A
Project Report
On

Steady state simulation of Plug Flow Reactor (PFR) in Aspen plus

Submitted by

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Under the guidance of

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CERTIFICATE

This is certified that the work contained in the thesis entitled ***"Steady State Simulation of Plug flow reactor (PFR) in Aspen plus"*** *submitted by* ***Banavathu Goutham Kumar (111CH0503)****, has been carried out under my supervision and this work has not been submitted elsewhere for a degree.*

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ABSTRACT

In this project work, we report Aspen-plus simulation of a cracking reaction *viz*. conversion of ethane to ethylene and hydrogen using plug flow reactor system. Ethane, which is produced in refineries isn't stored under normal temperature and pressure and is often sold at a cost lower than its production cost. However, cracking of ethane produces two very important compounds *viz*. ethylene and hydrogen which has very wide range of applications. Generally, in industry, cracking takes place in a fluidized bed catalytic cracker. In this work, the performance of plug flow reactor was studied to evaluate the process. Two contrastingly different routes were followed leading to the simulation. The first involved was the simulation of an adiabatic plug flow reactor at different operating conditions *viz*. feed flow rate, feed temperature, reactor temperature and pressure. The variation of diameter and length of the reactors were also studied in the overall performance of the system. Similarly, simulation studies were carried out for isothermal system as well. The performances of both the reactors were compared. It was observed that under a given set of conditions, isothermal plug flow reactor performed comparatively much better than its adiabatic counterpart.

CONTENT

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LIST OF SYMBOLS

A	Component A (reactant)	moles
B	Component B (reactant)	moles
C	Component C(product)	moles
C_A	Molar concentration of A	mol/m^3
$K_{(T)}$	Specific reaction rate	
α	Order of the reaction A	sec^{-1}
β	Order of the reaction B	sec^{-1}
PFR	Plug flow reactor	
K_0	pre-exponential factor	$kmol\ s^{-1}\ bar^{-2}\ (kg\ catalyst)^{-1}$
ε	Catalyst porosity	
E	Activation Energy	kcal/kmol
R	Ideal gas constant	J / mol K
T	Absolute temperature	(°K)
k_F	Forward reaction rate constant	s^{-1}
$K_{F(T)}$	Specific forward reaction rate constant	s^{-1}
K_{0F}	Forward pre exponential factor	s^{-1}
$K_{R(T)}$	Specific backward reaction rate constant	s^{-1}
k_R	backward reaction rate constant	s^{-1}
K_{0R}	Forward pre exponential factor	s^{-1}
K_{EQ}	Chemical equilibrium constant	
E_R	Activation energy for reverse reaction	kJ/mol
E_F	Activation energy for forward reaction	kJ/mol
FEHE	Feed Effluent Heat Exchanger	

P_j	Partial pressure of component j	bar
P	Total pressure in the system	bar
Y_j	Mole fraction	
W_{cat}	weight of catalyst	kg
Re	Reynolds number	
μ	Viscosity	$kgm^{-1}s^{-1}$
λ	Heat of reaction	kJ/kmol
c_{pA}	Heat capacity of A	$kJ\ kmol^{-1}\ K^{-1}$
c_{pB}	Heat capacity of B	$kJ\ kmol^{-1}\ K^{-1}$
c_{pC}	Heat capacity of C	$kJ\ kmol^{-1}\ K^{-1}$
M_A	Molecular weight of A	kg /kmol
M_B	Molecular weight of B	kg /kmol
M_C	Molecular weight of C	kg /kmol
D_P	Catalyst particle size	meters
ρ_{cat}	Catalyst bulk density	kg/m^3
γ	Ratio heat capacities	
U	Heat-transfer coefficient	$kW\ m^{-2}\ K^{-1}$
U_{FEHE}	Heat-transfer coefficient for feed effluent heat exchanger	$kW\ m^{-2}\ K^{-1}$
F_A	input of feed A	moles/sec
r_A	rate of reaction of A	mol/m^3 min
X_A	Fraction of A converted	
V	Volume	m^3

CHAPTER 1

INTRODUCTION

This chapter highlights the basics on adsorption science and technology. It focuses on novel materials called metal organic frameworks (or, MOFs). The background of the present thesis work is aptly explained. The objective of the work also properly highlighted.

1.1 Prelude

The major distinguishing properties of tubular reactors is their distributed-parameter nature, that is, variables like temperature and components (reactant, product) change with physical dimensions as well as with time. In regular plug flow reactor system we assume its vessel is cylindrical. Fluid will flows down word direction across the reactor length, and also the velocity profile is flat. So that there is no axial mixing will happens, and that radial gradients will not exist in composition or temperatures. The PFR is an empty vessel if no catalyst is used. If any catalyst packed inside the reactor then it is called as packed bed reactor. And also catalyst will affect the dynamic behaviour of the reactant because the process fluid having lower thermal capacitance than the catalyst mainly in the gas-phase system. The temperatures of both the catalyst and the process fluid vary with time. Under steady-state conditions the two temperatures are equal at any axial position. [1][2].

1.2 Applications of the PFR

Crude oil refining industries produces fuels like ethane, propane, butane etc. within process units of the refinery, which involve cracking and also reforming reactions in PFR. Reforming reactions are used to convert cyclical shaped saturated naphthenes into aromatics, which increases the octane numbers. Lighter hydrocarbons like butane and propane are alkylated to form high-octane C-8 material for blending into gasoline to increasing the quality of gasoline. Longer-chain hydrocarbons are converted lighter components by using catalytic or thermal cracking. All kinds of products are produced by using these cracking and reforming reactions. The unsaturated olefins generally used in different kinds of polymerization processes (ethylene and propylene) .For all those processes PFR can be utilized [1] [3].

Different kinds of materials that are used for housing, clothing, automobiles, construction, appliances, electronics, and healthcare come from processes that utilize PFRs. Reactors are important in the food and beverage industries, where farm products are processed [1].

1.2.1 Uses of hydrogen (H):

- Substantial amounts of Hydrogen is utilised in the oil refinery and synthetic industry.
- The main importance of hydrogen is for the processing ("upgrading") of fossil fuels, and in the production of NH_3 (Ammonia).
- The main utilization of Hydrogen in the petrochemical plant include dehydro-alkalation, dehydro-sulfurization and hydro-cracking.
- It is also used as a hydrogenating agent, to convert unsaturated fatty oils to saturated oils. And also in the preparation of methanol. It is the raw material for production of HCL.
- It is commonly used as a cooling agent in the power stations. [4]

1.2.2 Uses of ethylene (C_2H_4)

The areas of an ethylene plant are:

- It induces the leaf abscission, seed germination and also the growth of root hair.
- It affects the flowering in pineapples.
- It is used industrially mainly in polymerization processes to get polythene, poly vinyl chloride, which are used commercially.
- It is also used to produce ethyl alcohol which is industrially main important product [3]

1.3 Plug flow reactor basics:

- **Adiabatic:** Here heat transfer inside and outside of the reactor is not allowed. Temperature and composition vary with length. Radial temperature gradient will not exist because there is no heat in flow and out flow. Adiabatic temperature gradient depends on the per-pass conversion in the reactor, its heat capacity and the amount of the material sent to the reactor. If conversion is low then adiabatic temperature gradient also less [1] [5].

- **With heat transfer:** PFR is used as shell and tube heat exchanger. Process fluid flows inside the tubes and is heated or cooled by the heat transfer medium within the shell. Radial temperature change depends on the tube diameter, fluid velocities and fluid properties. If tube size increases then temperature gradient will also increases [1] [6].

- **Adiabatic with Intermediate Heat Transfer:** PFR systems use a series of adiabatic reactors with cooling or heating between the reactor-vessels. The process has more than one adiabatic reactors with fired furnaces between the reactors to material backup to the require reactor inlet temperature [6].

- **Adiabatic with "Cold-Shot Cooling":** Generally exothermic reactions are takes place in vessels with multiple catalyst beds. Since temperature increases through the bed. At the end of each bed, it is used adiabatically. Hot fluid is mixed with cold fluid leaving the bed to bring the temperature back down to get particular inlet temperature for downstream bed. This cold stream is some of the feed stream that has been bypassed around the reactor feed preheating system [1].

1.4 Research Objectives

- To study the effect of pressure, feed flow rate, feed temperature on the product formation in both isothermal and adiabatic PFR.
- To study the effect of change in length and diameter of the PFR on the formation of products.
- To study the effect of increasing the number of tubes in multi tube adiabatic PFR.
- To study temperature gradient across the PFR.

1.5 Background of present research work

Chemical reactors are important parts of different chemical, petroleum, polymer, bio-chemical processes because they convert raw materials into desirable chemicals. Generally many reactions occur normally the liquid or vapor phase. The PFR is used for both gas and liquid phases. In some cases the vessel is packed with a catalyst (solid). Some tubular reactors run adiabatically, heat generated or consumed by the reaction depend up on the reaction is endothermic or exothermic. The control of PFR can be quite difficult because of the distributed nature of the process. The main problem is to control temperature because it effects conversion and yield of the product [7] [8].

Ethane is not industrially used as a fuel because it cannot be stored as a liquid under certain pressure and temperature and so is less convenient to use than propane or butane, and also transporting requires extreme pressure or low temperature. No trucks, barges or trains are used for transporting and ships are not economical, pipelines are possible for transporting but it is very risky process [7] [9] [10].

There is simply not enough petrochemical demand to absorb all the ethane that refineries produce. The result is rejection of ethane sold as natural gas at fuel value less than being extracted and used as a petro-chemical feed stock [11]. But it can be cracked to produce hydrogen and ethylene; these products are industrially more beneficial.

Research has been done to convert ethane to ethylene and hydrogen which are having wide range of industrial applications by different methods. But the main problem is to achieve 100% product formation, and this reaction is highly exothermic in nature, so the operating is risky. In previous researches we found that there no appropriate work is done on this process by using plug flow reactor. The present work aims for 100% conversion by considering effect of different parameters to the product conversion.

CHAPTER 2

LITERATURE REVIEW

2.1 Basic laws of chemical kinetics and reaction equilibrium

The rate at which a chemical reaction can occurs in single-phase (homogeneous) systems mainly depends on the concentration of reactants & products, temperature of the system. Other variables may also effect the rate of the reaction such as pH, concentration of catalyst, inhibitor concentration and initiator concentration etc.

2.1.1 Kinetics of Power Law

An *irreversible* reaction occurring with two reactants making one product is expressed as

$$\mathbf{A + B \rightarrow C} \qquad (2.1)$$

The overall reaction rate k is expressed in terms of the number of moles of component A disappeared per unit volume per unit time. Generally rate of reaction depends on per mass of catalyst exist in the reactor. The number of moles of component B disappeared is same as the no. of moles of A which is same as the no. of moles of component C formed. The overall rate of reaction is depend up on temperature governed by the specific reaction rate $k_{(T)}$ and concentration term expressed in terms of mass or mole concentration ,mass or mole fraction, component vapour pressure or partial pressure, activity of the component [12]. Suppose the concentration term is expressed in molar concentrations terms

Then, for components A(C_A) and B(C_B), the overall rate of reaction equation expressed as

$$k = k_{(T)} C_A^{\alpha} C_B^{\beta} \qquad \mathbf{(2.2)}$$

The kinetic expression of the reaction is determined by the actual mechanism of the reaction. Generally more than one mechanism may give the exact or similar rate expression. In elementary reactions like cracking of ethane to ethylene and hydrogen the reaction order same as the stoichiometry. The single rate determining step concept is frequently used in the development of kinetic equations [1]. The specific reaction rate which is depend up on temperature is represented by $k_{(T)}$ expressed by the Arrhenius equation

$$k_{(T)} = k_0 e^{-E/RT} \tag{2.3}$$

The k_0 is a larger number (more than one). It depends on the units of concentration and the reaction order with respect to every component. The exponential term is a small +ve number, minimum value of this exponential term is 0 (E/RT value is ∞ at very low and absolute temperatures because the exponential is having -ve sign) and maximum value is 1(E/RT value is 0 at extreme temperatures),so at low temperature the E/RT term is large so the exponential is obviously small and produces a less specific rate of reaction, at extreme temperatures exponential term reaches to 1.The specific rate of reaction increases with increasing temperature [13]. The rate of change of $k_{(T)}$ with temperature depends on the activation energy value [12].

Generally in reverse reactions complete conversion never takes place, the expression written as:

$$\mathbf{A + B \Longleftrightarrow C} \tag{2.4}$$

The forward reaction rate can be expressed in terms of the molar concentrations of the reactants and products (C_A & C_B) which are dependent on the reaction orders α&β

can be written as

$$k_{\mathrm{F}} = k_{\mathrm{F(T)}} \mathrm{C}_{\mathrm{A}}^{\alpha} C_{\mathrm{B}}^{\beta} \tag{2.5}$$

With specific rate

$$k_{\mathrm{F(T)}} = k_{OF}\, \mathrm{e}^{\mathrm{-EF/RT}} \tag{2.6}$$

The rate of reaction of the reverse reaction is also written in terms of the molar concentration of product C_c which is dependent on the reaction order γ [1].

$$k_{\mathcal{R}} = k_{R(T)}\, C_C^{\gamma} \tag{2.7}$$

with the specific rate

$$k_{R(T)} = k_{0R} e^{-ER/RT} \tag{2.8}$$

The net overall rate of reaction is the difference between the rate of forward reaction k_F and the reverse reaction

$$k = k_F - k_{\mathcal{R}} = k_{F(T)} C_A^{\alpha} C_B^{\beta} - k_{R(T)}\, C_C^{\gamma} \tag{2.9}$$

Under the chemical equilibrium conditions, the overall rate of the net reaction is 0, which causes to the relationship between the specific rate of reactions of the forward & backward reactions and for the reaction, the chemical equilibrium constant (K_{EQ}) is

$$K_{EQ} = \frac{C_A^{\alpha} C_B^{\beta}}{C_C^{\gamma}} = \frac{K_{F(T)}}{K_{R(T)}} \tag{2.10}$$

$$K_{EQ} = \frac{K_{F(T)}}{K_{R(T)}} = \frac{K_{0F} e^{\frac{-E_F}{RT}}}{K_{0R} e^{\frac{-E_R}{RT}}} = \frac{K_{0F}}{K_{0R}} e^{\frac{E_R - E_F}{RT}} \tag{2.11}$$

The specific rate of reactions k_F & k_R depends up on temperature only, it is true for the chemical equilibrium constant K_{EQ} also. This temperature dependence is governed by the diff. between the reverse and forward reactions activation energies.

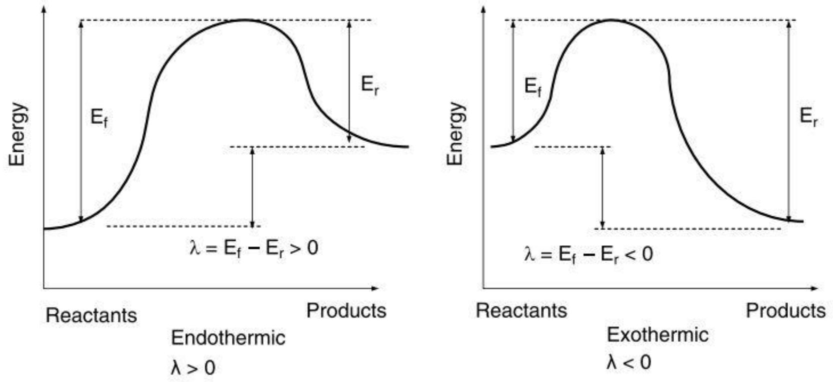


Figure 2. 1 Change in energies from Reactants to Products [1].

We can imagine the change in relative energy change from reactants to products shown in Figure 2.1. If the forward and reverse reaction's activation energies are same, the equilibrium constant is not depending up on temperature. If the activation energy of the forward reaction E_R is lesser than the activation energy of the backward reaction E_F, then extra energy transferred from reactants to products. Suppose activation energy of the forward reaction E_F more than backward reaction, then energy released from products to reactants. In thermodynamics the van't Hoff equation gives the relationship between temperature and chemical equilibrium constant [1]

$$\frac{d(\,lnK_{EQ}\,)}{dt} = (\frac{\lambda}{RT^2}) \qquad (2.12)$$

The reactions which are exothermic in nature having -ve heats of reaction, so the equilibrium constant decreases if temperature increases, but in the case of endothermic reactions the equilibrium constant of a reversible endothermic reaction increases with increasing temperature because they have positive heats of reaction.

After differentiating Eq.2.11 with respect to temperature substituting in Eq.2.12 gives the relationship between the heat of reaction λ and activation energies. .

$$\mathbf{E_F - E_R = \lambda} \qquad (2.13)$$

If the temperature increases then equilibrium constant of the exothermic irreversible reaction will decreases. And also the reverse reaction increases comparatively more faster than the forward reaction, that means at chemical equilibrium we get relatively more reactants than products and also Equilibrium constant will be low[1].

CHAPTER 3

PLUG FLOW REACTOR DESIGN

3.1 Introduction

In PFR composition of the fluid varies with length along the flow path, the material balance for a reaction component must be made for a differential element of volume dV. For reactant A material equation becomes

input = output + disappeared in reaction + accumulation

Here there is no accumulation.

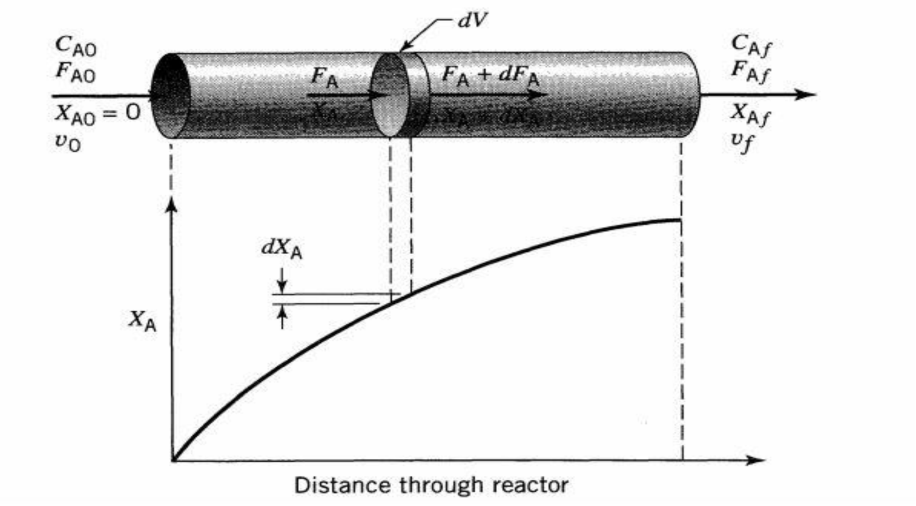


Figure 3.1 Plug flow reactor Notation [14]

Therefore

input = output + disappeared in reaction

Input of A (moles/time) = F_A

Output of A (moles/time) = $F_A + dF_A$

Disappearance of A
in reaction (moles/time) = $(-r_A)dV$

$$= \left(\frac{no.of\ moles\ of\ A\ reacting}{(volume\ of\ the\ fluid)\ (time)}(volume\ of\ element)\right)$$

Therefore

$$F_A = (F_A + dF_A) + (-r_A)dV \qquad (3.1)$$

⇨ $$dF_A\,[F_{A0}(1-X_A)] = -F_{A0}\,dX_A \qquad (3.2)$$

⇨ $$F_{A0}\,dX_A = (-r_A)\,dV \qquad (3.3)$$

This is the required equation for A in the differential section of the reactor of volume dV. F_A the feed rate is constant but r_A is certainly dependent on the conversion or concentration of materials [14]. Integrating the expression we get

$$\int_0^V \frac{dV}{F_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A} \qquad (3.4)$$

3.2 Different kinds of Plug flow reactor systems

3.2.1 Recycle Type of PFR

The unrecovered components are collected at the exit stream of the tubular reactor. The recovered reactants can be liquid or gas recycle. The liquid recycles are directly mixed with the fresh reactant if the reaction is in liquid phase for further continuation of the reaction. For liquid recycle system a regular distillation process is used to separate product and the unconverted material is again sent back to the reactor to add with fresh feed.

But if the reaction is in gas phase and after recycling products we get gas recycles then a vaporizer is used to pump to the reactor. In gas phase reacting system to recycle products we go for liquid-vapor distillation, lighter components are collected at the top of the distiller recycled back to blend with feed [1] [7].

3.2.2 Reaction Phase

PFR can be operated by a gas-phase or a liquid-phase reaction. In both types, temperature plays key role. In gas-phase reaction, the operating pressure is an important design variable, because rates of the reaction kinetics in most gas-phase reactions controlled by partial pressures of reactants, and also products. The compression costs of feed and product streams are generally affected by the pressure levels. Generally if the PFR operated at high pressures negative effect occurred on the reaction rates which is compensated by running the reactor at high temperatures in the fuel-fired reforming furnace [1].

3.2.3 Configuration of Heat Transfer

Feed temperature plays an important role to the product formation, so feed preheating is usually a curtail part of the plant design. A feed-effluent heat exchanger (FEHE) is used for an exothermic reactions conducted in an adiabatic reactor. The reactor effluent is maintained at extreme temperature to transfer heat to the cold reactor feed stream, which consists of the recycle stream and also fresh feed used to control the inlet temperature of the reactor some of the cold stream is bypassed around the FEHE. Maximum no. of systems have both a FEHE and a trim utility heat-input unit .The furnace is usually part of the process because it is needed for start up to get the initial high temperature required for the reaction to start. Therefore it is available to use a second manipulated variable for improved control. Another configuration utilizes “cold-shot” cooling. Some part of the cold reactor feed is bypassed around the upstream reactors and blended with the hot effluent from the reactor to lower the inlet temperature to the downstream catalyst bed [1].

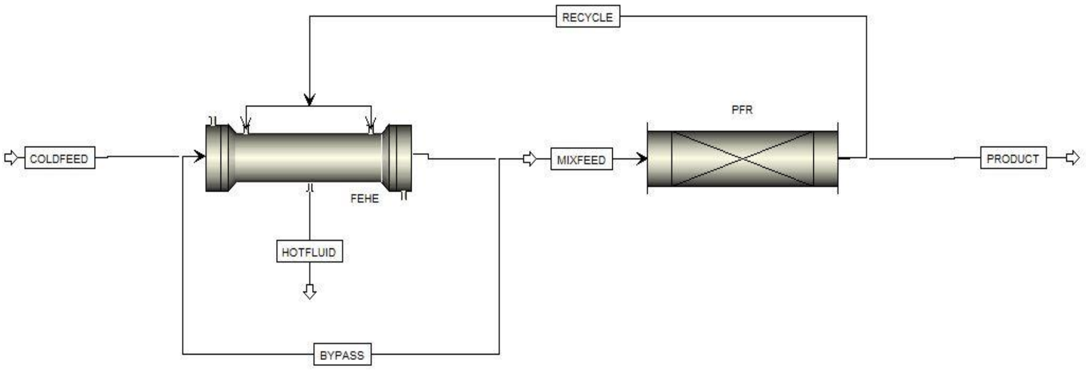


Figure 3.2 PFR with Feed Effluent Heat Exchanger

3.3 Plug flow reactors in Isolation

Both adiabatic and non-adiabatic PFRs are considered. The flow patterns, composition profiles, and temperature profiles in a real tubular reactor can often be quite complex. Temperature and composition may take place in both the radial and axial dimensions. Flow can be turbulent or laminar. Axial diffusion and conduction can occur. All of these potential complexities are eliminated when the "plug flow" assumption is made.

- The process fluid passes through the entire cross-sectional area of the reactor with uniform velocity.
- There is no radial change takes place. This assumption is fairly reasonable for adiabatic reactors.
- For non-adiabatic reactors, radial temperature changes are essential features. If diameters of the PFR kept small, the plug flow assumptions are more accurate. To get more accurate solutions the diameter of the PFR should be low.

3.3.1 Adiabatic PFR

If a gas-phase exothermic irreversible reaction takes place with two reactants and one product a PFR packed with a catalyst (solid), then the equations become

$$\mathbf{A} + \mathbf{B} \rightarrow \mathbf{C} \qquad (3.5)$$

The reaction rate mainly depends on the partial pressures of the reactants which is expressed as

$$\text{ƙ}=k_{(\mathrm{T})}P_A P_B \qquad (3.6)$$

$$=y_A y_B P^2 \boldsymbol{k_0}\, \mathbf{e}^{\mathbf{-E/RT}} \qquad (3.7)$$

The variables like pressure, temperature, no. of moles change with axial position: P(z), T(z), and $y_j(z)$

The ordinary differential equations explain the steady state adiabatic tubular reactor can be written in terms of axial length z as the independent variable. Alternatively the weight of catalyst w also used as independent variable. There are three main equations: a component balance on the product C_A pressure drop equation based on the Ergun equation, and energy balance. These equations explain how the molar flowrate of component C, the pressure P, and temperature T change down the length of the reactor. Under steady state conditions, the solid catalyst and the temperature of the gas are equal.

$$\frac{dF_C}{dw} = k \tag{3.8}$$

$$\frac{dT}{dW} = \frac{-\lambda k}{C_{pA}F_A + C_{pB}F_B + C_{pC}F_C} \tag{3.9}$$

$$\frac{dP}{dw} = \frac{-f L_R \rho V^2}{D_p W_{\text{cat}} 10^5} \tag{3.10}$$

$$f = \frac{(1-\varepsilon)}{\varepsilon^3}\left[1.75 + 150\frac{(1-\varepsilon)}{\text{Re}}\right] \tag{3.11}$$

In eq.(3.11) Re is the Reynolds number of the particle ($\text{Re} = D_p V \rho / \mu$).

The temperature and pressure vary with axial position of the reactor.
So the friction factor varies somewhat down the length of the reactor.

As the gas flows down the reactor and the reaction proceeds, the molar flow rate F_C increases, molar flow rate of A & B and Pressure decreases, but Temperature increases [15].

3.3.2 Non-adiabatic PFR

The main difference between adiabatic and isothermal or non-adiabatic systems is heating or cooling happen due to the process fluid which is flowing inside the tubular reactor. In exothermic irreversible reactions at the exit of the reactor maximum steady-state temperature occurred. In non-adiabatic reactors or any other cooled reactor system, steady state temperature possible at the axial position or along the path of the process fluid.

The component balance (material balance) & pressure change equations are not changed for both of the reactors. But the energy change is different for isothermal and non-isothermal reactors.

The energy change equation can be written as

$$\frac{dT}{dw} = \frac{-\lambda\Re - 4U(T - T_{\mathrm{st}})/(\rho_{\mathrm{cat}} D_{\mathrm{tube}})}{c_{p\mathrm{A}}F_{\mathrm{A}} + c_{p\mathrm{B}}F_{\mathrm{B}} + c_{p\mathrm{C}}F_{\mathrm{C}}} \tag{3.12}$$

In exothermic reactions more heat is generated inside the reactor this may affect the reactor performance, to overcome this problem steam is used as cooling agent. In this case reactor is worked as a shell & tube heat exchanger. Here temperature change not taking place along the axial position of the reactor. The overall heat transfer coefficient U depends up on the flow velocity of the fluids inside the reactor [1]. This is calculated by

$$U = 0.01545 + \frac{0.6885 \times 10^{-6}}{D_p}\mathrm{Re} \tag{3.13}$$

3.4 Single adiabatic plug flow reactor system with a gas recycle

Entire plant wise design considers all the equipment which are used in the plant: heat exchangers, gas recycle, tubular reactor, condenser, compressor, preheat furnace, separator, and distiller etc. The flow sheet is shown in fig3.3 [1] [7].

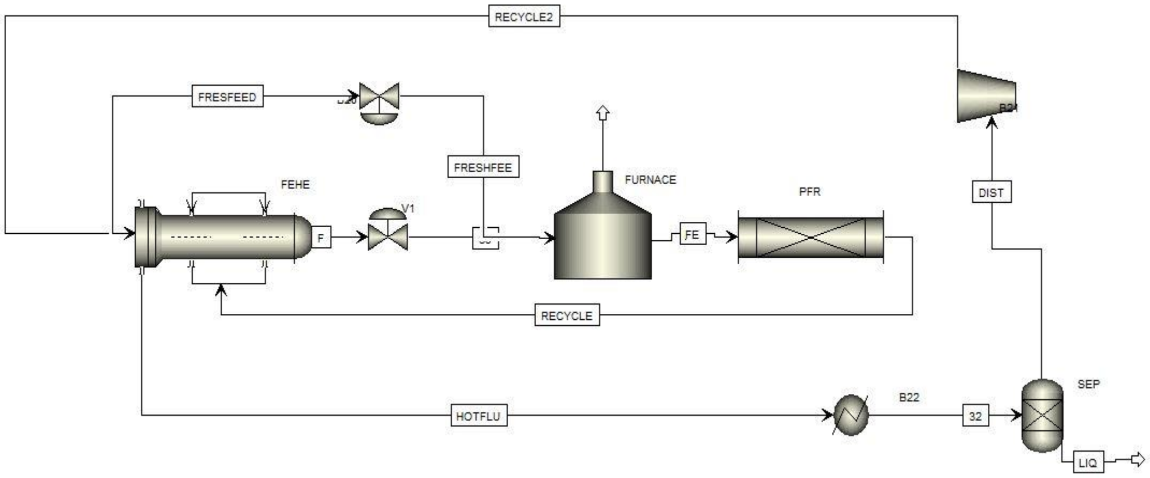


Figure 3.3 Single Adiabatic PFR Process

3.5 Multiple Adiabatic PFRS operating with Inter-stage cooling

In this process all the adiabatic reactors are connected in series and also a cooling system is connected after every reactor system. The feed which exits from one side of the reactor is directly cooled in the cooling chamber and again sent to the next reactor for further reaction. Heat exchangers are used to remove heat in this system. The flow sheet is shown in fig3.4 [1].

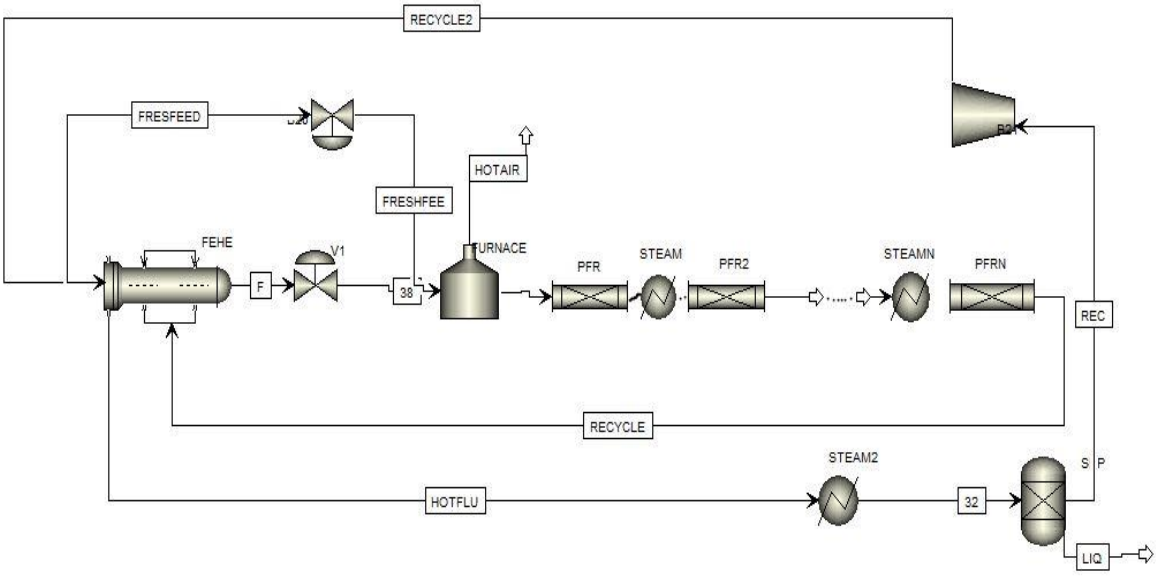


Figure 3.4 Adiabatic PFR with Inter-stage Cooling

3.6 Multiple adiabatic Plug flow rectors with cold shoot cooling

This process is used when a catalyst is present inside the reactor and the reactor is operating under adiabatic conditions. Generally if the feed is at extreme temperatures then it is condensed and added to the inlet of catalyst bed and blend with hot vapor (or gas) which is coming from upstream to decrease the extreme temperature of hot gas. The flow sheet is shown in fig3.5 [1] [16].

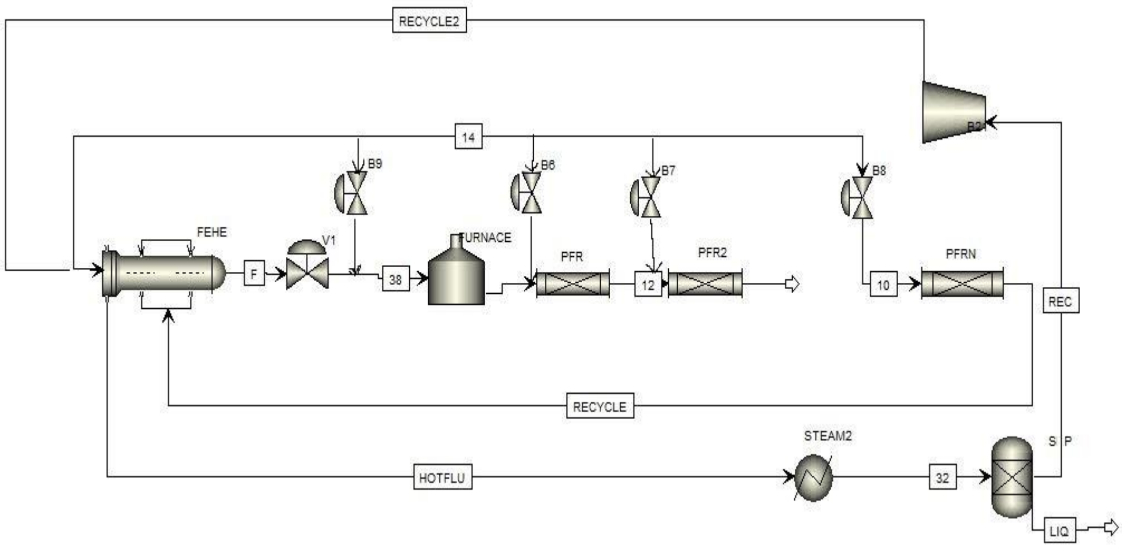


Figure 3.5 Adiabatic PFR with "Cold-Shot cooling"

3.7 Cooled reactor system

STHE is used for this process generally. Catalyst is fitted inside the reactor system, inside the shell stem is formed which is used as cooling agent. The liquid level in the shell is maintained by bringing boiling feed water to keep feeds are covered. Reactor inlet temperature and temperature of the steam are assumed to be equal [1] [15]. The design is shown in fig3.6.

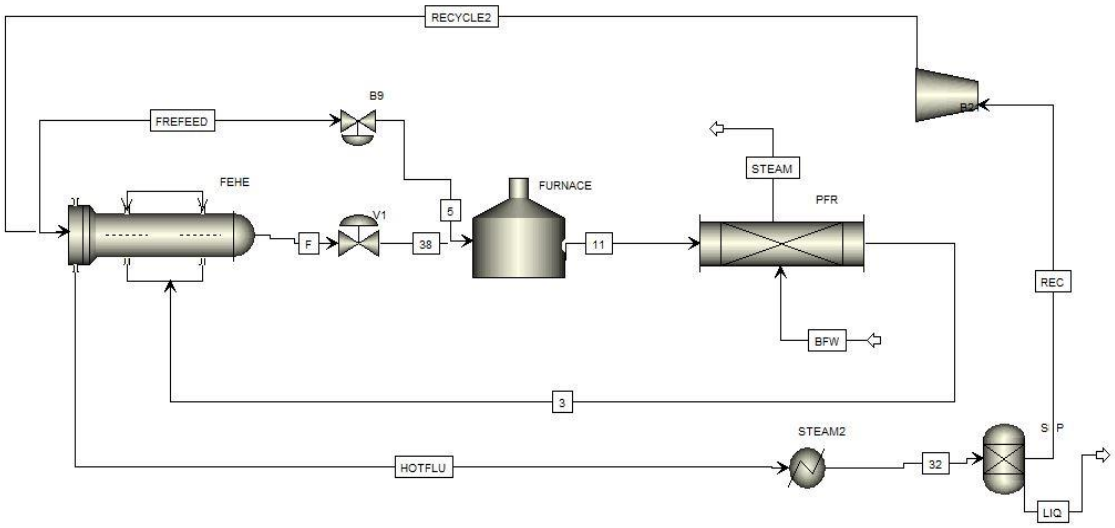


Figure 3.6 Cooled Reactor System

CHAPTER 4

SIMULATION WORK

4.1 ASPEN SOFTWARE

Aspen plus V8.4 is used for the plug flow reactor simulation. We studied particularly cracking of ethane to ethylene and hydrogen reactions in aspen plus. For that RPlug (PFR) is used.

Some key things about the process:

- The process is thermal cracking process.
- The reaction is irreversible and elementary.
- Operating the reactor isothermally and adiabatically at 1100K at a pressure of 6 atm.

$$C_2H_6\ (g) \rightarrow C_2H_4\ (g) + H_2\ (g) \qquad (4.1)$$

- $$\mathbf{A} \rightarrow \mathbf{B} + \mathbf{C} \qquad (4.2)$$
- Where A is gaseous ethane, B is gaseous ethylene, and C is gaseous hydrogen.
- F_{Ao} = 0.425 lbmol/s [17].
- k = $0.072 s^{-1}$ at 1000K [17].
- Activation Energy is E = 82 kcal/gmol [17].
- Assumed initial length=10m & diameter=1m.

The aim of this simulation is to get 100% conversion of ethane to ethylene and hydrogen.

To optimize this process steady state simulation is carried out.

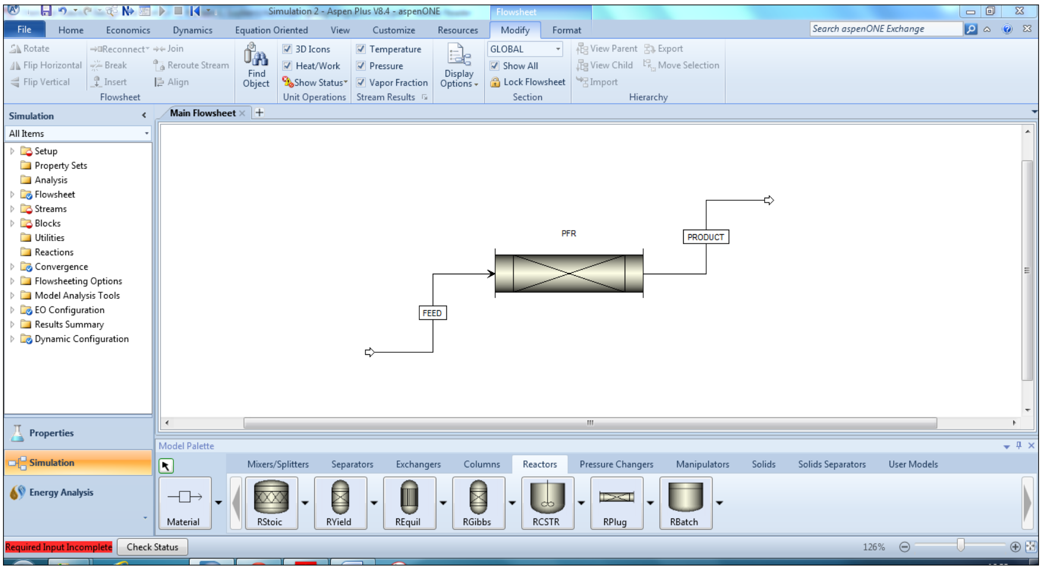
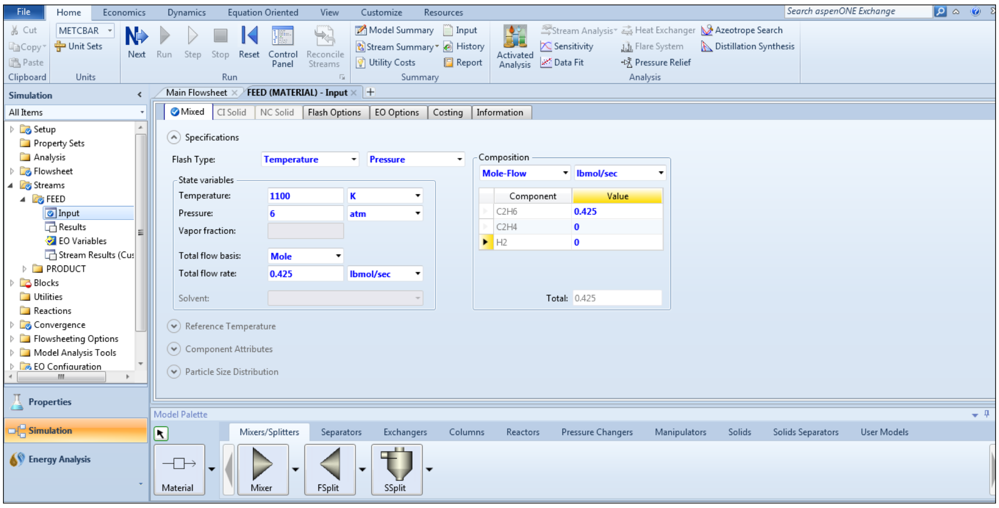


Figure 4.1Schematic diagram of PFR in ASPEN V8.4



Flash Type: Temperature Pressure

State variables

Temperature: 1100 K

Pressure: 6 atm

Vapor fraction:

Total flow basis: Mole

Total flow rate: 0.425 lbmol/sec

Solvent:

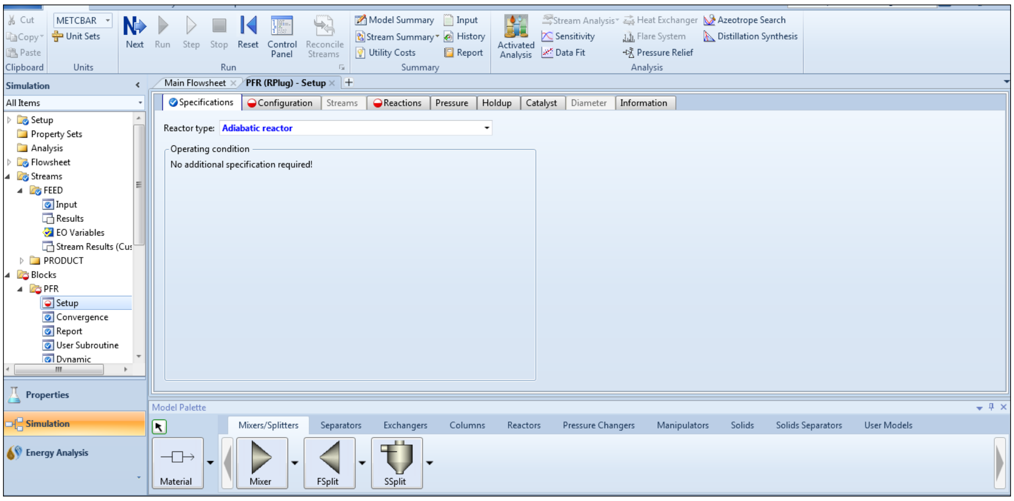
Composition

Mole-Flow lbmol/sec

Component	Value
C2H6	0.425
C2H4	0
H2	0

Total: 0.425

Figure 4.2 Feed input

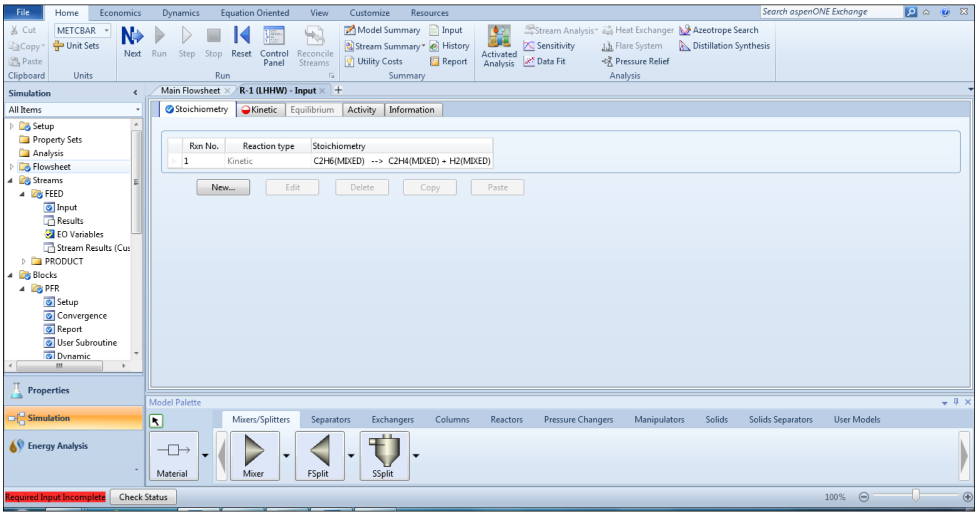


Reactor type: Adiabatic reactor

Operating condition

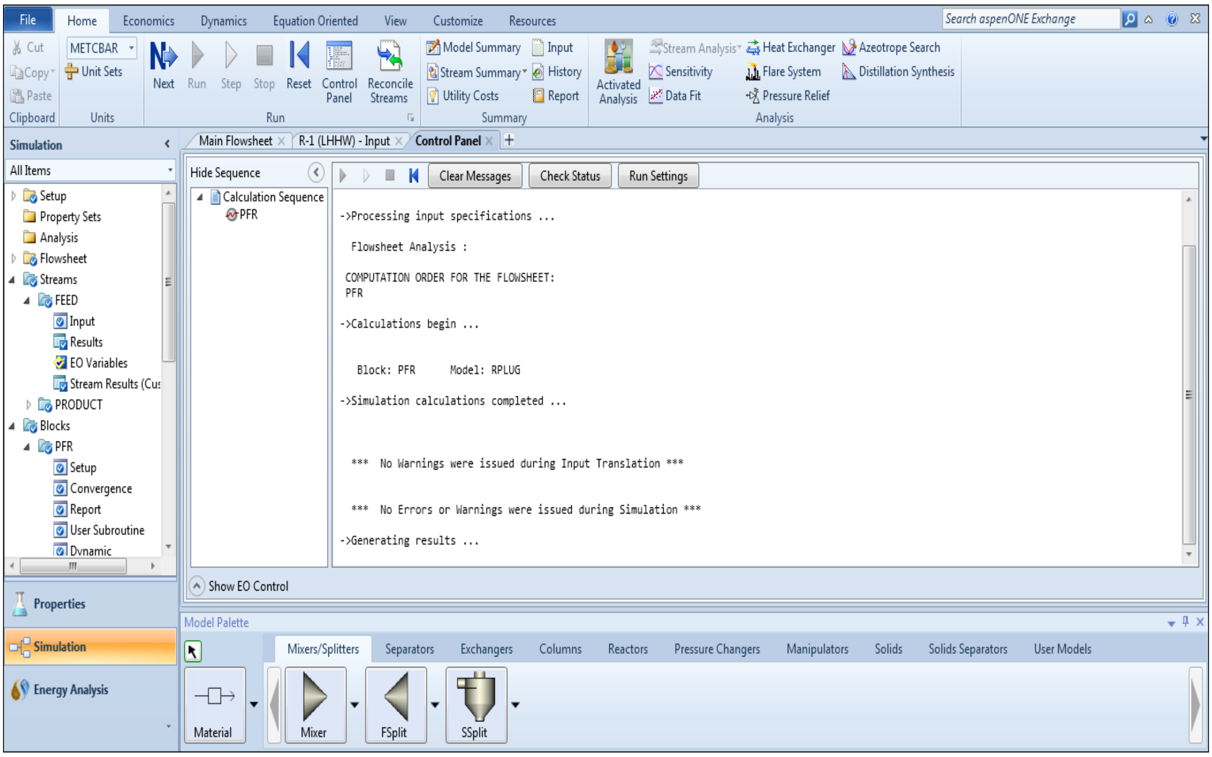
No additional specification required!

Figure 4.3 Selection of the reactor



Rxn No.	Reaction type	Stoichiometry
1	Kinetic	C2H6(MIXED) --> C2H4(MIXED) + H2(MIXED)

Figure 4.4 Cracking reaction



```
->Processing input specifications ...

 Flowsheet Analysis :

 COMPUTATION ORDER FOR THE FLOWSHEET:
 PFR

->Calculations begin ...


  Block: PFR      Model: RPLUG

->Simulation calculations completed ...



 ***  No Warnings were issued during Input Translation ***


 ***  No Errors or Warnings were issued during Simulation ***

->Generating results ...
```

Figure 4.5 Running status and checking the errors and warnings

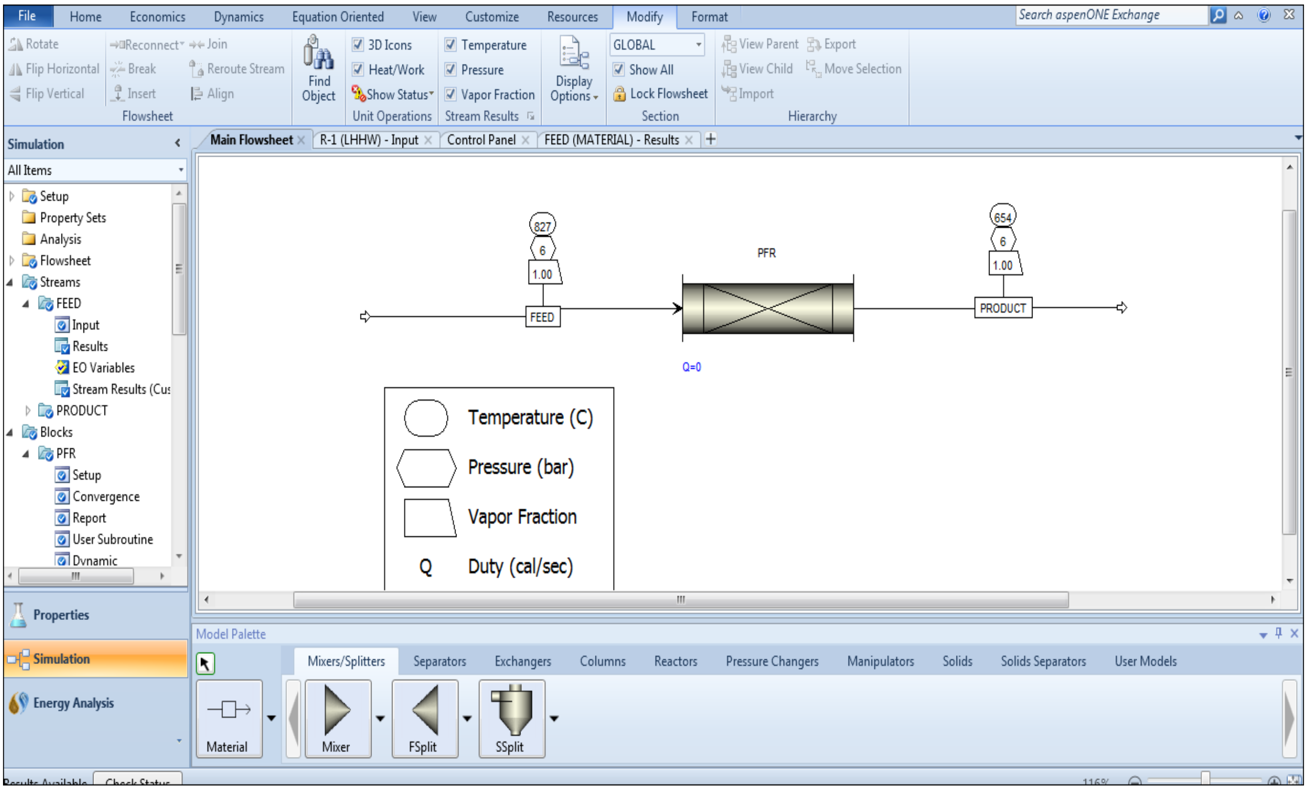
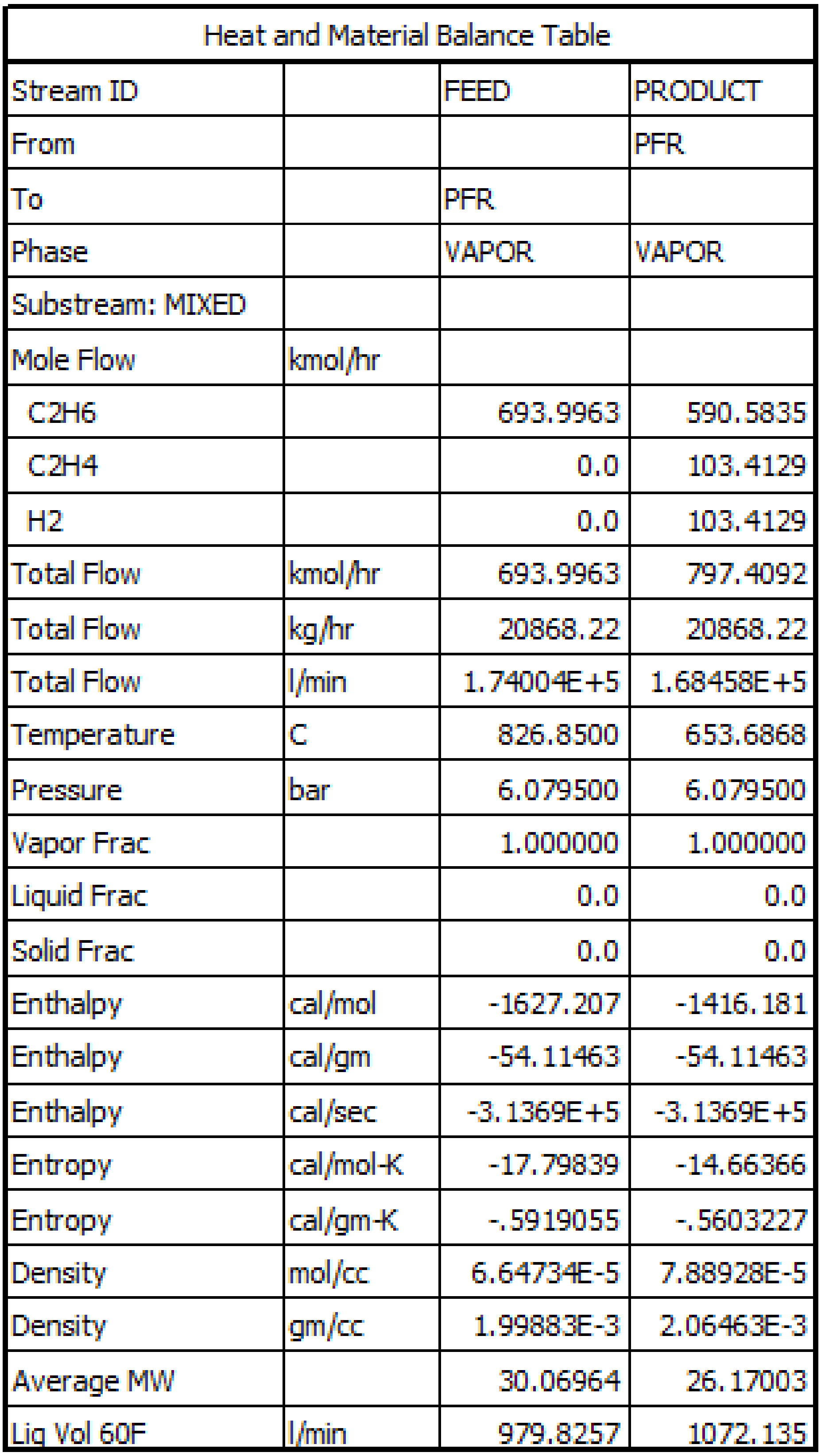


Figure 4.6 Flow sheet of PFR after completing simulation

Table 4.1 Material balance and Energy balance



Heat and Material Balance Table

Stream ID		FEED	PRODUCT
From			PFR
To		PFR	
Phase		VAPOR	VAPOR
Substream: MIXED			
Mole Flow	kmol/hr		
C2H6		693.9963	590.5835
C2H4		0.0	103.4129
H2		0.0	103.4129
Total Flow	kmol/hr	693.9963	797.4092
Total Flow	kg/hr	20868.22	20868.22
Total Flow	l/min	1.74004E+5	1.68458E+5
Temperature	C	826.8500	653.6868
Pressure	bar	6.079500	6.079500
Vapor Frac		1.000000	1.000000
Liquid Frac		0.0	0.0
Solid Frac		0.0	0.0
Enthalpy	cal/mol	-1627.207	-1416.181
Enthalpy	cal/gm	-54.11463	-54.11463
Enthalpy	cal/sec	-3.1369E+5	-3.1369E+5
Entropy	cal/mol-K	-17.79839	-14.66366
Entropy	cal/gm-K	-.5919055	-.5603227
Density	mol/cc	6.64734E-5	7.88928E-5
Density	gm/cc	1.99883E-3	2.06463E-3
Average MW		30.06964	26.17003
Liq Vol 60F	l/min	979.8257	1072.135

CHAPTER 5

RESULTS AND DISCUSSIONS

5.1 **Adiabatic reactor**

5.1.1 Effect of flow rate change to the product conversion

Table 5.1 Feed flow rate vs product conversion

S.no	Feed flow rate (kmol/hr)	Product flow rate(kmol/hr)	% of conversion
1	100	36.51058	16.56
2	150	52.46	15.86
3	200	76.73	15.36
4	250	82.49	14.96
5	300	96.8	14.63
6	350	110.77	14.35
7	400	124.43	14.11
8	450	137.83	13.89
9	500	151	13.7
10	550	163.93	13.52
11	600	176.67	13.35
12	650	189.22	13.20

13	700	201.62	13.06
14	750	213.85	12.93
15	800	225.93	12.81
16	850	237.86	12.69
17	900	249.61	12.58
18	950	261.38	12.48
19	1000	272.86	12.37

Table 5.2 Feed flow rate vs product conversion

S.no	**Feed flow rate (kmol/hr)**	**Feed flow rate(lbmol/hr)**	**Product flow rate(lbmol /hr)**	**% of conversion**
1	10	22.046	4.46	20.23
2	20	44.11	8.45	19.18
3	30	66.13	12.26	18.54
4	40	88.18	15.94	18.08
5	50	110.23	19.53	17.72
6	60	132.27	23.04	17.42
7	70	154.32	26.48	17.17
8	80	176.36	29.88	16.94
9	90	198.41	33.21	16.74

Table 5.3 Feed flow rate vs product conversion

S.no	**Feed flow rate (kmol/hr)**	**Feed flow rate(lbmol/hr)**	**Product flow rate(lbmol /hr)**	**% of conversion**
1	9	19.84	4.05	10.39
2	8	17.63	3.63	20.56
3	7	15.43	3.20	20.76
4	6	13.22	2.77	20.99
5	5	11.02	2.23	21.25
6	4	8.82	1.902	21.57
7	3	6.62	1.45	21.98
8	2	4.41	0.99	22.54
9	1	2.20	1.68	76.52

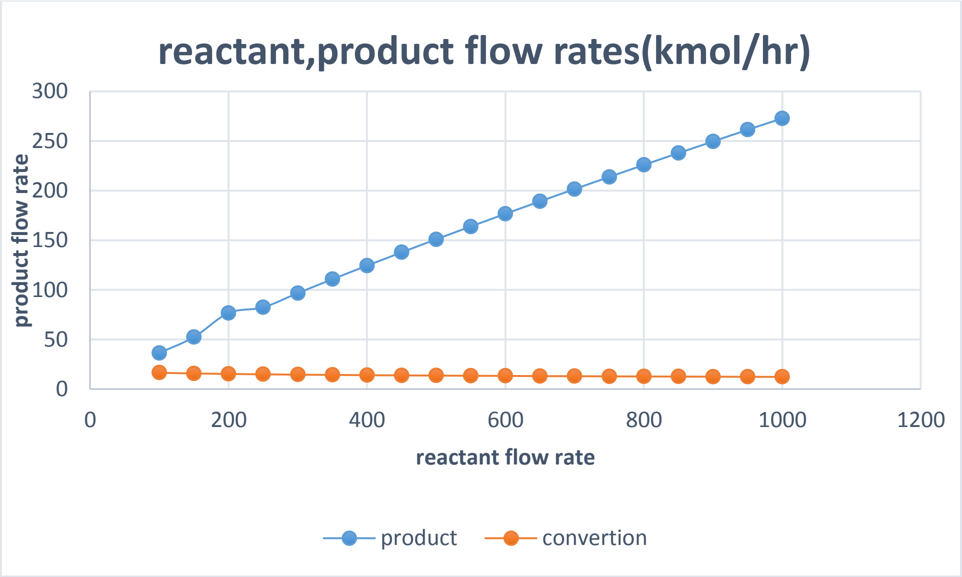


Figure 5.1 Feed flow rate vs product conversion

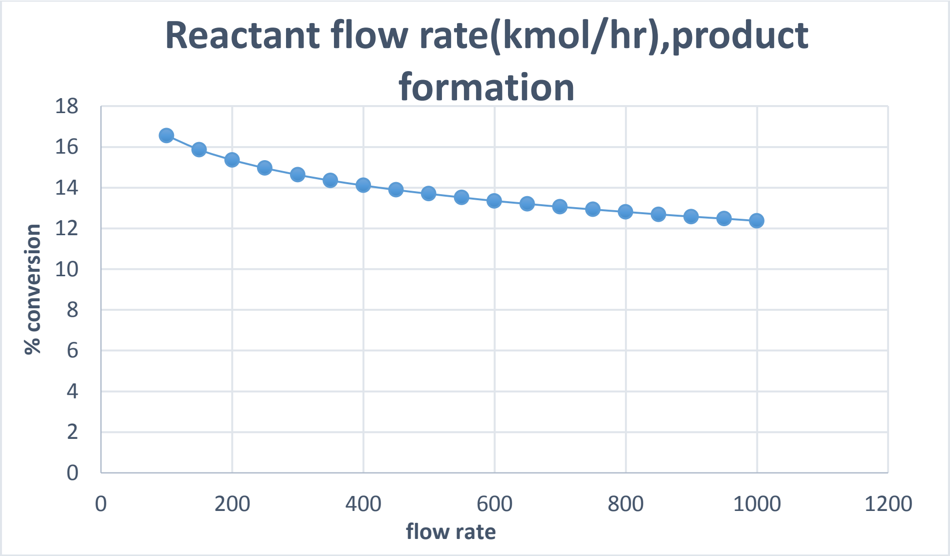


Figure 5.2 Feed flow rate vs product conversion

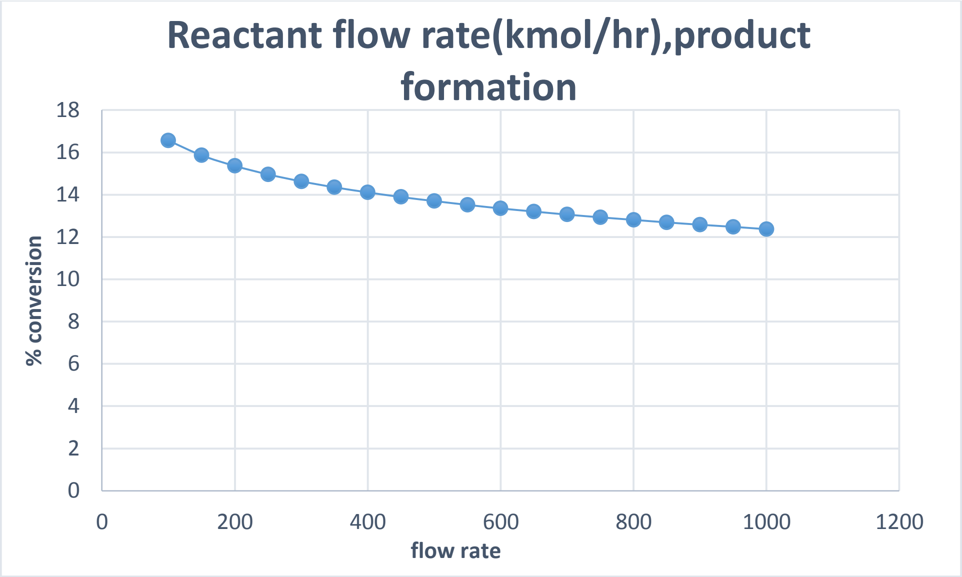


Figure 5.3 Feed flow rate vs % product conversion

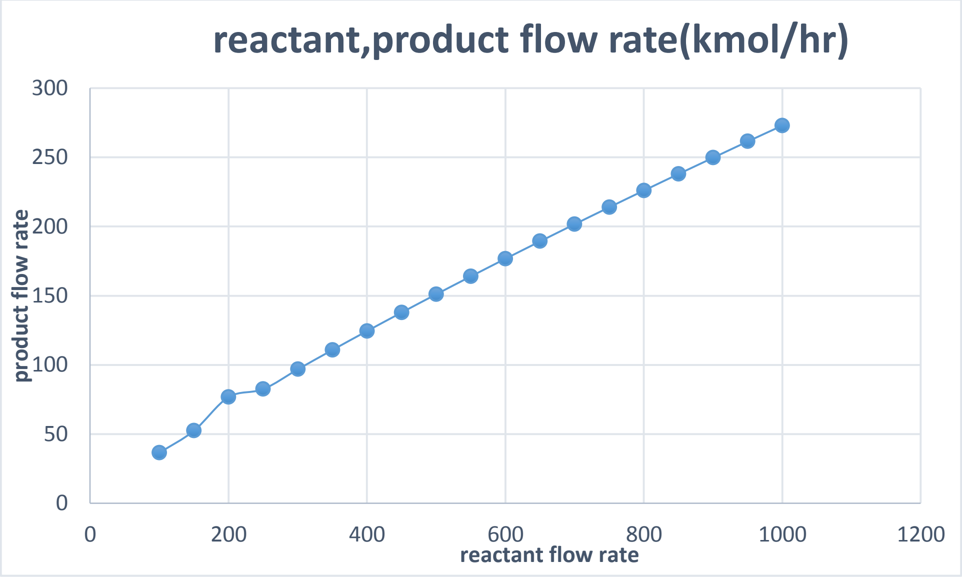


Figure 5.4 Feed flow rate vs product conversion

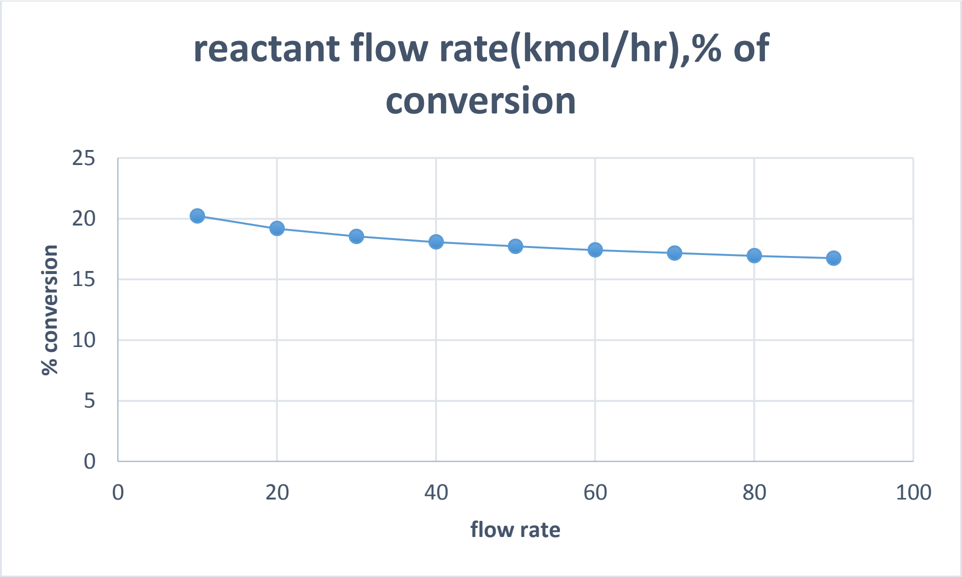


Figure 5.5 Feed flow rate vs product conversion

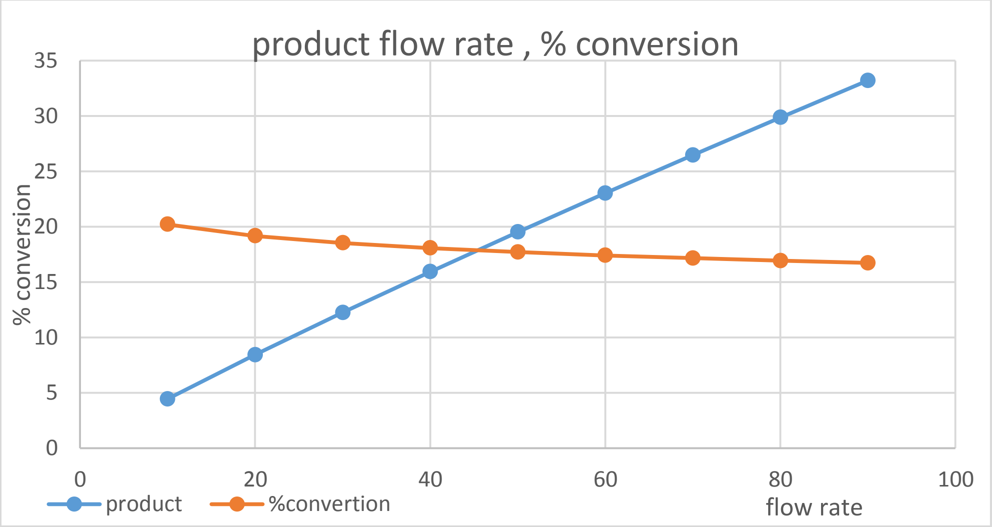


Figure 5.6 Product flow rate vs conversion

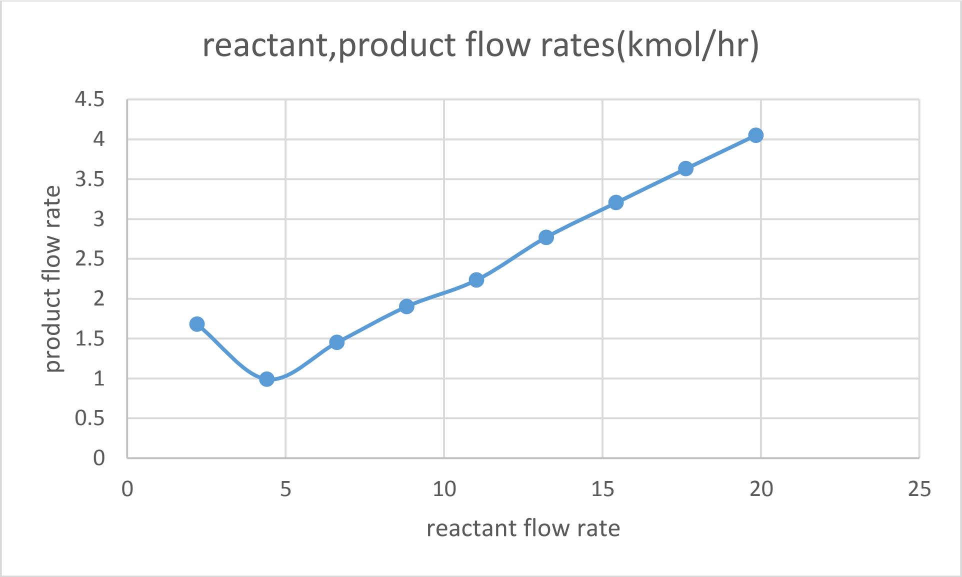


Figure 5.7 Reactant vs product flow rates

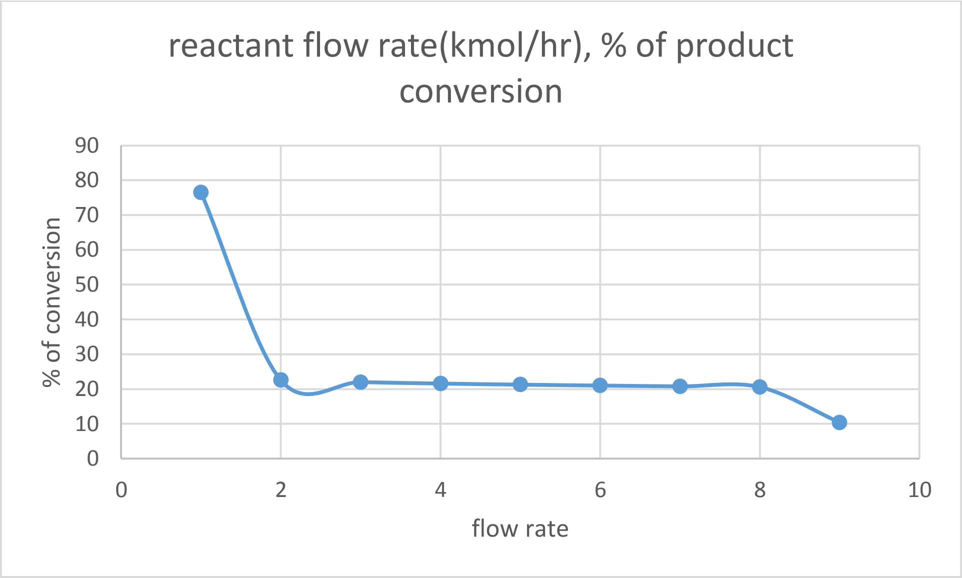


Figure 5.8 Feed flow rate vs conversion

5.1.2. Multi tube reactor

Table 5.4 No. of tubes vs product conversion

S.no	No. of tubes	Feed flow rate(kmol/hr)	Product flow rate(kmol /hr)	% of conversion
1	1	1530	200.13	13.08
2	2	1530	219.87	14.37
3	3	1530	231.06	15.102
4	4	1530	244.82	15.60
5	5	1530	262.77	16.002
6	10	1530	262.77	17.17
7	20	1530	280.15	18.31
8	30	1530	289.96	18.95
9	40	1530	296.80	19.4
10	50	1530	302.04	19.74
11	100	1530	317.89	20.77
12	200	1530	333.14	21.77
13	300	1530	341.83	22.3
14	400	1530	347.86	22.73
15	500	1530	352.5	23.04

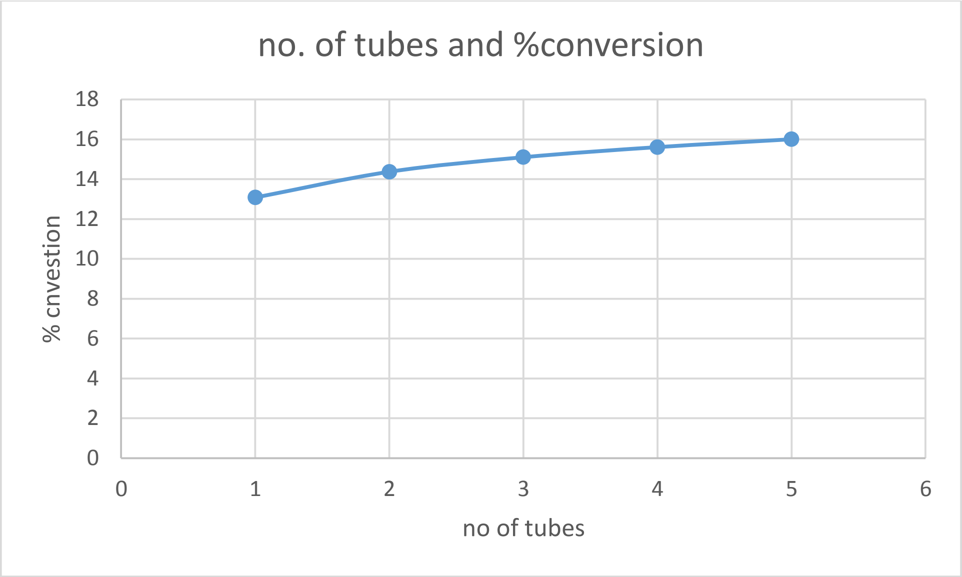


Figure 5.9 No. of tubes vs conversion

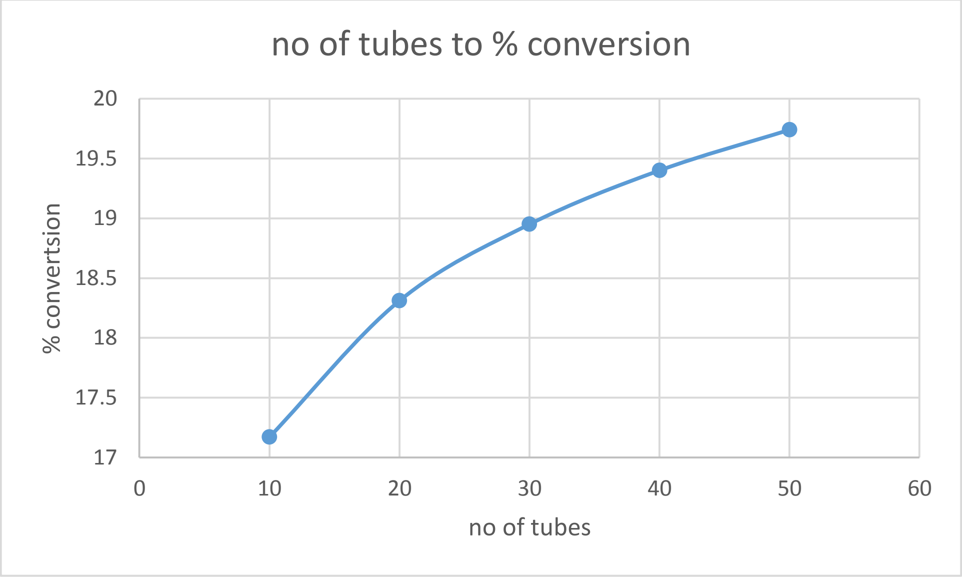


Figure 5.10 No. of tubes vs conversion

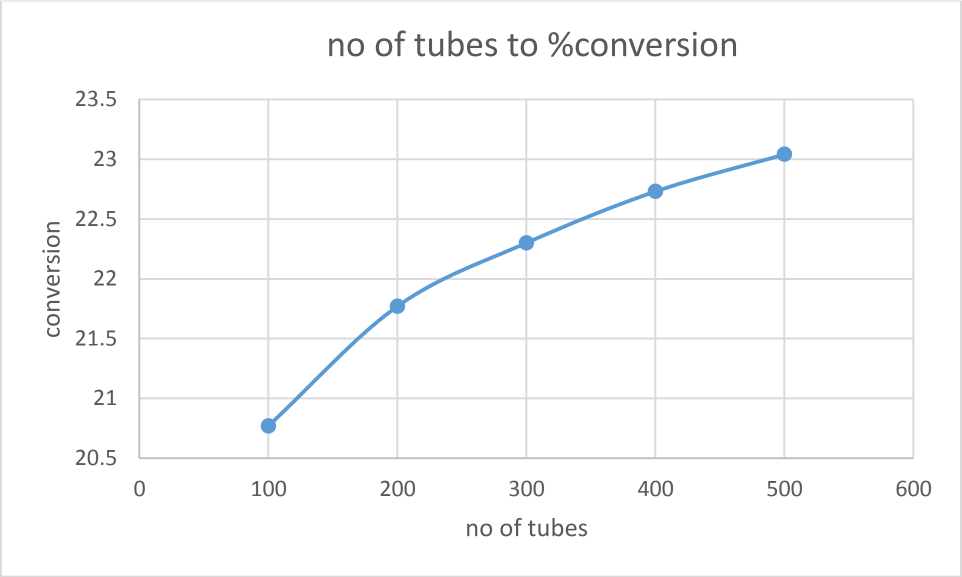


Figure 5.11 No. of tubes vs conversion

5.1.3. Effect of feed temperature to the product formation

Table 5.5 Feed temperature vs product formation

S.no	**Feed temperature**	**Feed flow rate(kmol/hr)**	**Product flow rate(kmol /hr)**
1	1100	1530	220.10
2	1200	1530	334.73
3	1300	1530	474.12
4	1400	1530	617.27
5	1500	1530	763.33
6	1600	1530	911.41
7	1700	1530	1060.47

8	1800	1530	1208.65
9	1900	1530	1352.61
10	2000	1530	1480.19

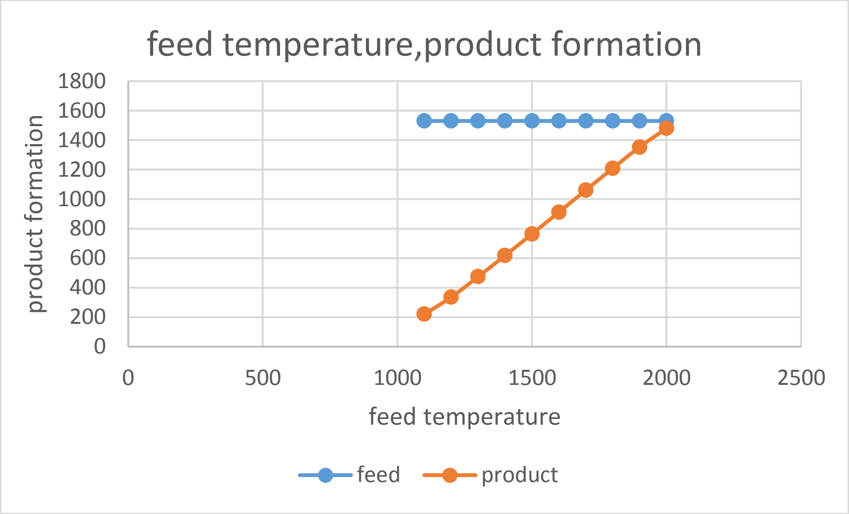


Figure 5.12 Feed temperature vs product formation

5.1.4 Effect of pressure

Table 5.6 Effect of pressure vs product formation

S.no	**Pressure(atm)**	**Feed flow rate(kmol/hr)**	**Product flow rate(kmol /hr)**
1	1	1530	145.45
2	2	1530	167.18
3	3	1530	179.60
4	4	1530	188.21

5	5	1530	194.81
6	6	1530	200.10
7	7	1530	204.60
8	8	1530	208.43
9	9	1530	211.79
10	10	1530	214.75
11	20	1530	233.95
12	30	1530	244.83
13	40	1530	252.38
14	50	1530	258.14
15	50	1530	258.14

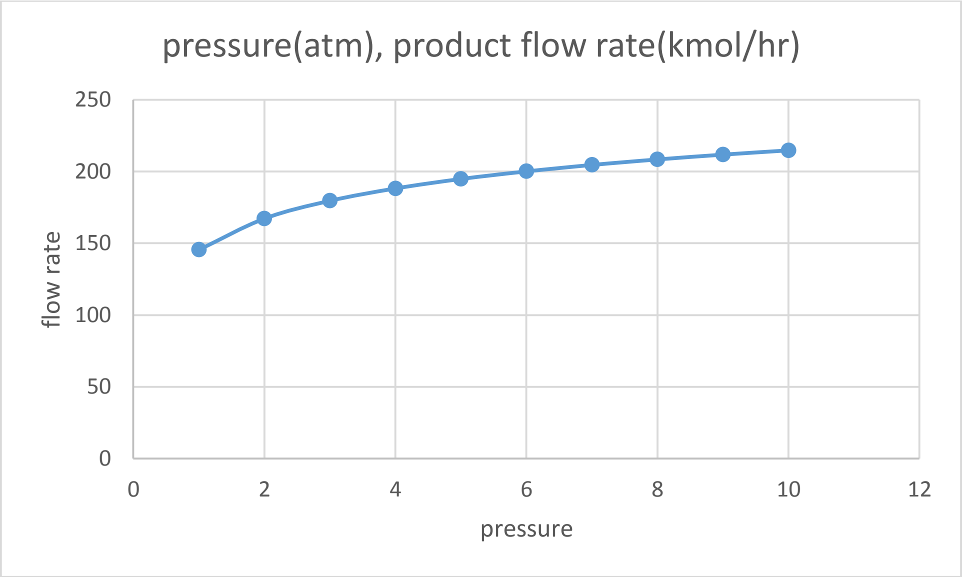


Figure 5.13 Effect of pressure vs product formation

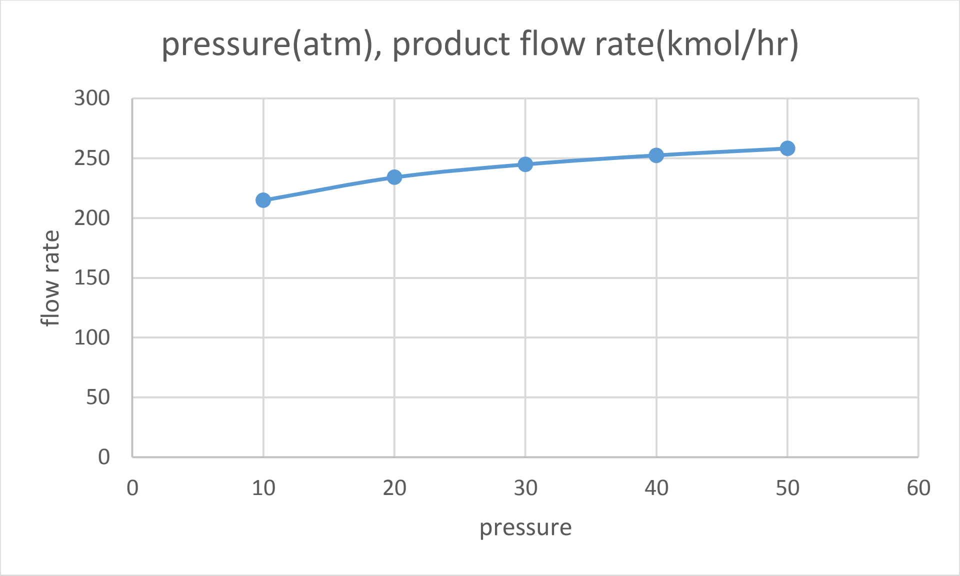


Figure 5.14 Effect of pressure vs product formation

5.1.5 Effect of length and diameter to the yield (input, output in kmol/hr)

Table 5.7 Effect of (L/D) to the product formation

L/D	C_2H_6	C_2H_6	C_2H_4	H_2
10/.4	694	628.69	65.31	65.30
10/.5	694	622.31	71.68	71.68
10/1	694	603.36	90.63	90.63
10/1.5	694	592.94	101.05	101.05
10/2	694	585.88	108.13	108.13
10/3	694	576.20	117.79	117.79

10/5	694	546.69	129.30	129.31
15/3	694	580.96	113.03	113.03

5.1.6 Effect of length and diameter (L/D) to the temperature gradient

Table 5.8 Effect of (L/D) to the temperature gradient

Reactor length(M)	10/.4	10/.5	L/D=10/1	10/2 LD	L/D=15/2
	tempetature1 (^{0}C)	Temperature2 (^{0}C)	Temperature3 (^{0}C)	Temperature4 (^{0}C)	Temperature5 (^{0}C)
0	826.85	826.85	826.85	826.85	826.85
1	775.31	764.78	730.70	697.18	687.65
2	758.80	747.84	713.77	681.02	671.79
3	748.84	737.81	704.01	671.79	662.74
4	741.73	730.77	697.16	665.33	656.43
5	736.21	725.24	691.92	660.39	651.57
6	731.71	720.77	687.66	656.43	647.64
7	727.91	717.01	684.08	653.10	644.34
8	724.64	713.77	681.00	650.25	641.50
9	721.77	710.92	678.30	647.67	639.01
10	719.20	708.38	675.90	645.41	636.79

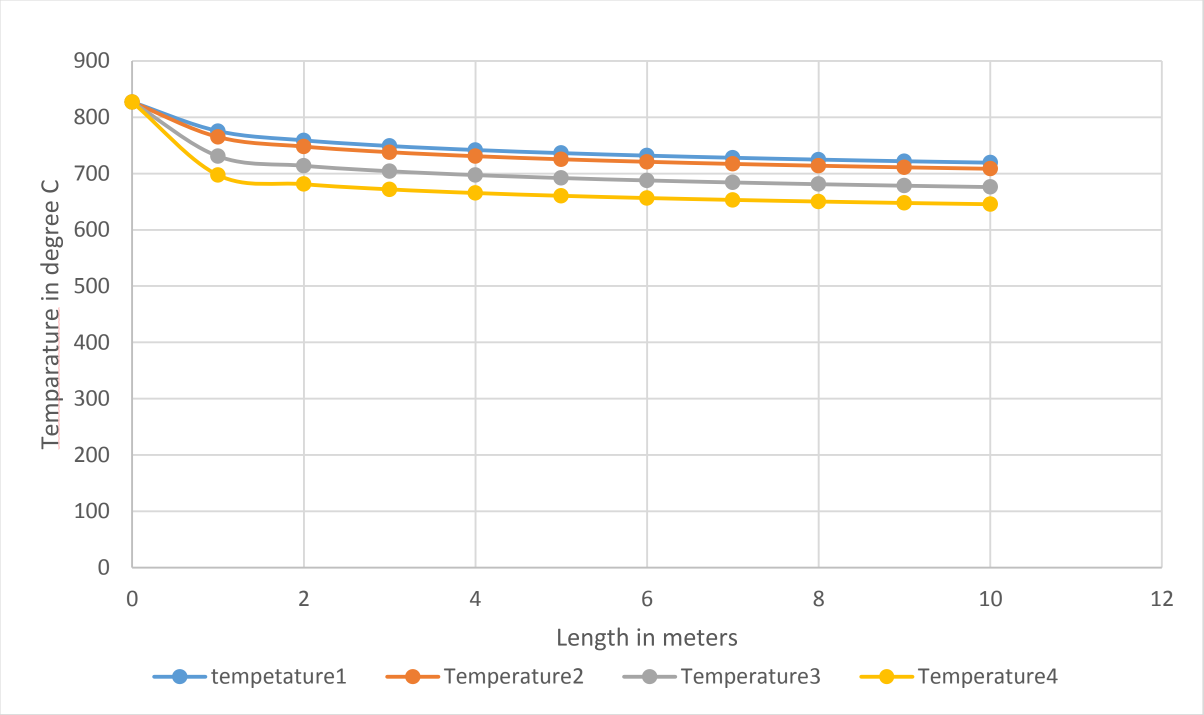


Figure 5. 15Temperature change with increasing of length

5.2 Isothermal PFR

5.2.1 Effect of feed flow rate to the product conversion

Table 5.9 Effect of feed flowrate to the product formation

S.no	Feed flow rate (kmol/hr)	Feed flow rate(lbmol/hr)	Product flow rate(lbmol /hr)	% of conversion
1	1000	2024.62	95.10	2128.84
2	900	1984.16	97.51	1934.90
3	800	1763.69	98.34	1734.47
4	700	1543.23	99.01	1528.10
5	600	1322.77	99.04	1316.23

6	500	1102.31	99.50	1100.22
7	400	881.84	99.81	881.44
8	300	661.38	99.95	661.35
9	200	440.92	99.99	440.92
10	100	220.46	100	220.46

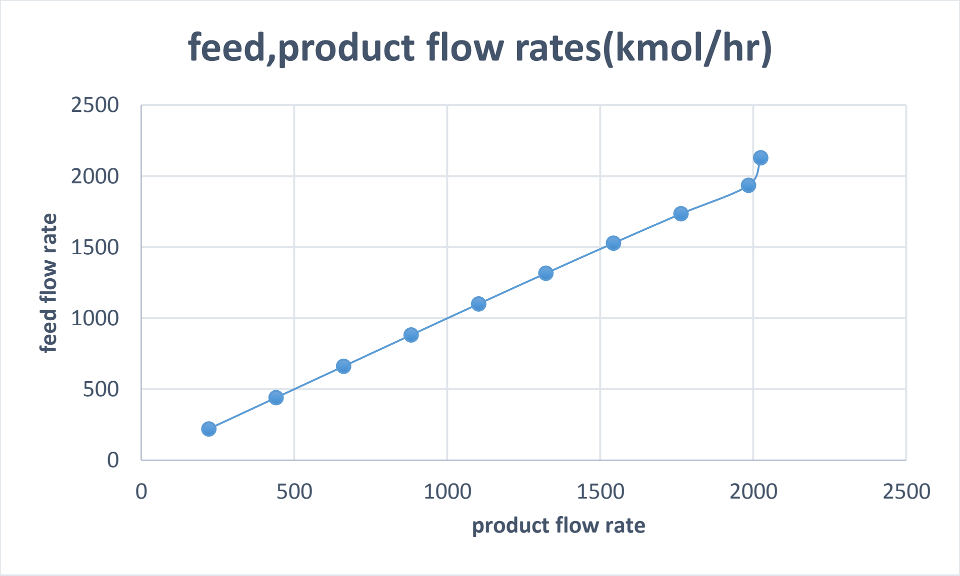


Figure 5.16 Effect of feed flowrate to the product formation

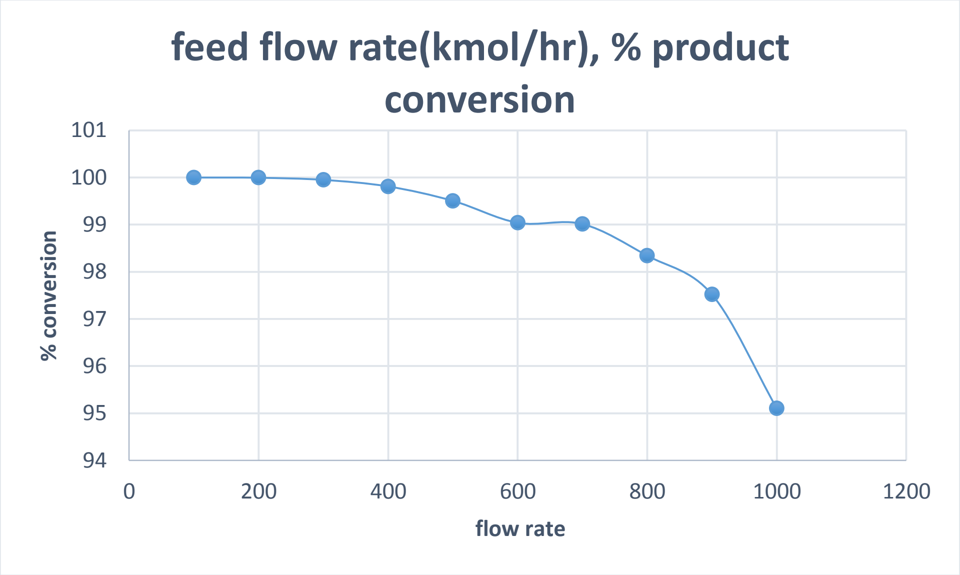


Figure 5.17 Effect of feed flow rate to the %conversion of the product

5.2.2. Effect of feed temperature to the product formation

Table 5.10 Effect of feed temperature to the product formation

S.no	Feed temparature	Feed flow rate(kmol/hr)	Product flow rate(kmol /hr)	% of conversion
1	1500	1530	1530	100
2	1400	1530	1530	100
3	1300	1530	1530	100
4	1200	1530	1530	100
5	1100	1530	1515.44	99.05
6	1000	1530	1257.13	82.17
7	1050	1530	997.65	65.21

8	1060	1530	1162.941	76.01
9	1070	1530	1305.71	85.34
10	1080	1530	1413.701	92.39
11	1090	1530	1481.911	96.86
12	1100	1530	1515.438	99.05

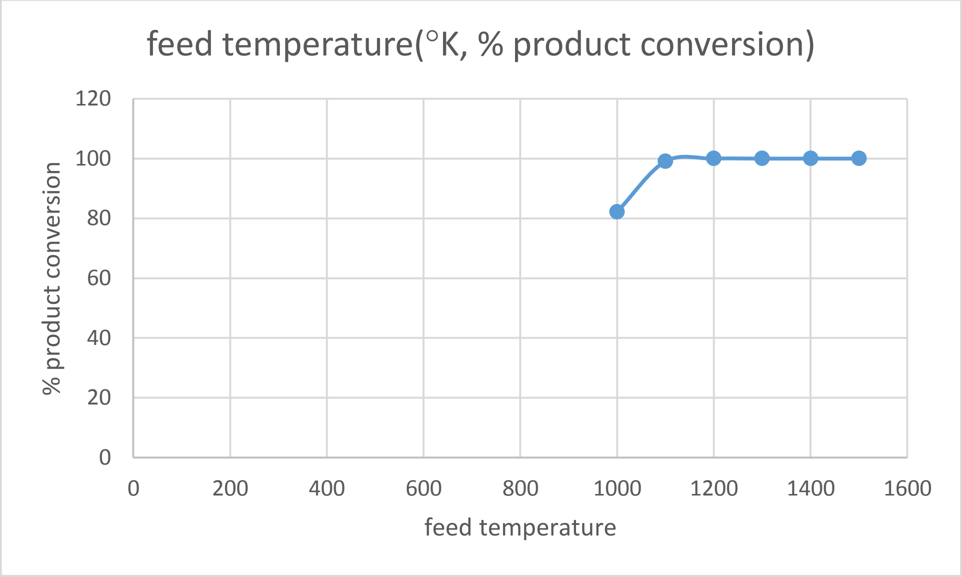


Figure 5.18 Effect of feed temperature to the product conversion

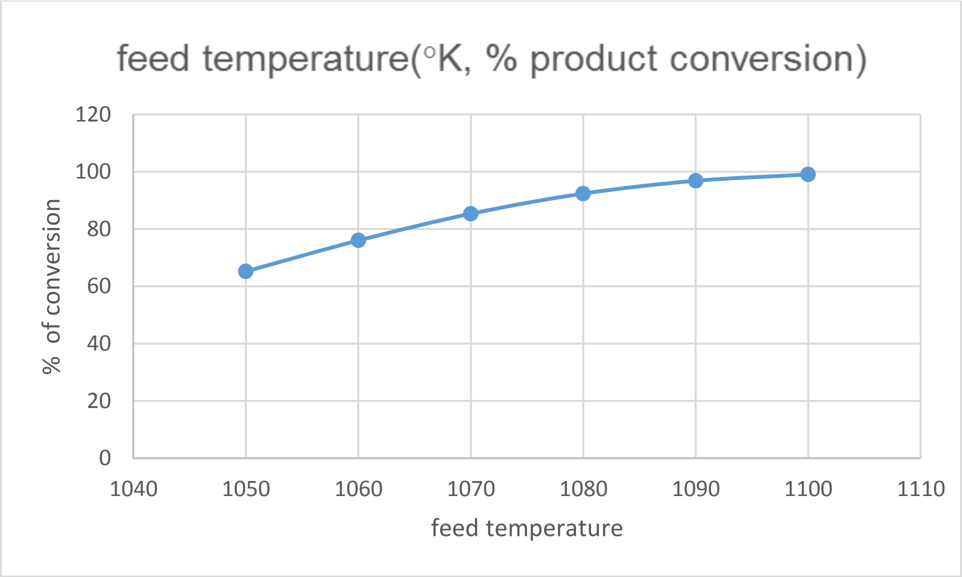


Figure 5.19 Effect of feed temperature to the % of product conversion

Table 5.11 Effect of feed temperature vs product formation

S.no	**Feed temperature**	**Feed flow rate(kmol/hr)**	Product flow rate(kmol /hr)	**% of conversion**
1	1055	1530	1082.19	70.73
2	1056	1530	1098.71	71.81
3	1057	1530	1115.06	72.87
4	1058	1530	1131.23	73.93
5	1059	1530	1147.18	74.97
6	1060	1530	1162.94	76.01
7	1050	1530	997.65	65.20
8	1040	1530	705.41	46.10
9	1030	1530	697.3	42.96

10	1020	1530	506.12	33.07
11	1010	1530	377.22	24.64
12	1000	1530	272.86	17.77

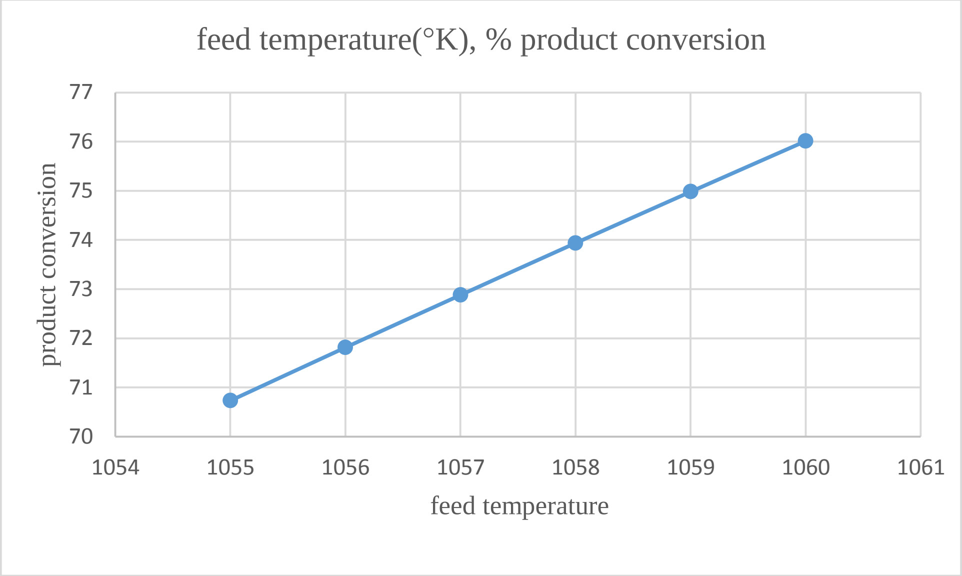


Figure 5.20 Effect of feed temperature vs % product conversion

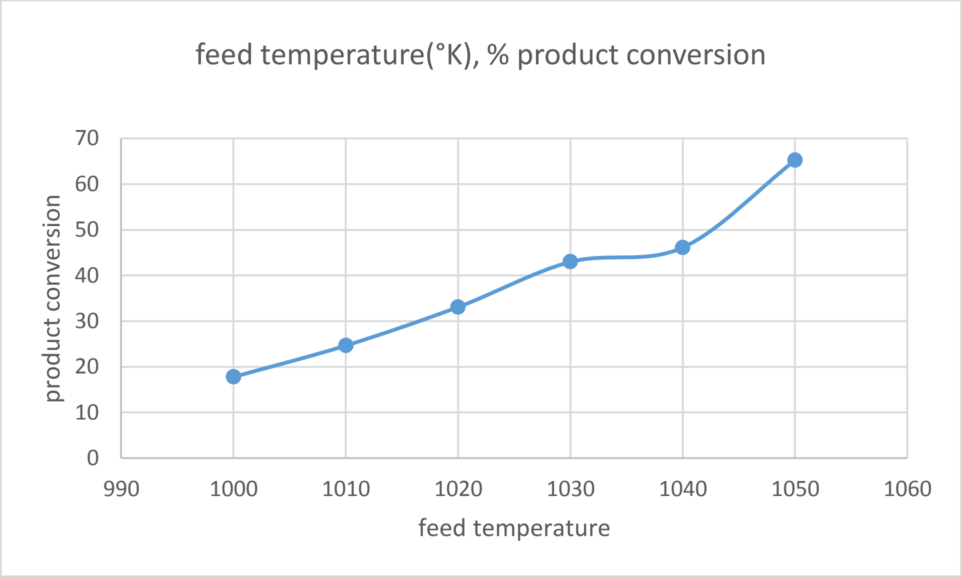


Figure 5.21 Effect of feed temperature vs % product conversion

5.2.3 Effect of pressure

Table 5.12 Effect of pressure vs product formation

S.no	Pressure(atm)	Feed flow rate(kmol/hr)	Product flow rate(kmol /hr)
1	1	1530	973.76
2	2	1530	1278.33
3	3	1530	1409.48
4	4	1530	1470.95
5	5	1530	1500.76
6	6	1530	1515
7	7	1530	1522
8	8	1530	1526
9	9	1530	1526.36
10	10	1530	1529

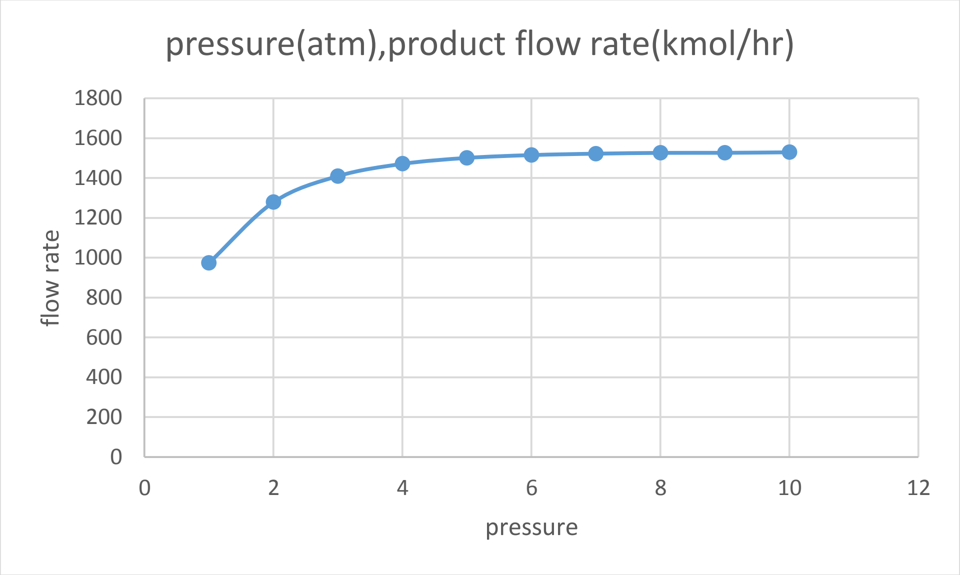


Figure 5.22 Effect of pressure vs product flow rate

5.2.4 Effect of length and diameter ratio (L/D) to the product formation

Table 5.13 Effect of (L/D) to the product conversion

L/D	C_2H_6	C_2H_6	C_2H_4	H_2
7/2	694.00	7.18397E-3	693.99	693.98
8/2	694.00	8.49335E-4	693.999	693.999
9/2	694.00	0	694.00	694.00
10/2	694.00	0	694.00	694.00
7/3	694.00	1.59942E-3	693.99	693.99
8/3	694.00	2.86591E-4	693.996	693.996
9/3	694.00	2.8457E-4	693.99	693.99
10/3	694.00	0	694.00	694.00
5/4	694.00	0	694.00	694.00

Discussion:

In adiabatic reactor:

- If length kept constant in adiabatic PFR, the yield of the product is increasing with the increasing in diameter size.
- Temperature gradient increasing with the increasing diameter size of PFR.
- Effect of feed flow rate to the product formation: if flow rate increases product formation decreases.
- Effect of feed temperature: product formation is increases with increasing with increasing the feed temperature.
- Effect of pressure: product formation is increases with increasing with increasing the pressure inside the reactor.
- Effect of no. of tubes: product formation increases with increasing no. of tubes.

In isothermal reactor:

- Product formation increases with increasing length while diameter size kept constant.
- Effect of feed flow rate: if flow rate increases product formation decreases.
- Effect of feed temperature: 1100°K is the optimum feed temperature at 6atm pressure and flow rate at 1530kmol/hr(694 lb mol/hr) and (L/D) (10m :0.1m)
- Effect of pressure: product formation is increases with increasing with increasing the pressure inside the reactor.
- Effect of reactor temperature: product formation increases with increasing the reactor temperature.

CHAPTER 6

CONCLUSIONS AND FUTURE WORKS

We have successfully simulated the cracking of ethane to ethylene and hydrogen using isothermal and adiabatic plug flow reactors. Effect of various process variables *viz*. feed flow rate, feed temperature, reactor temperature and pressure were studied. The variation of diameter and length of the reactors were also studied in the overall performance of the system. From the overall study, following conclusions are made:

a) Isothermal plug flow reactor achieves 100% conversion to products at 1100 K temperature, 6atm pressure and 100kmol/hr feed flow rate.
b) But with adiabatic PFR a highest percentage of 16.56 was achieved, keeping all the conditions same.
c) For adiabatic PFR product conversion is increasing while increasing the feed temperature but it is not recommended at high feed temperatures.
d) In isothermal PFR, at (L/D) ratio of 10/2 and 9/3 product of high purity (100%) were achieved.
e) In adiabatic PFR, at (L/D) ratio of 10/5, yields a product of purity of 18.6% only.

f) Finally, it can be concluded that under a given set of conditions, isothermal plug flow reactor performed comparatively much better than its adiabatic counterpart.

This cracking reaction is industrially important because hydrogen and ethylene are used in widely different industrial processes. As a future work, this study may further be extended to carry out dynamic simulation with control features. Similarly, a detailed cost optimization can be carried out to find the effectiveness of the plug flow process in comparison to fluidized bed catalytic cracker

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