	352.88676
Yard Improvements	1 % GRC	35.288676
Service Facilities	5 % GRC	176.44338
Land	2% GRC	70.577352
Total 1		**3917.043036**
INDIRECT COST		
Engineering and supervision	5 % GRC	176.44338
Construction Expenses	8 % GRC	282.309408
Contractor's Fee	1.5 % GRC	52.933014
Contingency	10 % GRC	352.88676
Total 2		**864.572562**
Total 1 + Total 2		**4781.615598**
Gross Root Capital (GRC)		3528.8676
Fix Capital Investment (FCI) = GRC + Total 1 + Total 2		**8310.483198**
Working Capital	12 % FCI	997.2579838
Start Up Cost	8 % FCI	664.8386558
Total Capital Investment (TCI)		**9972.579838**

Manufacturing Expenses			
	Specification	**Yearly Cost**	**Cost/kg product**
Direct Production Cost			
Raw Material			
Pentaerythritol	$ 59.00/kg	507,690.37	12.820464
Lauric Acid	$ 68.64/kg	3,346,970.31	84.51945216
Utilities			
Cooling Water	\$ 0.22/m^3	66.941028	0.00169043
Electricity	$ 0.046/kWh	525.71	0.013275506
LP Steam (Credit)	$ 0.001998/kg	3.36	0.00008492
Maintenance and Repairs	3 % FCI	249.31	0.006295821
Operating Supplies	0.5% FCI	41.55	0.001049303
Operating Labor	$ 0.003332/kg product	131.95	0.003332
Direct Supervision & Clerical Labor	15 % operating labor	19.79	0.0004998
Laboratory Charges	10 % operating labor	13.19	0.0003332
Patents and Royalties	0.1 % TPC	4,337.34	0.109528846
Indirect Production Cost			
Local Taxes	1 % FCI	83.10	0.002098607
Insurance	0.5 % FCI	41.55	0.001049303
Plant Overhead	7% TPC	303,613.96	7.667019228
Total Manufacturing Expenses, AME		**4,163,788.46**	105.1461731
General Expenses			
Administration Cost	15 % operating labor, supervision& maintenance.	60.16	0.001519143
Distribution & Selling Expenses	2 % TPC	86,746.85	2.190576922
Research & Development	2 % TPC	86,746.85	2.190576922
Total General Expenses, AGE		**173,553.85**	4.382672988
Total Production Cost, APC = AME + AGE (excluding depreciation)		4,337,342.31	109.5288461