

**Modeling and Simulation of Nonisothermal Plug Flow Reactor for Methanol
Synthesis Via Methyl Acetate Saponification**

by

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Dissertation submitted in partial fulfillment of
the requirement for the
Bachelor of Engineering (Hons)
(Chemical Engineering)

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CERTIFICATION OF APPROVAL

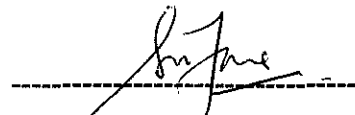
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Approved by,

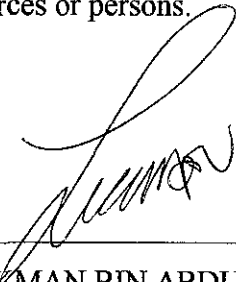
A handwritten signature in black ink, appearing to read 'Suzana', is written over a horizontal dashed line.

(Dr. Suzana Bte Yusup)

**Universiti Teknologi Petronas
Tronoh, Perak Darul Ridzuan
JULY 2004**

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 reference and acknowledgements, and that the original work contained herein have not been taken or done by unspecified sources or persons.



LUKMAN BIN ABDUL KARIM

ABSTRACT

Methanol usage has grown over the centuries since it was first isolated in 1667 by Robert Boyle. It is mainly used for antifreeze, fertilizers, alternative fuel and methyl tert-butyl ether (MTBE). Methanol is mainly produced in gas phase through steam reforming, water-gas shift reaction and direct oxidation. These processes use natural gas as raw materials and operate at extreme temperature and pressure. This report proposes an alternative way to synthesize methanol in liquid phase via saponification of methyl acetate and calcium hydroxide. A program that models and simulates the saponification of methyl acetate in a Plug Flow Reactor is developed using MATLAB Programming. Mole balance and energy balance which produce the ordinary differential equations is used to solve the conversion and temperature profile respectively. In this report, the comparison of using the adiabatic and heat effects of the reactor will be discussed with reference to the experimental data. The optimum operating conditions were found to be at 326K with 0.01M inlet concentration of methyl acetate. The net conversion of methyl acetate was 97%. The methyl acetate conversion rises as the temperature rises and the Cauchy numerical method best solves the ordinary differential equations of this saponification reaction.

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NOMENCLATURE

| | | |
|---|---|---|
| a | = | Heat Transfer Area (m^2/m^3) |
| C_a | = | Concentration of methyl acetate |
| C_b | = | Concentration of calcium hydroxide(mol/m^3) |
| C_c | = | Concentration of methanol (mol/m^3) |
| C_d | = | Concentration of calcium acetate (mol/m^3) |
| C_{ao} | = | Initial concentration of methyl acetate (mol/m^3) |
| C_{bo} | = | Initial concentration of calcium hydroxide (mol/m^3) |
| C_{pa} | = | Heat capacity of methyl acetate($\text{J}/\text{mol}.\text{°C}$) |
| C_{pb} | = | Heat capacity of calcium hydroxide ($\text{J}/\text{mol}.\text{°C}$) |
| C_{pc} | = | Heat capacity of methanol ($\text{J}/\text{mol}.\text{°C}$) |
| C_{pd} | = | Heat capacity of calcium acetate ($\text{J}/\text{mol}.\text{°C}$) |
| h | = | Step size |
| k_a | = | Reaction constant ($\mu\text{mol}/\text{g}_{\text{cat}}.\text{s}.\text{kPa}^2$) |
| R | = | Rate of reaction |
| r_a | = | Rate of reaction in term of methane conversion |
| T | = | Temperature ($\text{K}/\text{°C}$) |
| T_a | = | External gas temperature (°C) |
| T_o | = | Inlet / initial temperature (°C) |
| U | = | Overall heat transfer coefficient ($\text{W}/\text{m}^2.\text{K}$) |
| V | = | Volume of reactor (m^3) |
| X_a | = | Methane conversion |
| ΔH_{RXN} | = | Heat of reaction (J/mol) |
| ΔH_{298} | = | Heat of reaction at 298K (J/mol) |
| ΔC_p | = | Heat capacity ($\text{J}/\text{mol}.\text{°C}$) |

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CHAPTER 1

INTRODUCTION

1.1 Background of Study

Natural gas or liquid petroleum gas (LPG) is currently abundant throughout the world and with this, many chemical processes depend on it as feedstock including methanol synthesis. Nevertheless this natural resource is depleting with the passing of every tonne-using day. Please refer to Figure 1-1 and Figure 1-2. There are no longer massive reservoir left unfound and the new reservoirs are at remote areas [1]. Furthermore, the steam reforming, water-gas shift reaction and direct oxidation releases carbon dioxide (CO_2) and carbon monoxide (CO) to the atmosphere, which could cause air pollution. So, alternatives processes that differ from the conservative or mainstream methods are welcome as backup processes. These alternative methods should also take environmental concerns very seriously so the same intolerance doesn't happen again. The current methanol synthesis processes mentioned above also utilize high operating temperature (700 to 900°C) and pressure (30 to 35 bar) [2]. High operating temperature and pressure would increase the operating and maintenance cost of the already exuberant costing plant complex that is made of high heat, pressure and corrosion resistance material. This cost impact will affect the overall cost of the end product, which the every day users buy. The production cost will go down much if the operating temperature and pressure is at room temperature and pressure or at least moderately low. In short, there are many possibilities of upgrading and perfecting the methanol synthesis production or developing new methods to meet the needs of people without the harsh side effect to the environment.

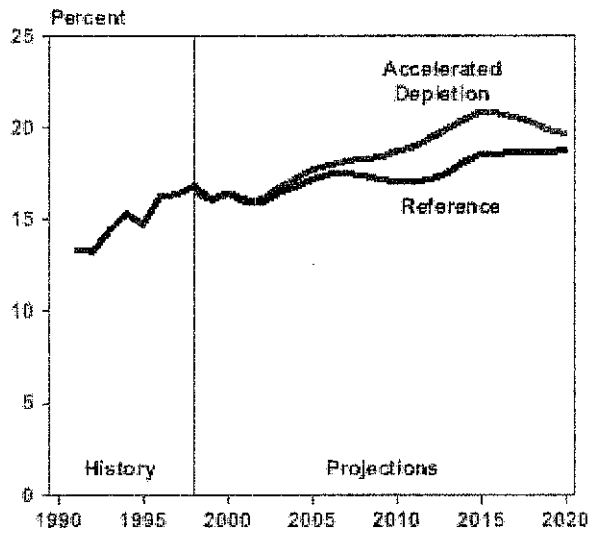


Figure 1-1: Ratio of offshore lower 48 natural gas production to proved reserves, 1991-2020 [3]

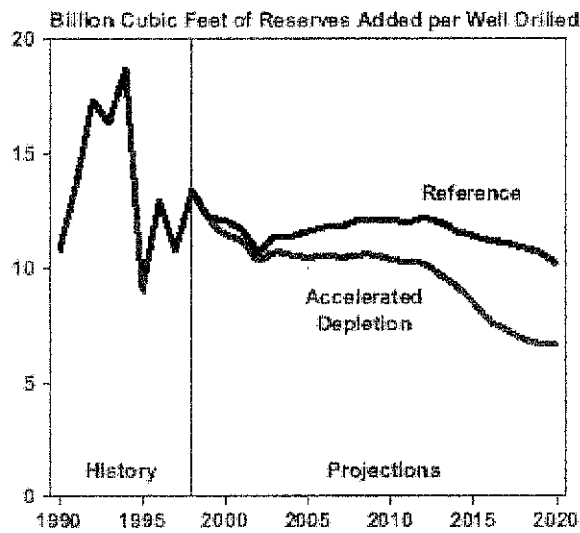


Figure 1-2: Finding rate per well for offshore lower 48 natural gas, 1990-2020

1.2 Problem Statement

The saponification of methyl acetate into methanol is a very attractive route of methanol synthesis in the liquid phase. This reaction offers several advantages because in order to maintain the methanol synthesis in liquid phase, the temperature cannot exceed the boiling point of the reactant and products. Low temperature and pressure will lower the operating and maintenance cost of the plant. Hazards in terms of temperature and pressure will become less for low operating conditions.

The saponification of methyl acetate uses liquid methyl acetate and liquid calcium hydroxide as reactant and will produce liquid methanol and liquid calcium acetate. The temperature will be in the range of 25°C to 55°C (methanol boiling point, 64.7°C, methyl acetate boiling point 57.1°C) [4]. The feed will enter a plug flow reactor (PFR) where variables such as the temperature, pressure, overall heat transfer coefficient, heat transfer area and the volumetric flow rate can be manipulated to determine the optimum conversion and temperature profiles.

A systematical way of estimating these variables is to model and simulate the reaction by MATLAB programming. By using mathematical modeling namely ordinary differential equations (ODE), the mole and energy balance can be simultaneously solved to produce conversion and temperature profiles. The profiles are used to monitor the occurrences with respect to temperature and conversion of methyl acetate along the PFR.

1.3 Objective and Scope of Study

The main objective of this project is to develop a MATLAB program that models and simulates the saponification of methyl acetate to form liquid methanol. This program will enable the user to manipulate the variables affecting the reaction such as the temperature, pressure, overall heat transfer coefficient, heat transfer area and the volumetric flow rate.

The second objective is to monitor the saponification of methyl acetate through the PFR via conversion of methyl acetate and temperature profiles. The profiles should be compatible with the theory. The saponification of methyl acetate will be treated as a reaction system and the nonisothermal plug flow reactor will be used as a reactor basis. Euler, Runge-Kutta, Adams, Cauchy methods etc are used to solve the ordinary differential equation posed by the mole and energy balance to come up with the profiles above. The best suitable method of solving the ordinary differential equation is chosen.

The third and last objective is to compare the results with experimental data. Even though the experiment of methyl acetate saponification has not been conducted manually due to the lack of chemicals at that time, moderately similar data was used as comparison.

The project work is divided into two parts; the first part is to model the system and the second part is to develop the program. This project is feasible to be performed in one semester period.

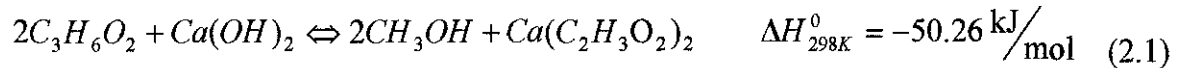
CHAPTER 2

LITERATURE REVIEW / THEORY

2.1 Reaction Mechanism

The synthesis of liquid methanol via the saponification of methyl acetate is given by the chemical equation below:

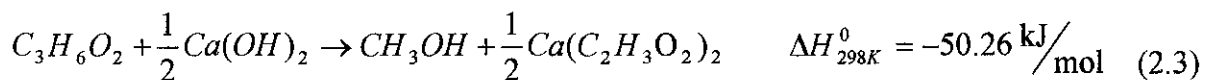
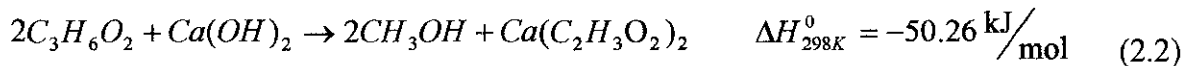
Methyl Acetate + Calcium Hydroxide \Leftrightarrow *Methanol + Calcium Acetate*



The reaction is exothermic and reversible. To simplify the modeling of the reaction, the reaction is treated as an irreversible reaction by applying the following assumptions:

- 1) The product of the reaction is removed fast enough as it is formed. Thus, the reaction shifts to the right.
- 2) No reactions or sub-reactions occur other than the main reaction above.
- 3) No phase change occurs. The reaction is in liquid form only.

The new chemical equation is given by:



Since this reaction has not been done experimentally, the **rate constant** (k) and the reaction rate (r_A) had to be theoretically assumed.

$$k = k_1 \exp\left(A\left(\frac{1}{273} - \frac{1}{T}\right)\right) \quad (2.4)$$

From the general rate constant equation above, values of k_1 and A are inserted. The values are taken from real ethyl acetate saponification, which is assumed to have the same values for k_1 and A as the methyl acetate saponification [5].

$$k = 0.39175 \exp\left(5472.7\left(\frac{1}{273} - \frac{1}{T}\right)\right) \quad (2.5)$$

The **reaction rate** is formed based on equation 2.3 and is expanded accordingly. The assumption made is that the concentrations of reactant A (methyl acetate) and reactant B (calcium hydroxide) are initially of the same value.

$$r_A = -kC_A C_B^{1/2} \quad (2.6)$$

$$r_A = -kC_A^{3/2} \quad (2.7)$$

$$r_A = -k(C_{A0} - C_{A0}X)^{3/2} \quad (2.8)$$

$$r_A = -k(C_{A0}^3 - 3C_{A0}^2X + 3C_{A0}X^2 - C_{A0}^3X^3)^{1/2} \quad (2.9)$$

2.2 Mole Balance

The mole balance of the reactants in PFR is used to create the conversion profile along reactor volume and describe in equation (2.10). Since the reaction is exothermic, conversion, X will increase along reactor volume, V as shown in Figure 2-1 [6].

$$\frac{dX}{dV} = \frac{-r_A}{F_{A0}} \quad (2.10)$$

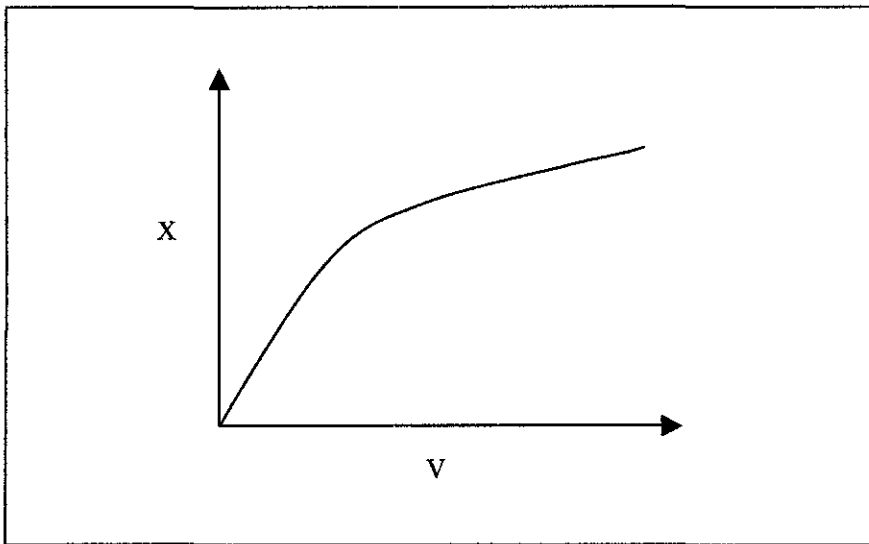


Figure 2-1: Conversion profile along reactor volume

2.3 Energy Balance

2.3.1 Heat effect PFR

Heat effect of PFR equations are used in order to create the temperature profile along the reactor volume. The PFR reactor (Figure 2-2) is modeled with the assumptions that:

- 1) Radial heat gradient does not exist in the reactor.
- 2) The heat flux through the reactor wall per unit volume is as shown in Figure 2-3 below.

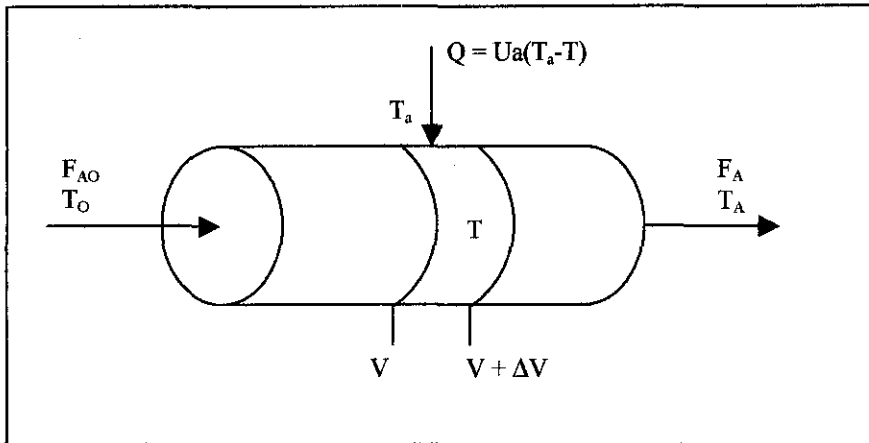


Figure 2-2: PFR with heat effect.

Energy balance of the PFR with heat effect is shown in equation (2.11) [6].

$$\frac{dT}{dV} = \frac{Ua(T_a - T) + (r_A)(\Delta H_{RXN})}{F_{AO}[C_{P_A} + X\Delta C_P]} \quad (2.11)$$

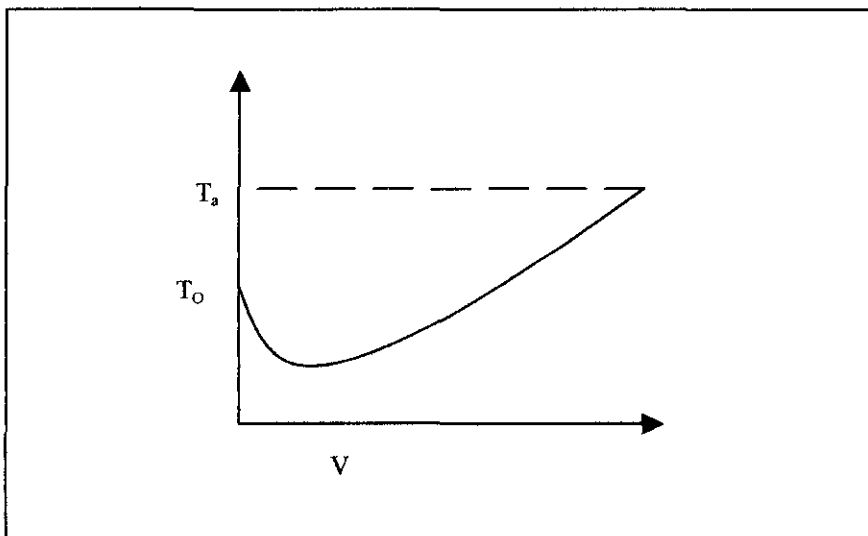


Figure 2-3: Temperature profile along reactor volume with heat effect of PFR

2.4 Thermodynamic Properties

The thermodynamic properties of the reactants, products and the reaction itself are essential to the modeling of the saponification of methyl acetate. The properties being used are the heat capacity and heat of formation of each reactant and product.

The table below lists the heat of formation [4]:

| Chemicals | Function | Heat of Formation, (J/mol) |
|-------------------|----------|-------------------------------|
| Methyl Acetate | Reactant | -445,900.0 |
| Calcium Hydroxide | Reactant | -1,000,812.8 |
| Methanol | Product | -239,200.0 |
| Calcium Acetate | Product | -1,514,730.0 |

Table 2-1: List of heat of formation

| Chemicals | Heat Capacity, C_p (J/mol.K) |
|-------------------|--|
| Methyl Acetate | $57.308 + 6.3751 \times 10^{-1}T - 2.1308 \times 10^{-3}T^2 + 3.0569 \times 10^{-6}T^3$ (valid for 176K – 456K) |
| Calcium Hydroxide | 89.5 (valid for 276K – 373K) |
| Methanol | $40.152 + 3.1046 \times 10^{-1}T - 1.0291 \times 10^{-3}T^2 + 1.4598 \times 10^{-6}T^3$ (valid for 176K – 461K) |
| Calcium Acetate* | $-416.831 + 3.5896T - 6.6188 \times 10^{-3}T^2 + 4.4587 \times 10^{-6}T^3$ (valid for 276K – 373K) |

Table 2-2: List of heat capacities

*Heat capacity belongs to succinic acid, $C_4H_6O_4$ due to the unavailability of calcium acetate heat capacity

2.5 Reactor

Tubular quartz reactor also known as PFR is used as the reactor basis. In PFR, the reactants are continually consumed as they flow down the length the reactor. In modeling PFR, assumption has to be made that the concentration varies continuously in the axial direction through the reactor. Adiabatic PFR is assumed that no heat added or released from the reactor and no work done into the reactor.

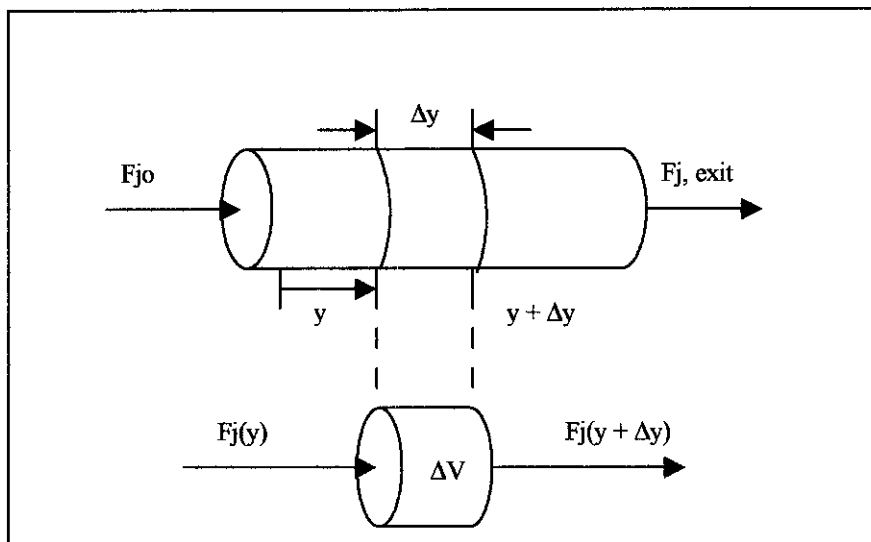


Figure 2-4: Plug Flow Reactor (PFR)

2.6 Literature Review Methanol Synthesis Processes

86% of the world methanol is produced from natural gas via steam reforming, water-gas shift reaction and direct oxidation [2]. The minor methanol synthesis comes from the biomass process [7] and Carnol process [8]. The difference between the three processes is mainly due to the feed that is available at the place and environmental issues. The table below lists the process description, advantages and disadvantages of the three processes.

Table 2-3: List of methanol synthesis processes

| PROCESS | REFERENCES | FEED | DESCRIPTION | ADVANTAGES | DISADVANTAGES |
|--|---|--|--|--|---|
| Steam Reforming. Water-Gas Shift Reaction | R.J. Farrauto and C.H. Bartholomew, 1998, <i>Fundamentals of Industrial Catalytic Processes, Blackie Academic & Professional.</i> | Natural Gas | Converts hydrocarbon in natural gas to light gases – high in H ₂ and CO. Steam used as oxidant. CO and H ₂ reacts further to form methanol. | Established and available technology. Natural gas currently abundant. High productivity. | Utilizes extreme temperature (700 to 900°C) and pressure (30 to 35 bar). CO and CO ₂ emission. |
| Biomass | Vogt, Kristina, 2004 Program in Forest Systems. & Bio--Energy, CFR, University off Washington | - Pulp Mill Black liquor - Forest Residues - Wood Residues - Soybean-Cake | Feed/raw materials subjected to heat and pressure to release gas. The gas goes to gas conditioning and catalytic heating. The product is distilled and methanol is purified. | Low CO and CO ₂ emission. More environmentally friendly. | Higher or equivalent cost as conventional methods. |
| Carnol Process | Steinberg, Meyer, <i>The Carnol System for Methanol Production</i> | Recovered Carbon Dioxide, CO ₂ from coal fired power plants | CO ₂ reacted with H ₂ forming methanol | Reduce up to 56% CO ₂ in power plant emission. | Lower production capacity. |

CHAPTER 3

METHODOLOGY / PROJECT WORK

3.1 Methodology

The project consists of two parts, modeling the related equations and developing the MATLAB program for methyl acetate saponification to form liquid methanol. The purpose of modeling is to describe the system in a mathematical form, which results in nonlinear equations that will be used to predict the temperature and conversion profiles along the reactor.

In this research project, numerical solution is used to solve the emerging ordinary differential equations. Six numerical methods (Euler, Modified Euler, Runge-Kutta, Adams, Adams Moulton and Cauchy) are used to solve the equation and the best numerical method will be chosen.

MATLAB programming involves developing two programs. The first program is the main program, whereby the user will need to introduce all necessary information. The program then calls the MATLAB function program to solve the ordinary differential equation and plot the result. The numerical methods programs are readily available in textbooks and MATLAB function. The project work is summarized in a block flow diagram in Figure 3-1.

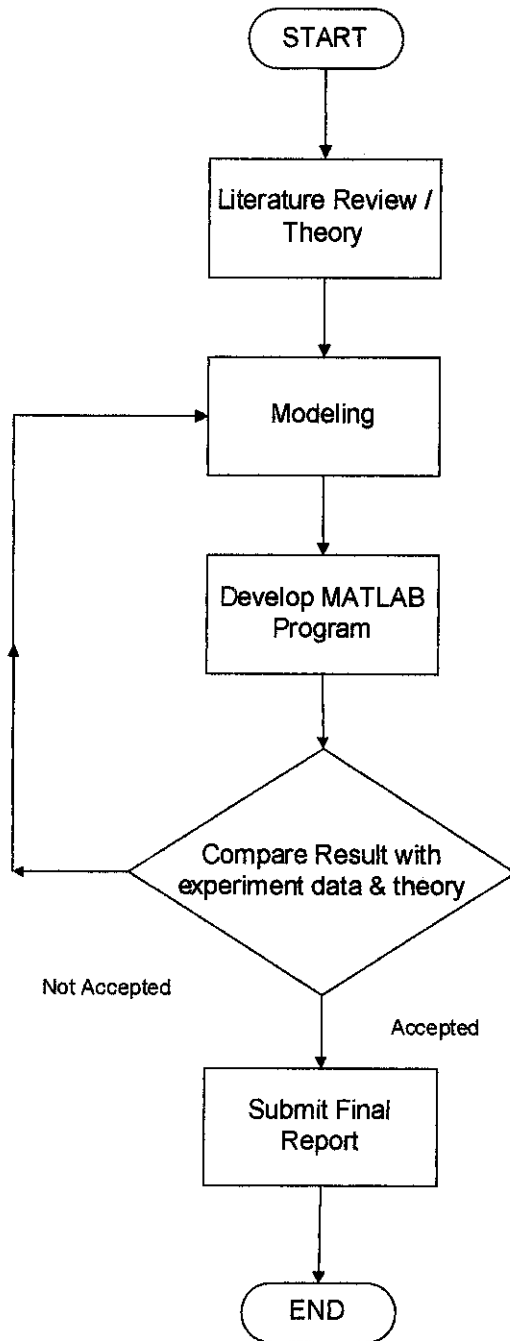


Figure 3-1: Project work flow chart

3.2 Mathematical Formulation

3.2.1 Mathematical formulation: Modeling the mole and energy balance.

The mole balance given by equation 2.10 and the energy balance given by equation 2.11 form the non linear equations that will be solved by the various numerical methods. The reaction constant (k) in equation, reaction rate (r_A) in equation, heat capacities in table and the heat of reaction are also included in the function program.

3.2.2 Mathematical formulation: Modeling temperatures along reactor volume.

The stoichiometric of the chemical equation 2.3 is used to relate the heat of reaction of each reactant and product in the equation below:

$$\Delta H^{\circ}_{RXN}(T_R) = \frac{1}{2}H^{\circ}_{CalciumAcetate} + H^{\circ}_{Methanol} - \frac{1}{2}H^{\circ}_{CalciumHydroxide} - H^{\circ}_{MethylAcetate} \quad (3.1)$$

The heat capacities of each component listed in table 2.2 follows the general arrangement of:

$$C_{p_i} = \alpha_i + \beta_i T + \gamma_i T^2 + \chi_i T^3 \quad (3.2)$$

Each of the sub components in the heat capacity is related by

$$\Delta\alpha = \frac{1}{2}\alpha_{CalciumAcetate} + \alpha_{Methanol} - \frac{1}{2}\alpha_{CalciumHyroxide} - \alpha_{MethylAcetate} \quad (3.3)$$

$$\Delta\beta = \frac{1}{2}\beta_{CalciumAcetate} + \beta_{Methanol} - \frac{1}{2}\beta_{CalciumHyroxide} - \beta_{MethylAcetate} \quad (3.4)$$

$$\Delta\gamma = \frac{1}{2}\gamma_{CalciumAcetate} + \gamma_{Methanol} - \frac{1}{2}\gamma_{CalciumHyroxide} - \gamma_{MethylAcetate} \quad (3.5)$$

$$\Delta\chi = \frac{1}{2}\chi_{\text{CalciumAcetate}} + \chi_{\text{Methanol}} - \frac{1}{2}\chi_{\text{CalciumHydroxide}} - \chi_{\text{MethylAcetate}} \quad (3.6)$$

By using equation 3.1 to equation 3.6, the heat of the methyl acetate can be formed as a function of temperature as follows [6]:

$$\begin{aligned} \Delta H_{RXN}(T) = & H_{RXN}^{\circ}(T_R) + \Delta\alpha(T - T_R) + \frac{\Delta\beta}{2}(T^2 - T_R^2) + \frac{\Delta\gamma}{3}(T^3 - T_R^3) \\ & + \frac{\Delta\chi}{4}(T^4 - T_R^4) \end{aligned} \quad (3.7)$$

3.3 Solution to Ordinary Differential Equation

The numerical methods used to solve the mole and energy balance equations 2.10 and 2.11 are Euler Method, Modified Euler, Runge-Kutta, Adams, Adams-Moulton and Cauchy method.

3.3.1 Euler Method

The general equation for the Euler Method is [9]:

$$y_{i+1} = y_i + f(x_i, y_i)h + O(h^2) \quad (3.8)$$

A new value of y is predicted using the slope (equal to the first derivative at the original value of x) to extrapolate over the step size h.

3.3.2 Runge – Kutta Method

This method are based on approximating a function using its Taylor series expansion; thus, a first order Runge - Kutta method uses a first order Taylor series expansion, a second order of Runge - Kutta method uses a second order Taylor series expansion and so on. For this project the 2 to 5th order of Runge - Kutta method will be modeled and used to solve ordinary differential equations. Equation (3.9), (3.10), (3.11) and (3.12) are the 2nd, 3rd, 4th and 5th order of Runge – Kutta respectively [9].

$$\begin{aligned}
y_{i+1} &= y_i + \frac{1}{2}(k_1 + k_2) + O(h^3) \\
k_1 &= hf(x_i, y_i) \\
k_2 &= hf(x_i + h, y_i + k_1)
\end{aligned} \tag{3.9}$$

$$\begin{aligned}
y_{i+1} &= y_i + \frac{1}{6}(k_1 + 4k_2 + k_3) + O(h^4) \\
k_1 &= hf(x_i, y_i) \\
k_2 &= hf\left(x_i + \frac{h}{2}, y_i + \frac{k_1}{2}\right) \\
k_3 &= hf(x_i + h, y_i + 2k_2 - k_1)
\end{aligned} \tag{3.10}$$

$$\begin{aligned}
y_{i+1} &= y_i + \frac{1}{6}(k_1 + 2k_2 + 3k_3 + k_4) + O(h^5) \\
k_1 &= hf(x_i, y_i) \\
k_2 &= hf\left(x_i + \frac{h}{2}, y_i + \frac{k_1}{2}\right) \\
k_3 &= hf\left(x_i + \frac{h}{2}, y_i + \frac{k_2}{2}\right) \\
k_4 &= hf(x_i + h, y_i + k_3)
\end{aligned} \tag{3.11}$$

$$\begin{aligned}
y_{i+1} &= y_i + \frac{1}{90}(7k_1 + 32k_2 + 12k_3 + 32k_4 + 7k_5 + 7k_6) + O(h^6) \\
k_1 &= hf\left(x_i + \frac{h}{2}, y_i + \frac{k_1}{2}\right) \\
k_2 &= hf\left(x_i + \frac{h}{4}, y_i + \frac{3k_1}{16} + \frac{k_2}{16}\right) \\
k_3 &= hf\left(x_i + \frac{h}{2}, y_i + \frac{k_3}{2}\right) \\
k_4 &= hf\left(x_i + \frac{3h}{4}, y_i - \frac{3k_2}{16} + \frac{6k_3}{16} + \frac{9k_4}{16}\right) \\
k_5 &= hf\left(x_i + h, y_i + \frac{k_1}{7} + \frac{4k_2}{7} + \frac{6k_3}{7} - \frac{12k_4}{7} + \frac{8k_5}{7}\right) \\
k_6 &= hf\left(x_i + h, y_i + \frac{k_1}{7} + \frac{4k_2}{7} + \frac{6k_3}{7} - \frac{12k_4}{7} + \frac{8k_5}{7}\right)
\end{aligned} \tag{3.12}$$

3.3.3 Adams Method

The general equation for Adams Method is given by [9]:

$$y_{i+1} = y_i + \frac{23d_i}{12} f_i - 16f_{i-1} + 5f_{i-2} \quad (3.13)$$

3.3.4 Cauchy Method

The Cauchy method [9] is ideal for solving stiff equations with low orders. Some applications must deal with a large system of coupled differential equations, modeling processes that are occurring at substantially at different rates. This is the essence of the notion *stiffness* of a differential equation.

One of the best ways to deal with a stiff system is to use an implicit method to compute the approximation. If the system is linear, the implicitness can be dealt with by solving a linear system; if the system is non-linear, the some kind of root finding scheme must be used to solve the nonlinear equations or predictor-corrector method will be used.

CHAPTER 4

RESULTS / DISCUSSION

4.1 MATLAB Program

Nine MATLAB programs are developed to model and simulate the saponification of methyl acetate.

- a) Program that allow the user to input the reaction variables (Main.m).
- b) Program that contains the ordinary differential equation (ODE) of the mole and energy balance (Function.m).
- c) Program that contain the Euler method on solving the ODE (Euler.m).
- d) Program that contain the Modified Euler method on solving the ODE (MEuler.m).
- e) Program that contain the Runge-Kutta method on solving the ODE (RK.m).
- f) Program that contain the Adams method on solving the ODE (Adams.m).
- g) Program that contain the Adams Moulton method on solving the ODE (AdamsMoulton.m).
- h) Program to execute Cauchy method to solve the ODE (Cauchy.m)
- i) Program that supports the Cauchy method (CauchyS.m)

The first program is the main program Main.m. The flow diagram showing basic structure of the program is given in Figure 4-1. This program will ask the user to input all required parameters for the reaction.

Upon acquiring all the required information, the program will call MATLAB function program Euler.m, MEuler.m, RK.m, Adams.m and AdamsMoulton.m accordingly. To Cauchy method is executed separately due to its programming

codes. All the MATLAB functions are used to find the temperature and conversions profile along PFR volume.

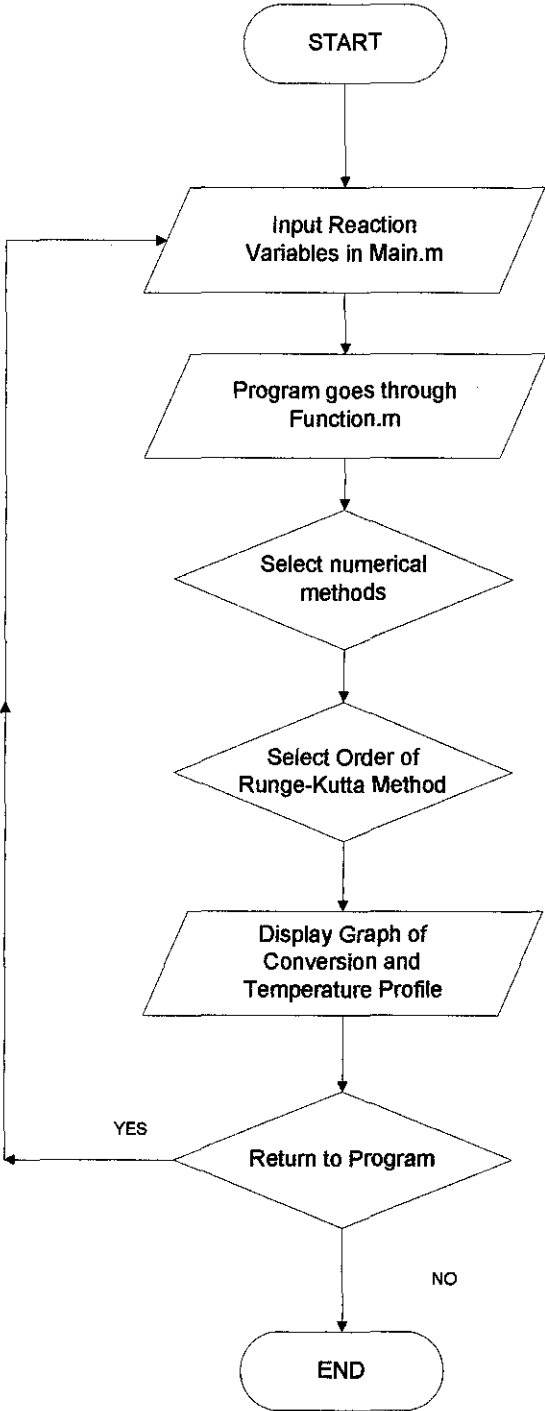


Figure 4-1: Flow diagram for Main.m

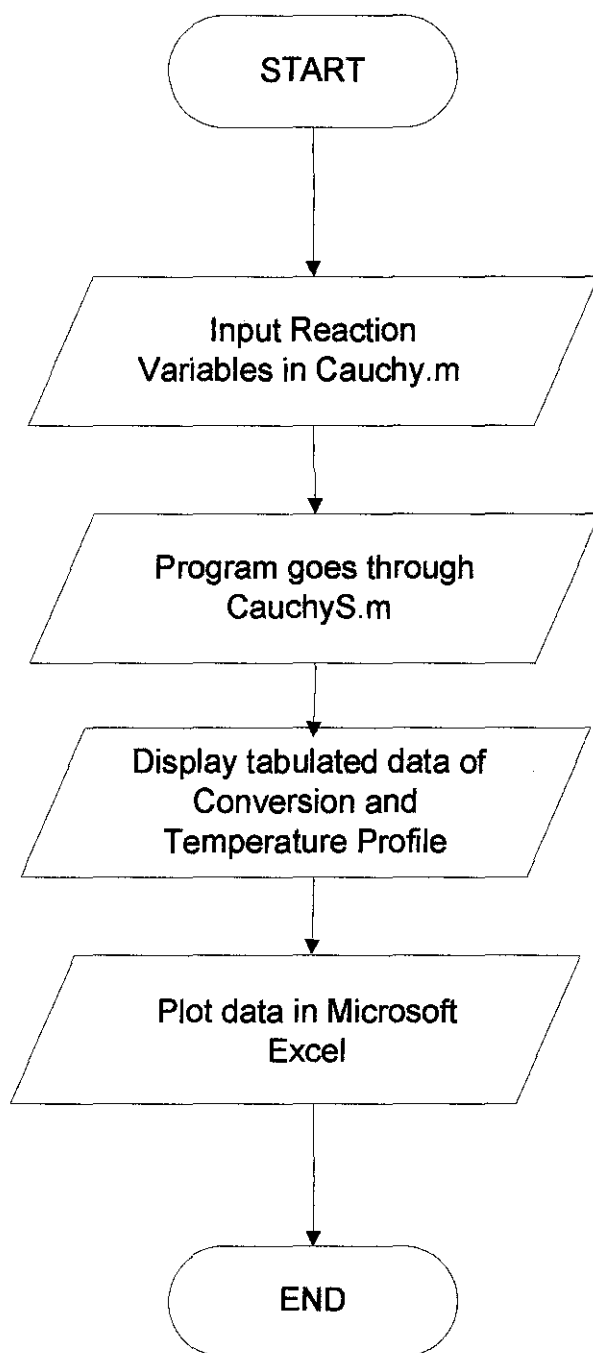


Figure 4-2: Flow diagram for Cauchy.m

```

case 3          % Runge-Kutta
n = input('\n Order of the Runge-Kutta method (2-5) = ');
if n < 2 | n > 5
    n = 2;
end
[V,y] = RK(fname,0,VR,h,[X0,T0],n,T0,CA0,FA0,U,a,Ta);
if k > 1
    lgnd = [lgnd ','];
end
lgnd = [lgnd 'RK' int2str(n) ''];
case 4          % Adams
[V,y] = Adams(fname,0,VR,h,[X0,T0],T0,CA0,FA0,U,a,Ta);
if k > 1
    lgnd = [lgnd ','];
end
lgnd = [lgnd 'Adams'];
case 5          % Adams-Moulton
[V,y] = AdamsMoulton(fname,0,VR,h,[X0,T0],T0,CA0,FA0,U,a,Ta);
if k > 1
    lgnd = [lgnd ','];
end
lgnd = [lgnd 'Adams-Moulton'];
end
x(k,:) = y(1,:); % Conversion
t(k,:) = y(2,:); % Temperature
end
if met
clf
% Plotting the results
subplot(2,1,1), plot(V/VR,x(1:lmethod,:))
ylabel('Conversion, X(%)')
title('(a) Methyl Acetate Conversion Profile')
subplot(2,1,2), plot(V/VR,t(1:lmethod,:))
xlabel('Ratio of Total Volume, V/V_R')
ylabel('Temperature, T(K)')
title('(b) Temperature Profile')
lgnd = [lgnd ''];
eval(lgnd)
end
end
change = input('\n\n Do you want to repeat the solution with different input data (0/1)? ');
end

```

4.2.2 Function.m

```

function fnc = Ex5_3_func(V,y,T0,CA0,FA0,U,a,Ta)
% Function Ex5_3_func.M
% This function contains the pair of ordinary differential
% equations introduced in Example 5.3. The name of this function
% is an input to the main program Example5_3.m and will be
% called by the selected ODE solver.

X = y(1); % Conversion
T = y(2); % Temperature

k = 0.39175*exp(5472.7*(1/298-1/T)); % Rate constant
dHR = -50258.6-270.3215*(T-298)+0.733875*(T^2-298^2)-7.359e-4*(T^3-298^3)+1.580625e-7*(T^4-298^4);

% Heat of reaction
CpA = 57.308 + 6.3751e-1*T - 2.1308e-3*T^2 + 3.0569e-6*T^3; % Heat capacity of A
CpB = 89.5; % Heat capacity of B
CpC = 40.152 + 3.1046e-1*T - 1.0291e-3*T^2 + 1.4598e-6*T^3; % Heat capacity of C
CpD = -416.831 + 3.5896*T - 6.6188e-3*T^2 + 4.4587e-6*T^3; % Heat capacity of D
dCp = CpD + CpC - CpB - CpA;

```

```
rA = -k * (CA0^3 - 3*X*CA0^3 + 3*(X^2)*CA0^3 - (CA0^3)*(X^3))^(1/2);
```

```
% Mole balance and energy balance
fnc = [-rA/FA0; (U*a*(Ta-T)+rA*dHR)/(FA0*(CpA+X*dCp))];
```

4.2.3 Function Program – Euler.m [5]

```
function [x,y] = Euler(ODEfile,xi,xf,h,yi,varargin)
% EULER Solves a set of ordinary differential equations by
% the Euler method.
%
% [X,Y]=EULER('F',XI,XF,H,YI) solves a set of ordinary
% differential equations by the Euler method, from XI to XF.
% The equations are given in the M-file F.M. H is the length
% of interval and YI is the vector of initial values of the
% dependent variable at XI.
%
% [X,Y]=EULER('F',XI,XF,H,YI,P1,P2,...) allows for additional
% arguments which are passed to the function F(X,P1,P2,...).
%
% See also ODE23, ODE45, ODE113, ODE15S, ODE23S, MEULER, RK,
% ADAMS, ADAMSMOULTON
```

```
% (c) N. Mostoufi & A. Constantinides
% January 1, 1999
```

```
% Initialization
if isempty(h) | h == 0
    h = (xf - xi)/99;
end
```

```
yi = (yi(:).)'; % Make sure it's a column vector
```

```
x = [xi:h:xf]; % Vector of x values
if x(end) ~= xf
    x(end+1) = xf;
end
d = diff(x); % Vector of x-increments
```

```
y(:,1) = yi; % Initial condition
```

```
% Solution
for i = 1:length(x)-1
    y(:,i+1) = y(:,i) + d(i) * feval(ODEfile,x(i),y(:,i),varargin{:});
end
```

4.2.4 Function Program – MEuler.m [5]

```
function [x,y] = MEuler(ODEfile,xi,xf,h,yi,varargin)
% MEULER Solves a set of ordinary differential equations by
% the modified Euler (predictor-corrector) method.
%
% [X,Y]=MEULER('F',XI,XF,H,YI) solves a set of ordinary
% differential equations by the modified Euler (the Euler
% predictor-corrector) method, from XI to XF.
% The equations are given in the M-file F.M. H is the length of
% interval and YI is the vector of initial values of the dependent
% variable at XI.
%
% [X,Y]=MEULER('F',XI,XF,H,YI,P1,P2,...) allows for additional
% arguments which are passed to the function F(X,P1,P2,...).
%
% See also ODE23, ODE45, ODE113, ODE15S, ODE23S, EULER, RK,
% ADAMS, ADAMSMOULTON
```

```
% (c) N. Mostoufi & A. Constantinides
% January 1, 1999
```



```

% Initialization
if isempty(h) | h == 0
    h = (xf - xi)/99;
end

yi = (yi(:).)';           % Make sure it's a column vector

x = [xi:h:xf];           % Vector of x values
if x(end) ~= xf
    x(end+1) = xf;
end
d = diff(x);             % Vector of x-increments

y(:,1) = yi;             % Initial condition
% Solution
for i = 1:length(x)-1
    % Predictor
    y(:,i+1) = y(:,i) + d(i) * feval(ODEfile,x(i),y(:,i),varargin{:});
    % Corrector
    y(:,i+1) = y(:,i) + d(i) * feval(ODEfile,x(i+1),y(:,i+1),varargin{:});
end

```

4.2.5 Function Program – RK.m [5]

```

function [x,y] = RK(ODEfile,xi,xf,h,yi,n,varargin)
% RK Solves a set of ordinary differential equations by the
% Runge-Kutta method.
%
% [X,Y]=RK(F',XI,XF,H,YI,N) solves a set of ordinary differential
% equations by the Nth-order Runge-Kutta method, from XI to XF.
% The equations are given in the M-file F.M. H is the length of
% interval. YI is the vector of initial values of the dependent
% variable at XI. N should be an integer from 2 to 5. If there
% are only five input arguments or the sixth input argument is an
% empty matrix, the 2nd-order Runge-Kutta method will be performed.
%
% [X,Y]=RK(F',XI,XF,H,YI,N,P1,P2,...) allows for additional
% arguments which are passed to the function F(X,P1,P2,...).
%
% See also ODE23, ODE45, ODE113, ODE15S, ODE23S, EULER, MEULER,
% ADAMS, ADAMSMOULTON

% (c) N. Mostoufi & A. Constantinides
% January 1, 1999

% Initialization
if isempty(h) | h == 0
    h = (xf - xi)/99;
end

if nargin == 5 | isempty(n) | n < 2 | n > 5
    n = 2;
end
n = fix(n);

yi = (yi(:).)';           % Make sure it's a column vector

x = [xi:h:xf];           % Vector of x values
if x(end) ~= xf
    x(end+1) = xf;
end
d = diff(x);             % Vector of x-increments

y(:,1) = yi;             % Initial condition
% Solution

switch n

```

```

case 2    % 2nd-order Runge-Kutta
for i = 1:length(x)-1
    k1 = d(i) * feval(ODEfile,x(i),y(:,i),varargin{:});
    k2 = d(i) * feval(ODEfile,x(i+1),y(:,i)+k1,varargin{:});
    y(:,i+1) = y(:,i) + (k1+k2)/2;
end
case 3    % 3rd-order Runge-Kutta
for i = 1:length(x)-1
    k1 = d(i) * feval(ODEfile,x(i),y(:,i),varargin{:});
    k2 = d(i) * feval(ODEfile,x(i)+d(i)/2,y(:,i)+k1/2,varargin{:});
    k3 = d(i) * feval(ODEfile,x(i+1),y(:,i)+2*k2-k1,varargin{:});
    y(:,i+1) = y(:,i) + (k1+4*k2+k3)/6;
end
case 4    % 4th-order Runge-Kutta
for i = 1:length(x)-1
    k1 = d(i) * feval(ODEfile,x(i),y(:,i),varargin{:});
    k2 = d(i) * feval(ODEfile,x(i)+d(i)/2,y(:,i)+k1/2, ...
        varargin{:});
    k3 = d(i) * feval(ODEfile,x(i)+d(i)/2,y(:,i)+k2/2, ...
        varargin{:});
    k4 = d(i) * feval(ODEfile,x(i+1),y(:,i)+k3,varargin{:});
    y(:,i+1) = y(:,i) + (k1+2*k2+2*k3+k4)/6;
end
case 5    % 5th-order Runge-Kutta
for i = 1:length(x)-1
    k1 = d(i) * feval(ODEfile,x(i),y(:,i),varargin{:});
    k2 = d(i) * feval(ODEfile,x(i)+d(i)/2,y(:,i)+k1/2, ...
        varargin{:});
    k3 = d(i) * feval(ODEfile,x(i)+d(i)/4,y(:,i)+3*k1/16+k2/16, ...
        varargin{:});
    k4 = d(i) * feval(ODEfile,x(i)+d(i)/2,y(:,i)+k3/2, ...
        varargin{:});
    k5 = d(i) * feval(ODEfile,x(i)+3*d(i)/4,y(:,i)-3*k2/16+ ...
        6*k3/16+9*k4/16,varargin{:});
    k6 = d(i) * feval(ODEfile,x(i+1),y(:,i)+k1/7+4*k2/7+ ...
        6*k3/7-12*k4/7+8*k5/7,varargin{:});
    y(:,i+1) = y(:,i) + (7*k1+32*k3+12*k4+32*k5+7*k6)/90;
end
end

```

4.2.6 Function Program – Adams.m [5]

```

function [x,y] = Adams(ODEfile,xi,xf,h,yi,varargin)
% ADAMS Solves a set of ordinary differential equations by the
% Adams method.
%
% [X,Y]=ADAMS(F',XL,XF,H,YI) solves a set of ordinary
% differential equations by the Adams method, from XI to XF.
% The equations are given in the M-file F.M. H is the length
% of the interval and YI is the vector of initial values of
% the dependent variable at XI.
%
% [X,Y]=ADAMS(F',XL,XF,H,YI,P1,P2,...) allows for additional
% arguments which are passed to the function F(X,P1,P2,...).
%
% See also ODE23, ODE45, ODE113, ODE15S, ODE23S, EULER, MEULER,
% RK, ADAMSMOULTON

% (c) N. Mostoufi & A. Constantinides
% January 1, 1999

% Initialization
if isempty(h) | h == 0
    h = (xf - xi)/99;
end

yi = (yi(:).');          % Make sure it's a row vector

```

```

x = [xi:h:xf];          % Vector of x values
if x(end) ~= xf
    x(end+1) = xf;
end
d = diff(x);          % Vector of x-increments

% Starting values
[a,b]=RK(ODEfile,x(1),x(3),h,yi,3,varargin{:});
y(:,1:3) = b;
for i = 1:3
    f(:,i) = feval(ODEfile,x(i),y(:,i),varargin{:});
end

% Solution
for i = 3:length(x)-1
    y(:,i+1) = y(:,i) + d(i)/12 * (23*f(:,i) - 16*f(:,i-1) + 5*f(:,i-2));
    f(:,i+1) = feval(ODEfile,x(i+1),y(:,i+1),varargin{:});
end

```

4.2.7 Function Program – AdamsMoulton [5].

```

function [x,y] = AdamsMoulton(ODEfile,xi,xf,h,yi,varargin)
% ADAMSMOULTON Solves a set of ordinary differential equations by
% the Adams-Moulton method.
% [X,Y]=ADAMSMOULTON('F',XI,XF,H,YI) solves a set of ordinary
% differential equations by the Adams-Moulton method, from XI to
% XF. The equations are given in the M-file F.M. H is the
% length of interval and YI is the vector of initial values of
% the dependent variable at XI.
%% [X,Y]=ADAMSMOULTON('F',XI,XF,H,YI,P1,P2,...) allows for
% additional arguments which are passed to the function% F(X,P1,P2,...).
%% See also ODE23, ODE45, ODE113, ODE15S, ODE23S, EULER, MEULER,
% RK, ADAMS
% (c) N. Mostoufi & A. Constantinides
% January 1, 1999
% Initialization

if isempty(h) | h == 0
    h = (xf - xi)/99;
end

yi = (yi(:)');          % Make sure it's a column vector
x = [xi:h:xf];          % Vector of x values
if x(end) ~= xf
    x(end+1) = xf;
end
d = diff(x);          % Vector of x-increments
% Starting values
[a,b] = RK(ODEfile,x(1),x(4),h,yi,4,varargin{:});
y(:,1:4) = b;
for i = 1:4
    f(:,i) = feval(ODEfile,x(i),y(:,i),varargin{:});
end

% Solution
for i = 4:length(x)-1
    % Predictor
    y(:,i+1) = y(:,i) + d(i)/24 * (55*f(:,i) - 59*f(:,i-1) ...
    + 37*f(:,i-2) - 9*f(:,i-3));
    f(:,i+1) = feval(ODEfile,x(i+1),y(:,i+1),varargin{:});
    % Corrector
    y(:,i+1) = y(:,i) + d(i)/24 * (9*f(:,i+1) + 19*f(:,i) ...
    + 5*f(:,i-1) + f(:,i-2));
    f(:,i+1) = feval(ODEfile,x(i+1),y(:,i+1),varargin{:});
end

```

4.2.8 Function Program – Cauchy.m [5]

```
% Cauchy.m
% Program that stores the values and cauchy function.

clc
% Input data
T0 = 298; %input (' Inlet temperature (K)           = ');
P0 = 101325; %input (' Inlet pressure (Pa)           = ');
v0 = 0.002; %input (' Inlet volumetric flow rate per tube(m3/s) = ');
X0 = 0; %input (' Inlet conversion of acetone       = ');
VR = 0.001; %input (' Volume of the reactor (m3)/1000 = ');
Ta = 298; %input (' Ambient temperature (K)         = ');
U = 110; %input (' Overall heat transfer coefficient (W/m2.K) = ');
a = 150; %input (' Heat transfer area (m2/m3)        = ');
k1 = 0.39175; %input (' Specific reaction rate (1/s)   = ');
E = 5472.7; %input (' Activation energy (J/mol)       = ');

CA0 = 0.1;          % Input concentration (mol/m3)
FA0 = v0 * CA0;    % Input molar flow rate (mol/s)

[X T]=ode23s('CauchyS',0:1,[0 333])
```

4.2.9 Function Program – CauchyS.m

```
function fnc = Ex5_3_func(V,y,T0,CA0,FA0,U,a,Ta)
% Function CauchyS.m
% This program provides the functions to be solved by Cauchy.m

X = y(1);          % Conversion
T = y(2);          % Temperature

T0 = 298; %input (' Inlet temperature (K)           = ');
P0 = 101325; %input (' Inlet pressure (Pa)           = ');
v0 = 0.002; %input (' Inlet volumetric flow rate per tube(m3/s) = ');
X0 = 0; %input (' Inlet conversion of acetone       = ');
VR = 0.001; %input (' Volume of the reactor (m3)/1000 = ');
Ta = 298; %input (' Ambient temperature (K)         = ');
U = 110; %input (' Overall heat transfer coefficient (W/m2.K) = ');
a = 150; %input (' Heat transfer area (m2/m3)        = ');
k1 = 0.39175; %input (' Specific reaction rate (1/s)   = ');
E = 5472.7; %input (' Activation energy (J/mol)       = ');
CA0 = 0.1;

FA0 = v0 * CA0;    % Input molar flow rate (mol/s)

k = 0.39175*exp(5472.7*(1/298-1/T));          % Rate constant
dHR = -50258.6-270.3215*(T-298)+0.733875*(T^2-298^2)-7.359e-4*(T^3-298^3)+1.580625e-7*(T^4-298^4);

% Heat of reaction
CpA = 57.308 + 6.3751e-1*T - 2.1308e-3*T^2 + 3.0569e-6*T^3; % Heat capacity of A
CpB = 89.5; % Heat capacity of B
CpC = 40.152 + 3.1046e-1*T - 1.0291e-3*T^2 + 1.4598e-6*T^3; % Heat capacity of C
CpD = -416.831 + 3.5896*T - 6.6188e-3*T^2 + 4.4587e-6*T^3; % Heat capacity of D
dCp = CpD + CpC - CpB - CpA;
rA = -k * (CA0^2 - 2*X*CA0^2 + (CA0^2)*(X^2)); % Reaction rate
% Mole balance and energy balance
fnc = [-rA/FA0; (U*a*(Ta-T)+rA*dHR)/(FA0*(CpA+X*dCp))];
```

4.3 Sample Run

| Variable | Value |
|---|--------|
| Inlet temperature (K) | 333 |
| Inlet Pressure (Pa) | 101325 |
| Inlet volumetric flow rate (m ³ /s) | 0.002 |
| Initial conversion of Methyl Acetate | 0 |
| Volume of the reactor (m ³) | 0.001 |
| External gas temperature (C) | 298 |
| Overall heat transfer coefficient (W/m ² .K) | 110 |
| Heat Transfer Area (m ² /m ³) | 150 |

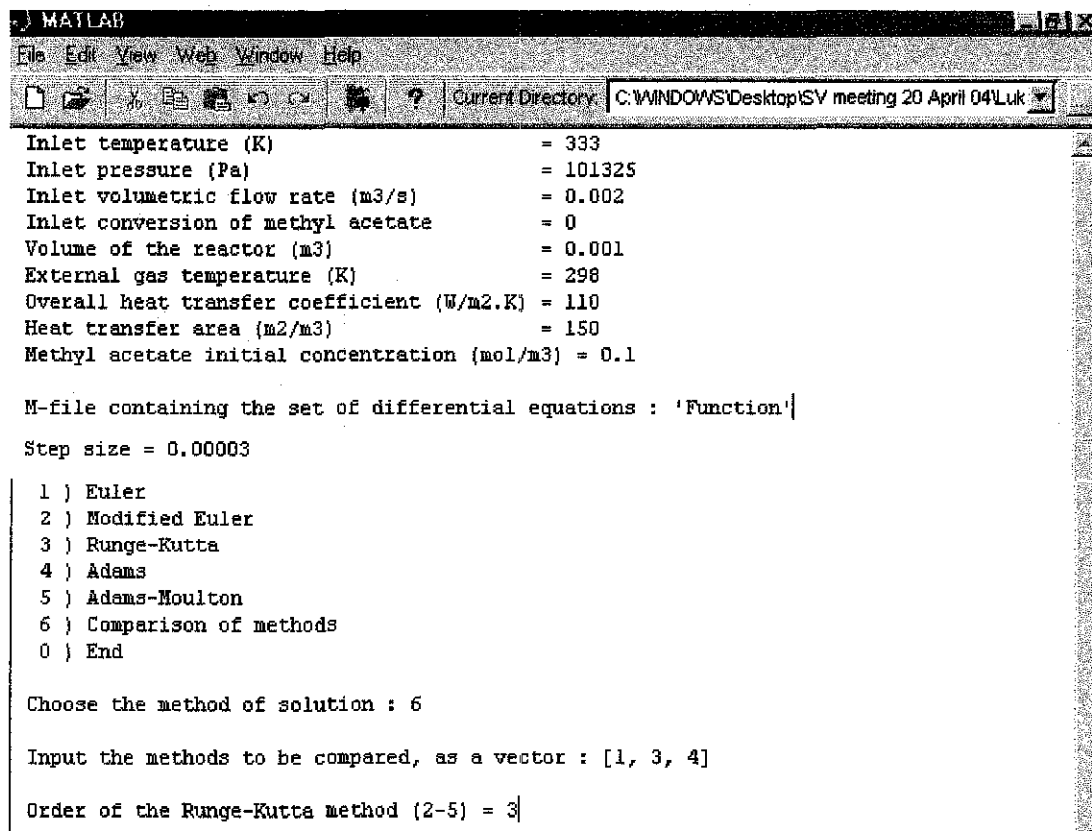
Table 4-1: Reaction variables for sample calculation

4.3.1 Running the Program

Running the MATLAB program requires to user to type “Main” at command prompt in MATLAB Command Window. The program run is shown in Figure 4-1. The figure also shoes that “Comparing Methods” has chosen. This will command will compare the results in the conversion and temperature profiles by the chosen methods.

To run the Cauchy method, simply type “Cauchy” in the workspace of MATLAB.

4.3.2 Sample Test Run



```
MATLAB
File Edit View Web Window Help
Current Directory: C:\WINDOWS\Desktop\SV meeting 20 April 04\Luk

Inlet temperature (K)           = 333
Inlet pressure (Pa)             = 101325
Inlet volumetric flow rate (m3/s) = 0.002
Inlet conversion of methyl acetate = 0
Volume of the reactor (m3)      = 0.001
External gas temperature (K)    = 298
Overall heat transfer coefficient (W/m2.K) = 110
Heat transfer area (m2/m3)      = 150
Methyl acetate initial concentration (mol/m3) = 0.1

M-file containing the set of differential equations : 'Function'

Step size = 0.00003

1 ) Euler
2 ) Modified Euler
3 ) Runge-Kutta
4 ) Adams
5 ) Adams-Moulton
6 ) Comparison of methods
0 ) End

Choose the method of solution : 6

Input the methods to be compared, as a vector : [1, 3, 4]

Order of the Runge-Kutta method (2-5) = 3
```

Figure 4-3: Display input

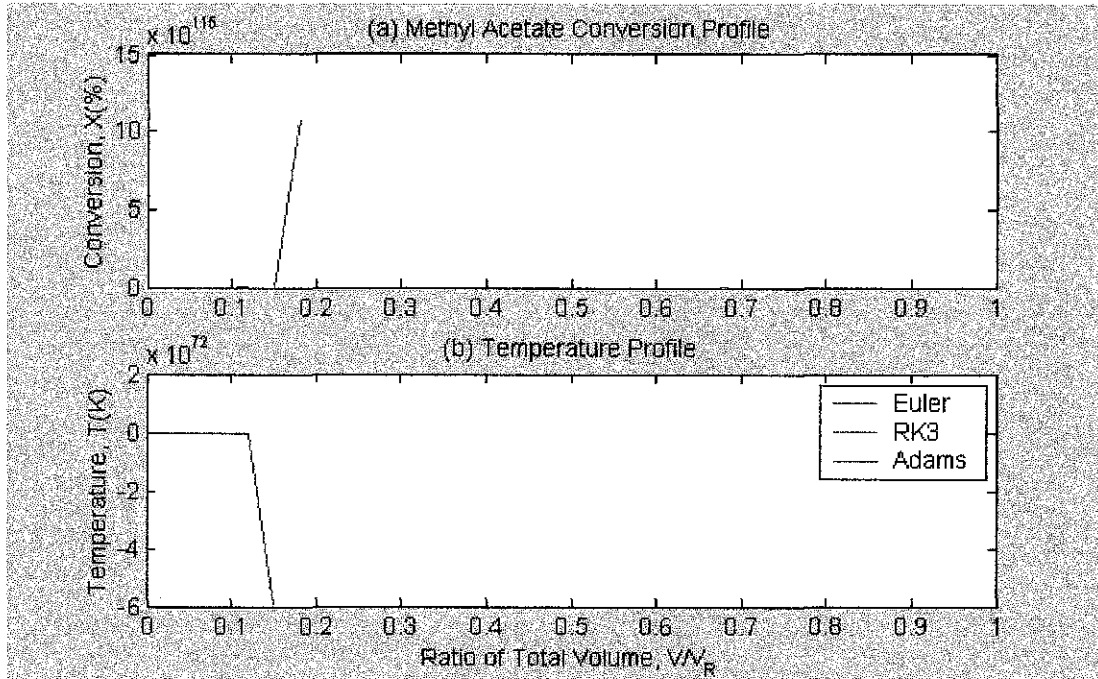


Figure 4-4: Methyl Acetate conversion and temperature profiles along the PFR volume according to settings in Table 4-1 and Figure 4-3

The Methyl Acetate conversion and temperature profiles shown in Figure 4-4 shows extreme and impossible trend values for both profiles. The conversion shoots up to 10^{15} % and the temperature drops to -6^{72} Kelvin. From the three numerical methods compared (Euler, Runge-Kutta and Adams) above, only Euler and Adams managed to show the results even though it is not practical.

It is found out later it project that the cause of the impractical results was the mole and energy balance equations. Those two equations were found out be stiff equations, which meant the numerical method must solve both equations simultaneously.

Cauchy method, a type of numerical method to solve stiff ordinary differential equation was introduced in the system. The preliminary results show logical and

practical values. A couple of variables namely temperature and methyl acetate inlet concentration was managed to be varied using the Cauchy method.

4.3.2 Cauchy.m Sample Run Result

Temperature variance at 303K, 326K and 328K with the following constants:

Initial concentration : 0.1Molar
Pressure : 1 atm
Overall heat transfer coefficient : 110 W/m².K
Heat transfer area : 150 m²/m³

Methyl Acetate initial concentration variance at 0.01M, 0.1M and 1.0M with the following constants:

Temperature : 303K
Pressure : 1 atm
Overall heat transfer coefficient : 110 W/m².K
Heat transfer area : 150 m²/m³

Methyl Acetate Conversion Profile at Varied Temperatures

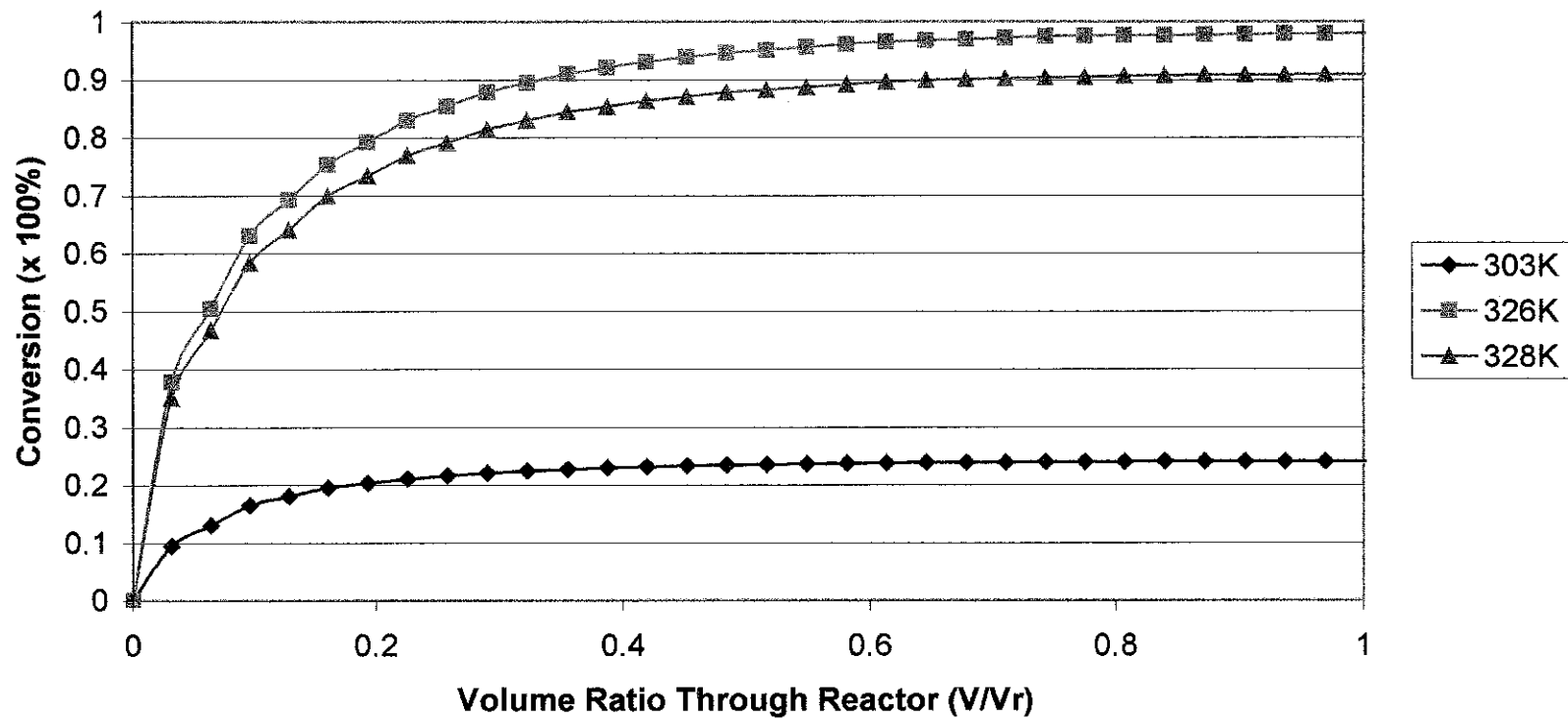


Figure 4-5: Methyl Acetate conversion profile for varied temperature heating settings

Temperature Profile for Varied Temperature Settings

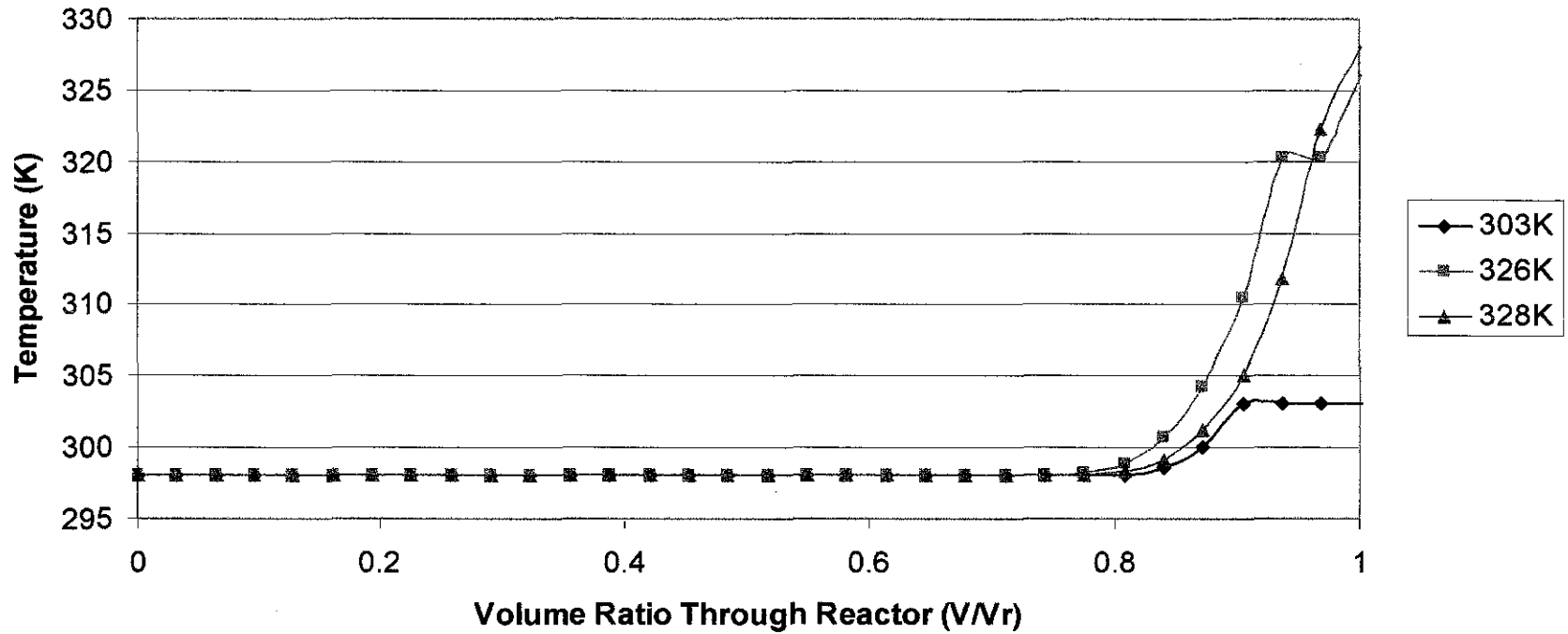


Figure 4-6: Temperature profile for varied temperature heating settings along the PFR

Methyl Acetate Saponification Conversion Profile

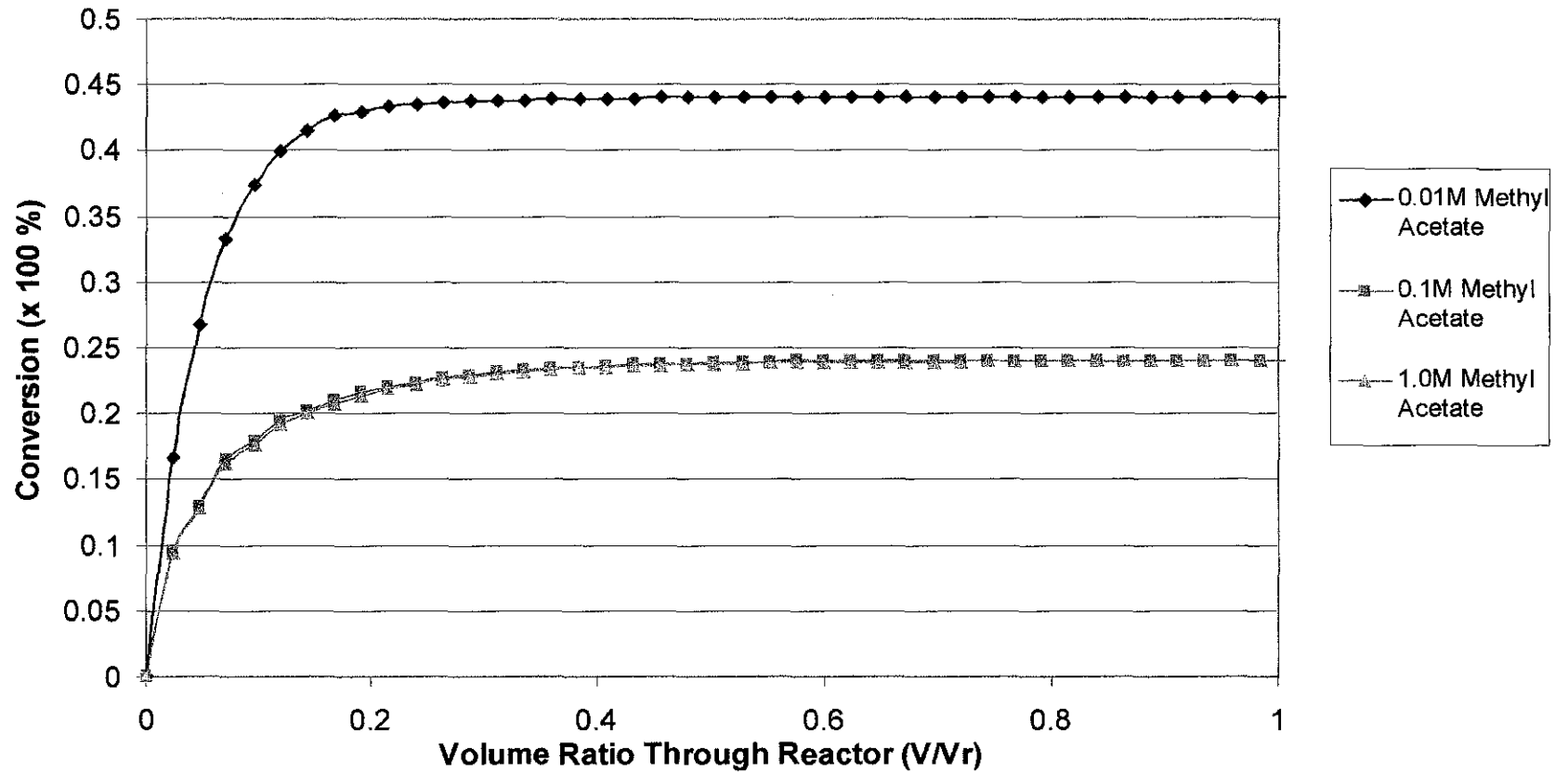


Figure 4-7: Methyl Acetate conversion profile for varied inlet concentration settings

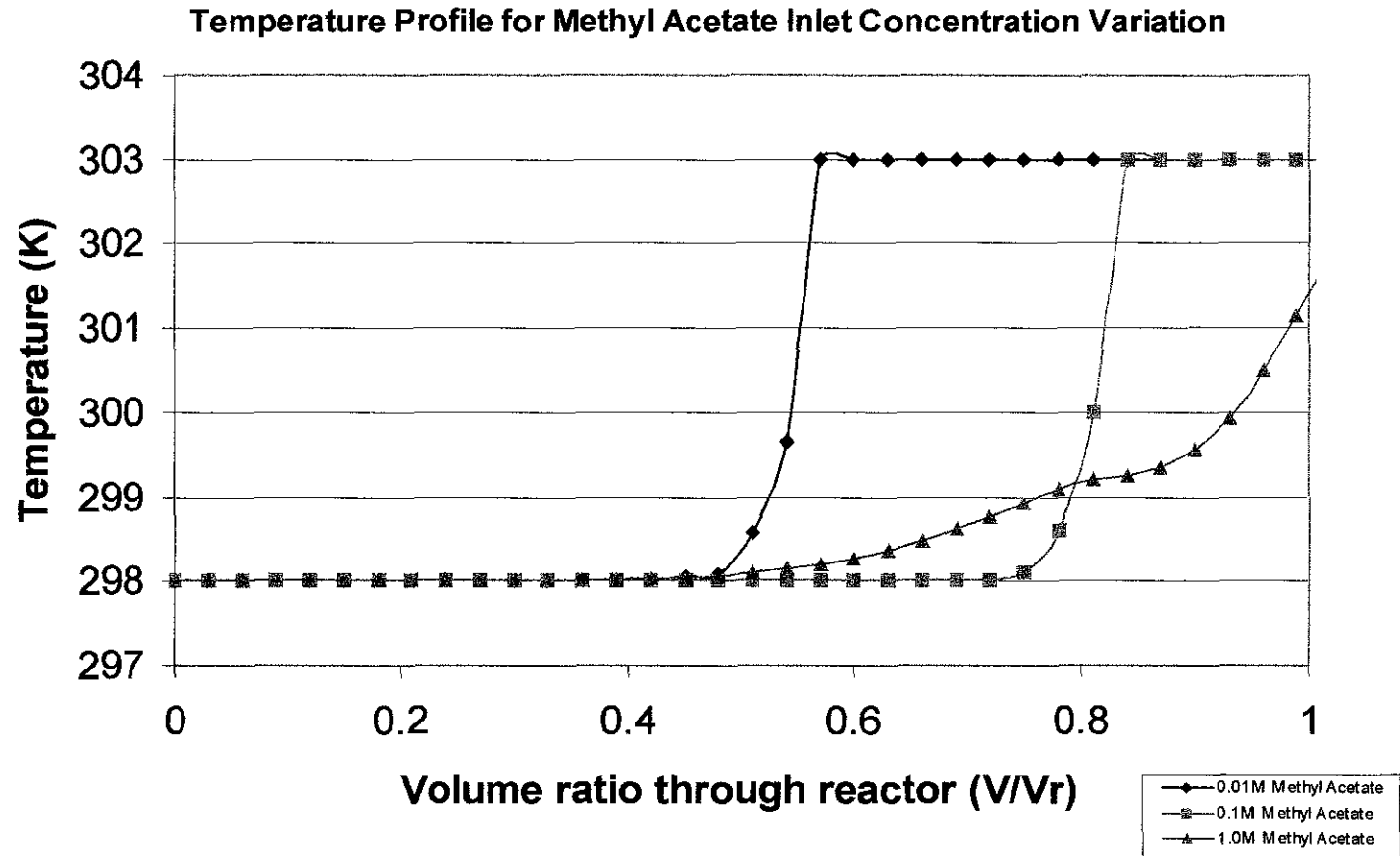


Figure 4-8: Temperature profile for varied inlet concentration setting

Conversion vs. Temperature for Batch, Autoclave & Plug Flow Reactors

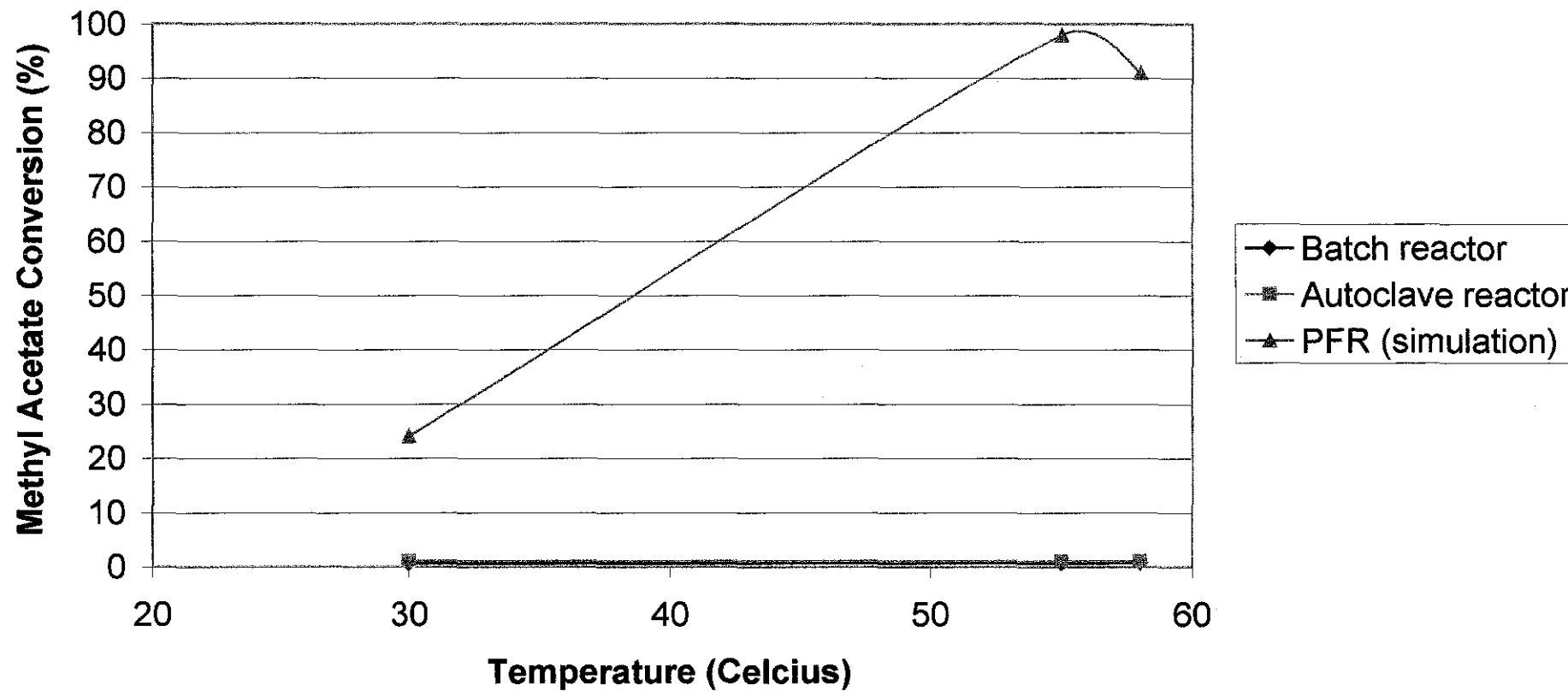


Figure 4-9: Comparison of conversions between experimental and simulation with respect to temperature

4.4 Discussion

4.4.1 Temperature variance

Figure 4-5 shows the methyl acetate conversion profile along the PFR at 303K, 326K and 328K. Each temperature were assumed to be heated from 298K. 303K represent the ambient room temperature at Tronoh, Perak where the project was done. 326K is the optimum temperature to yield maximum conversion, found out by experimenting on the program codes and 328K is the maximum allowable operating temperature before methanol (one of the product) and methyl acetate are boiled to vapor at 337.7K and 330.1K respectively.

The conversions at 303K, 326K and 328K are 24%, 97% and 74% respectively. The conversion rises as the temperature rises up to 326K, which is the highest conversion recorded. This is due to the addition of kinetic energy from the heat supplied. Higher heat provides more kinetic energy to the molecules to break existing bonds and become available to react with other reactants, thus converging into other compounds. The conversions become less from 326K to 328K due to high volatility of the methyl acetate and methanol as the temperature nears the boiling point of each of the compounds.

Compared to experimental values [10], in batch and continuous stirred tank reactor, the conversion increases from 300K to 323K. Please refer to Table 4-2 below and Figure 4-9. Figure 4-10 zooms at the experimental results only. Even though the experimental conversion is much less than this project's simulated results, the increasing trend of conversion in the particular temperature range justifies the findings of both sources.

| Temperature (°C) | Methyl Acetate Conversion (%) | |
|------------------|-------------------------------|--------|
| | Batch reactor | CSTR |
| 27 | 0.556 | 0.9724 |
| 30 | 0.6 | 0.9806 |
| 40 | 0.648 | 0.9822 |
| 50 | 0.782 | 0.989 |

Table 4-2: Experimental data of methyl acetate saponification at various temperatures

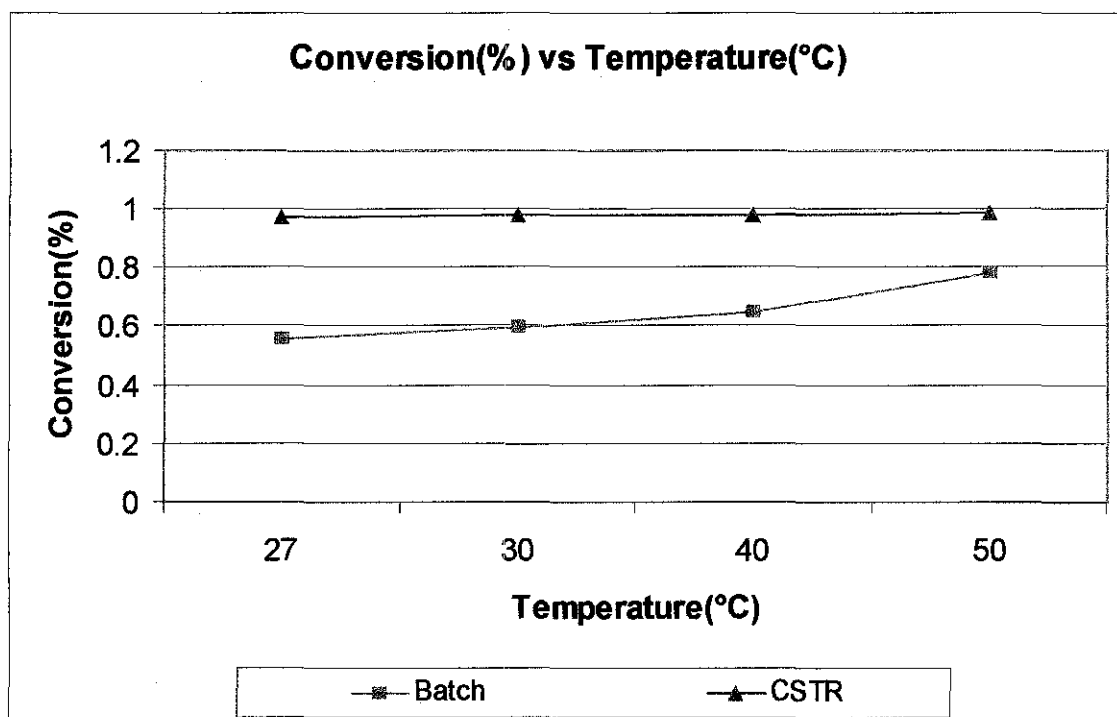


Figure 4-10: Experimental results of saponification of methyl acetate for Conversion vs. temperature

The corresponding temperature profile of the temperature variance is given by Figure 4-6. The profile shows that at all three heating temperatures show very little temperature increment along 80% of the reactor volume before rising up to its respective set point temperatures. The quickest response was the 298K to 326K heating. The most stable respond was the 298K to 303 heating due to the little temperature change.

4.4.2 Methyl Acetate inlet concentration variance

The conversion profile in Figure 4-7 that has a variation of inlet concentration (0.01M, 0.1M and 1.0M) shows a decreasing trend. The simulation was done at 303K. The highest (43%) conversion was gained from 0.01M inlet concentration of methyl acetate. 0.1M and 1.0M inlet concentration gained conversions of 24% and 23% respectively. The overall low conversion is due to the lack of heat supplied.

The program utilizes a small study-base PFR that is relatively small compared to the industrial tubular reactor. This factor causes the PFR to be crowded by molecules if the inlet concentration is high enough. Thus reaction is limited. This is emphasized by the lack of motion due to the lack of energy from heat. At 0.01M, the molecules are free to move and react, thus the high conversion.

The temperature profile for the above inlet concentration variance is given by Figure 4-8. The reactions were heated from 298K to 303K. The fastest response was the 0.01M inlet concentration at 55% through the PFR followed by the 1.0M and 0.1M. The inlet concentration stabilizes at 303K before leaving the PFR but the inlet concentration 1.0M only reached 301.5K.

4.4.3 Method of solving ODE

The best method to solve the mole and energy balance is proven to be the Cauchy method. This method succeeded where other numerical methods failed. The program code for Cauchy method is available in the MATLAB cache. The user or programmer has to model the mole balance, energy balance and the thermodynamics properties of the reaction in order to call the Cauchy method to solve the ordinary differential equations.

CHAPTER 5

CONCLUSION

The modeling and simulation of methyl acetate saponification to form methanol has been developed by using the reactions thermodynamic properties and more importantly, the mole and energy balance.

The conversion and temperature profiles along the PFR volume are compatible with the theory stated in Chapter 2. As the operating temperature becomes higher, the resulting conversion also increases to a limit due to the volatility and low boiling point of methanol. The optimum temperature is at 326K to yield conversion up to 97%. The conversion-temperature trends coincide with the experimental results proven by Sri Lisaharnie Mustapa [10]

In solving the ordinary differential equations (ODE), Cauchy method is the best method with respect to this project. This is due to the ability of the numerical method to deal with stiff equation at low order.

The MATLAB program codes developed can be used to predict the conversion and temperature profiles along PFR volume for the larger reactor scale. For this project, the small reactor scale is used to predict the conversion and temperature profile along the reactor volume.

Finally the project's objectives have been met. It recommends that reversible reaction of methyl acetate saponification has to be considered in modeling the conversion and temperature profile along PFR volume by other students who are interested. In addition, the student should include the errors while solving the resulting of ordinary differential equation.

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APPENDICES

Varying the temperature

Conversion (x 100%)

| Volume Ratio | 303K | 326K | 328K |
|--------------|--------|--------|--------|
| 0 | 0 | 0 | 0 |
| 0.0323 | 0.0945 | 0.3779 | 0.3501 |
| 0.0646 | 0.1295 | 0.504 | 0.4665 |
| 0.0969 | 0.1646 | 0.6301 | 0.5829 |
| 0.1292 | 0.1796 | 0.6919 | 0.6406 |
| 0.1615 | 0.1945 | 0.7538 | 0.6983 |
| 0.1938 | 0.2024 | 0.7914 | 0.7334 |
| 0.2261 | 0.2103 | 0.8291 | 0.7686 |
| 0.2584 | 0.2153 | 0.8535 | 0.7913 |
| 0.2907 | 0.2202 | 0.8779 | 0.814 |
| 0.323 | 0.2235 | 0.8939 | 0.8288 |
| 0.3553 | 0.2268 | 0.9099 | 0.8437 |
| 0.3876 | 0.2289 | 0.9204 | 0.8534 |
| 0.4199 | 0.2311 | 0.9309 | 0.8632 |
| 0.4522 | 0.2326 | 0.9385 | 0.8705 |
| 0.4845 | 0.234 | 0.946 | 0.8779 |
| 0.5168 | 0.235 | 0.9509 | 0.8821 |
| 0.5491 | 0.236 | 0.9558 | 0.8864 |
| 0.5814 | 0.2367 | 0.9604 | 0.8913 |
| 0.6137 | 0.2375 | 0.9649 | 0.8963 |
| 0.646 | 0.2379 | 0.9671 | 0.8984 |
| 0.6783 | 0.2384 | 0.9692 | 0.9005 |
| 0.7106 | 0.2388 | 0.9716 | 0.9018 |
| 0.7429 | 0.2392 | 0.974 | 0.903 |
| 0.7752 | 0.2394 | 0.975 | 0.9045 |
| 0.8075 | 0.2396 | 0.9761 | 0.906 |
| 0.8398 | 0.2398 | 0.9767 | 0.9067 |
| 0.8721 | 0.24 | 0.9774 | 0.9074 |
| 0.9044 | 0.2401 | 0.9781 | 0.9077 |
| 0.9367 | 0.2401 | 0.9788 | 0.9081 |
| 0.969 | 0.2401 | 0.9791 | 0.9085 |
| 1.0013 | 0.2401 | 0.9795 | 0.9089 |

Temperature (K)

| Volume Ratio | 303K | 326K | 328K |
|--------------|----------|----------|----------|
| 0 | 298 | 298 | 298 |
| 0.0323 | 298 | 298 | 298 |
| 0.0646 | 298 | 298 | 298 |
| 0.0969 | 298.0001 | 298 | 298.0001 |
| 0.1292 | 298.0001 | 298.0001 | 298.0001 |
| 0.1615 | 298.0001 | 298.0001 | 298.0001 |
| 0.1938 | 298.0002 | 298.0001 | 298.0002 |
| 0.2261 | 298.0002 | 298.0002 | 298.0003 |
| 0.2584 | 298.0004 | 298.0003 | 298.0005 |
| 0.2907 | 298.0006 | 298.0006 | 298.0007 |
| 0.323 | 298.0009 | 298.001 | 298.001 |
| 0.3553 | 298.0013 | 298.0014 | 298.0015 |
| 0.3876 | 298.0019 | 298.0027 | 298.0021 |
| 0.4199 | 298.0026 | 298.0036 | 298.0029 |
| 0.4522 | 298.0034 | 298.0047 | 298.0038 |
| 0.4845 | 298.0045 | 298.0059 | 298.005 |
| 0.5168 | 298.0058 | 298.0073 | 298.0063 |
| 0.5491 | 298.0072 | 298.0088 | 298.0077 |
| 0.5814 | 298.0086 | 298.0102 | 298.0092 |
| 0.6137 | 298.0101 | 298.0114 | 298.0105 |
| 0.646 | 298.0112 | 298.0118 | 298.0116 |
| 0.6783 | 298.0118 | 298.012 | 298.0118 |
| 0.7106 | 298.0118 | 298.0116 | 298.0122 |
| 0.7429 | 298.0127 | 298.0139 | 298.0105 |
| 0.7752 | 298.0082 | 298.1782 | 298.0221 |
| 0.8075 | 298.093 | 298.8886 | 298.2452 |
| 0.8398 | 298.5889 | 300.6954 | 299.0959 |
| 0.8721 | 300.001 | 304.2764 | 301.1469 |
| 0.9044 | 303 | 310.4416 | 305.0968 |
| 0.9367 | 303 | 320.1931 | 311.7809 |
| 0.969 | 303 | 320.1931 | 322.2146 |
| 1.0013 | 303 | 326 | 328 |

Varying the inlet concentration of Methyl acetate

Conversion (x 100%)

| Volume Ratio | 0.01M | 0.1M | 1.0M |
|--------------|--------|--------|--------|
| 0 | 0 | 0 | 0 |
| 0.024 | 0.1666 | 0.0945 | 0.0937 |
| 0.048 | 0.2664 | 0.1295 | 0.1277 |
| 0.072 | 0.333 | 0.1646 | 0.1617 |
| 0.096 | 0.3733 | 0.1796 | 0.1767 |
| 0.12 | 0.3997 | 0.1945 | 0.1917 |
| 0.144 | 0.4141 | 0.2024 | 0.1999 |
| 0.168 | 0.4255 | 0.2103 | 0.208 |
| 0.192 | 0.4296 | 0.2153 | 0.2132 |
| 0.216 | 0.4337 | 0.2202 | 0.2184 |
| 0.24 | 0.435 | 0.2235 | 0.2218 |
| 0.264 | 0.4362 | 0.2268 | 0.2252 |
| 0.288 | 0.4368 | 0.2289 | 0.2275 |
| 0.312 | 0.4374 | 0.2311 | 0.2298 |
| 0.336 | 0.4379 | 0.2326 | 0.2313 |
| 0.36 | 0.4384 | 0.234 | 0.2328 |
| 0.384 | 0.4387 | 0.235 | 0.2338 |
| 0.408 | 0.4389 | 0.236 | 0.2348 |
| 0.432 | 0.4393 | 0.2367 | 0.2355 |
| 0.456 | 0.4397 | 0.2375 | 0.2363 |
| 0.48 | 0.4399 | 0.2379 | 0.2367 |
| 0.504 | 0.44 | 0.2384 | 0.2372 |
| 0.528 | 0.4401 | 0.2388 | 0.2377 |
| 0.552 | 0.4401 | 0.2392 | 0.2382 |
| 0.576 | 0.4402 | 0.2394 | 0.2384 |
| 0.6 | 0.4402 | 0.2396 | 0.2386 |
| 0.624 | 0.4402 | 0.2398 | 0.2387 |
| 0.648 | 0.4403 | 0.24 | 0.2389 |
| 0.672 | 0.4403 | 0.2401 | 0.239 |
| 0.696 | 0.4403 | 0.2401 | 0.2392 |
| 0.72 | 0.4403 | 0.2401 | 0.2393 |
| 0.744 | 0.4403 | 0.2401 | 0.2394 |
| 0.768 | 0.4404 | 0.2401 | 0.2394 |
| 0.792 | 0.4404 | 0.2401 | 0.2394 |
| 0.816 | 0.4404 | 0.2401 | 0.2395 |
| 0.84 | 0.4404 | 0.2401 | 0.2395 |
| 0.864 | 0.4404 | 0.2401 | 0.2395 |
| 0.888 | 0.4404 | 0.2401 | 0.2395 |
| 0.912 | 0.4404 | 0.2401 | 0.2395 |
| 0.936 | 0.4404 | 0.2401 | 0.2395 |
| 0.96 | 0.4404 | 0.2401 | 0.2396 |
| 0.984 | 0.4404 | 0.2401 | 0.2396 |
| 1.008 | 0.4404 | 0.2401 | 0.2396 |

Temperature (K)

| Volume Ratio | 0.01M | 0.1M | 1.0M |
|--------------|----------|----------|----------|
| 0 | 298 | 298 | 298 |
| 0.03 | 298 | 298 | 298 |
| 0.06 | 298 | 298 | 298 |
| 0.09 | 298.0001 | 298.0001 | 298.0001 |
| 0.12 | 298.0001 | 298.0001 | 298.0001 |
| 0.15 | 298.0001 | 298.0001 | 298.0001 |
| 0.18 | 298.0001 | 298.0002 | 298.0002 |
| 0.21 | 298.0001 | 298.0002 | 298.0003 |
| 0.24 | 298.0001 | 298.0004 | 298.0007 |
| 0.27 | 298.0001 | 298.0006 | 298.0014 |
| 0.3 | 298.0001 | 298.0009 | 298.0028 |
| 0.33 | 298.0001 | 298.0013 | 298.0052 |
| 0.36 | 298.0001 | 298.0019 | 298.0092 |
| 0.39 | 298.0001 | 298.0026 | 298.0157 |
| 0.42 | 298.0009 | 298.0034 | 298.0258 |
| 0.45 | 298.05 | 298.0045 | 298.0409 |
| 0.48 | 298.082 | 298.0058 | 298.0629 |
| 0.51 | 298.5801 | 298.0072 | 298.0939 |
| 0.54 | 299.64 | 298.0086 | 298.1365 |
| 0.57 | 303 | 298.0101 | 298.1932 |
| 0.6 | 303 | 298.0112 | 298.2668 |
| 0.63 | 303 | 298.0118 | 298.3596 |
| 0.66 | 303 | 298.0118 | 298.4732 |
| 0.69 | 303 | 298.0127 | 298.6076 |
| 0.72 | 303 | 298.0082 | 298.7605 |
| 0.75 | 303 | 298.093 | 298.9248 |
| 0.78 | 303 | 298.5889 | 299.0903 |
| 0.81 | 303 | 300.001 | 299.2005 |
| 0.84 | 303 | 303 | 299.2467 |
| 0.87 | 303 | 303 | 299.3389 |
| 0.9 | 303 | 303 | 299.5542 |
| 0.93 | 303 | 303 | 299.9339 |
| 0.96 | 303 | 303 | 300.4796 |
| 0.99 | 303 | 303 | 301.1537 |
| 1.02 | 303 | 303 | 301.876 |
| 1.05 | 303 | 303 | 302.6264 |