A
DISSERTATION REPORT
ON

"MODELING AND SIMULATION OF POLYPROPYLENE PRODUCTION USING ASPEN AND OPTIMIZATION

Submitted for partial fulfillment of the requirement
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Submitted By:
PRATAP REDDY N
Enrolment No. : 09412011

Under the Guidance of :
Dr. Y.S. NEGI
(Professor)
Department of Polymer & Process Engineering
IIT Roorkee

DEPARTMENT OF POLYMER & PROCESS ENGINEERING
INDIAN INSTITUTE OF TECHNOLOGY ROORKEE
SAHARANPUR CAMPUS
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When one is so closely involved with an organization for a period of over four years, it becomes a monumental task to try to acknowledge all the people who have influenced you in various different ways. However, it also becomes imperative, due to the valuable contributions that they make towards your life and work, to attempt to perform this task right at the beginning.

I express my deep sense of gratitude towards my guide Dr. Y.S. NEGI for his extreme help and support in spite of his busy and hectic schedule and making this thesis a success.

Date: 6th June, 2014

PRATAP REDDY N

N. Pratap Reddy

CANDIDATE DECLARATION

I hereby declared that the work which is being presented in this Dissertation Report entitled **"Modelling and Simulation of Polypropylene Production Using ASPEN and Optimization"** in partial fulfilment of the requirement for the award of the degree of Integrated M.Tech in Polymer Science and Technology from IIT Roorkee is an authentic record of my own work carried out under the supervision of **Dr. Yuvraj Singh Negi** (Professor) Department of Polymer and Process Engineering, IIT ROORKEE.

I have not submitted the matter embodied in this dissertation report for the award of any other degree or diploma.

Date: 08-05-2014
Place: IIT Roorkee, Saharanpur Campus,
Saharanpur

PRATAP REDDY N
N Pratap Reddy

This is to certify that the above statement made by the candidate is correct to the best of our knowledge.

Dr. Y.S.NEGI
(Professor-IIT Roorkee)
Department of Polymer & Process Engineering
IIT ROORKEE

ABSTRACT

With the increasing demand of polymer products, there are abundant opportunities for upstream petrochemical industries to enhance their present capacity and deliver optimum quality products to the downstream industries to make the whole system efficient and profitable. Currently the market in India, predicted to have a huge demand-supply gap of Polypropylene of around 1795 KTA for 2015 on the basis of 2009, with CAGR of 13% (2005-06 to 2011-12). This large gap must be filled by adopting a sustainable way of optimization for the existing and new plants to meet the goals of high efficiency and profitability with minimum energy usage and waste generation. With the advent of computers and simulating software like ASPEN PLUS® it is possible to design and optimize a particular process. Proper design can significantly reduce production cost as well as provide make the process safe and reduce environmental hazards. The materials, unit operations and processes involved are identified and steady state simulation is done. Each unit is taken into consideration and some variables are optimized to give better yield and energy efficiency. The model considers the important issues of physical property and thermodynamic model selections, polymer properties, and catalyst characterization, in addition to the traditional Ziegler-Natta polymerization kinetics. This Model development involves basic chemical engineering principles and improved software tools, Polymers Plus and Aspen Plus. We consider a Ziegler-Natta catalyst with multiple catalyst sites. This steady state simulation of Polypropylene is based on the Physical property data and design of real life plants. The results obtained from simulation are matching with the industry for which the process is modeled with the same operating parameters and physical property data.

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CHAPTER 1

INTRODUCTION

1.1 SYSTEM CONSIDERED

The system considered for study, simulation and optimization is a polypropylene production plant. The process described by UNIPOL flowsheet is taken as base for simulating the system. This process description provides relevant and valuable data required for the simulation of the process.

Raw materials fed to the plant are benzene

- ☐ Refinery grade Propene obtained from Naphtha
- ☐ Ziegler-Natta Catalyst (Titanium Tetrachloride)
- ☐ Magnesium chloride (Promoter)
- ☐ Donor (Di isobutyl phthalate or 2,4-pentadiol di benzoate)
- ☐ Hydrogen

Various unit operations and processes are required to be taken care of which are described in some detail below. The major units in the process plant are the reactor section and the separator section.

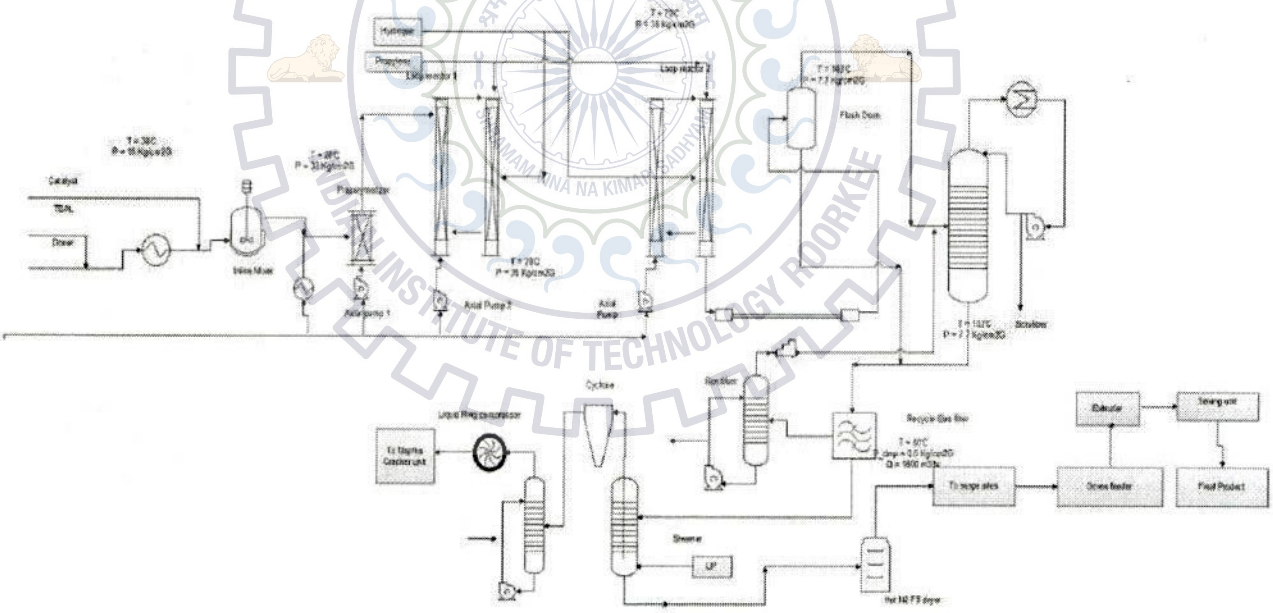


Figure 1-1. UNIPOL Flow sheet design in E-draw 6.0

1.2 RELEVANCE

The scope for application of plastics is increasing significantly and, more and more sectors in the economy started using plastics of account of their multiple benefits. Today, petrochemicals are vital inputs to all critical sectors of the economy including agriculture, infrastructure, automobile, construction, consumer goods, telecommunication, packaging and healthcare. Developing polypropylene production process with optimum and efficient performance will result in high profitability and production with minimum energy requirements. These objectives can be achieved by designing plants to deliver better quality products according to the demand of the markets with a maximum degree of flexibility that can be obtained.

Propylene obtained for the process is sourced from Naphtha obtained from the upstream process, which is present in surplus due to its replacement by Natural Gas in power plants and manufacturing of Fertilizers. This Surplus Naphtha is cracked to extract variety of monomers for the production of polymers. Average throughput of propylene by Naphtha cracker is estimated to be 11% of the feed. But with the availability of the advanced technology it can be extended up to 20%, with the optimum expense of Gasoline Production. Fluidized Catalytic crackers are widely used to achieve desired results and performance. Homopolymers, Random copolymers and heterophasic copolymers are produced from the bulk polymerisation using spheripol technology. The simulation performed here is purely based on the production of homopolymers, data required for the simulation involving production of heterophasic copolymers were not present in adequate amount.

Ziegler-Natta catalyst titanium tetrachloride supported on magnesium chloride along with triethyl aluminium is used to carry out the polymerisation at low kinetics at prepolymerization reactor. Slurry obtained is from this reactor is injected in the series of two loop reactors with propylene, both integrated with axial pumps to maintain a continuous uniform flow. Mixture from reactors is fed to flash drum through a flash line, which separates polymer and enterained monomer gas. Monomer gas is passed through propylene scrubber at high pressure, obtained monomer gas is washed and condensed to recycle it back. Bottoms of scrubber and flash drum are proceed through a recycle gas filter at low pressures to remove residual gas remained in the polymer. Residual gas obtained from recycle gas filter is fed to the propylene scrubber at high pressure and the polymer powder is sent to steamer in order to inactivate the remaining part of catalyst and remove soluble monomers. Obtained powder is dried off by hot nitrogen gas to obtain desired product with the required quality.

Designing of plant, using simulation is beneficial as it reduces calculations time and improves the accuracy when compared to methods otherwise used. There are various simulation program, used in the industries depending on their applicability with concerned process. ASPEN PLUS is very reliable and useful software to handle polymerization problems as it supports wide range of properties parameters in polymer processing. Designing of plant, using simulation is beneficial as it reduces calculations time and improves the accuracy when compared to methods otherwise used. There are various simulation program, used in the industries depending on their applicability with concerned process.

ASPEN PLUS is very reliable and useful software to handle polymerization problems as it supports wide range of properties parameters in polymer processing. Use of ASPEN plus simulation will have major business benefits : -

1. Reducing Human Errors.

2. Efficient and high profitability design.

3. Enhanced operational and control flexibility.

4. Minimize time requirements.

5. Reduce complexities in process networks and eliminate process bottle necks.

Process modeling and simulation is a better choice adopted by chemical engineer's today in almost every area of process engineering, due to its reliable payoff in reduced efforts and minimum time utilization. OPEX can be reduced by obtaining optimum operating process parameters by involving various optimization techniques. ASPEN Plus supports process optimization using inbuilt complex and SQP methods, and also from sensitive analysis.

In the present work the polypropylene production plant is simulated using ASPEN PLUS ® and the sizes, the temperature and other relevant parameters are obtained by optimization. MATLAB®, MS Excel and Origin Pro 8.0 are used to plot graphs in the following simulation from which an optimum conditions are estimated .

1.3 OBJECTIVE OF THE PROJECT

Considering the importance of the present process, work was undertaken to design and simulate the polypropylene production process using ASPEN PLUS ® software. The objectives of the present project are following.

- To design a Ziegler-Natta catalyst based polypropylene production process and study the sensitivity analysis.
- To minimize the loss of material along with a greater production of polypropylene and low requirement of energy.

CHAPTER 2

LITERATURE REVIEW

2.1. ZIEGLER-NATTA CATALYSTS

Ziegler-Natta catalysts for propylene polymerization have enhanced much since their discovery in the fifties, including changes in catalyst precursors, cocatalysts, internal and external electron donors. Internal donors are used during catalyst manufacturing to maximize the fraction of stereospecific sites; external donors are added during the polymerization to replace internal donors lost due to alkylation and reduction reactions with the cocatalyst. In addition to its use for passivation (poison scavenging), the cocatalyst is used to activate the catalyst by the reduction and alkylation of the transition metal.

First and second generation Ziegler-Natta catalysts were composed of crystalline $TiCl_3$ in four different geometries: α = hexagonal, β = fiber or chain, γ = cubic, and δ = alternating between hexagonal and cubic. Three of these geometries, α, γ and δ, have high stereoselectivity and can be activated with a diethylaluminum cocatalyst. The δ-$TiCl_3$ complex has the highest activity towards propylene polymerization and is obtained as porous particles with relatively small diameters (20-40 μm). The controlled fragmentation of catalyst particles during polymerization was one of the major challenges to the development of heterogeneous Ziegler- Natta catalysts (Cerruti, 1999).

The introduction of electron donors (Lewis bases) during polymerization to increase catalyst stereoselectivity and productivity led to 2nd generation Ziegler-Natta catalysts. Because most of the potential active sites are located inside $TiCl_3$ crystals where they cannot promote polymerization, 1st and 2nd generation catalysts have poor productivities per mole of titanium, and require post-reactor steps to remove catalyst residues (deashing). Their lower stereoselectivities also demand a post-reactor step to extract atactic polypropylene from the final product. The elimination of these two post-reactor steps was the main driving force behind the development of new types of heterogeneous Ziegler-Natta catalysts.

A new catalyst generation came about when $TiCl_4$ was supported on porous $MgCl_2$ particles. These 3rd generation ($TiCl_4/MgCl_2$) Ziegler-Natta catalysts had very high activities and stereoselectivities. Shell (1960) produced the first 3rd generation catalyst using $TiCl_4$ supported on $MgCl_2$ with high activity and controlled stereoselectivity using several types of electron donors. The activity of 3rd generation catalysts can be as high as 27 kg-polypropylene per gram of catalyst, which is almost six times higher than that of a typical 2nd generation catalyst. Polypropylene resins made with 3rd generation catalysts have an isotacticity index (II) of 92-97%, while those produced with 2nd generation catalysts have only an II of 88-93%. (The isotacticity index measures the fraction of isotactic polypropylene – or, more correctly, the fraction of polypropylene insoluble in boiling heptane – in the resin.) Therefore, one of the biggest advantages of 3rd generation catalysts is the elimination of post-reactor steps for atactic polypropylene removal and catalyst deashing (Cerruti, 1999).

Fourth generation Ziegler-Natta catalysts are also composed of $TiCl_4$ supported on porous $MgCl_2$, but with controlled morphology and with slightly better productivity. In the early eighties, a new class of olefin polymerization catalyst appeared in the form of metallocene complexes. Metallocenes produce polyolefins with properties that are more uniform than those made with Ziegler-Natta catalysts, and have been used particularly for the production of differentiated commodity polyethylene and polypropylene resins.

2.1.1. TiCl4/MgCl2 Catalysts

A typical $TiCl_4/MgCl_2$ catalyst is prepared in four main temperature-controlled steps: digestion, activation, washing, and drying. The digestion step includes the reaction of an organo-magnesium (MgOR) compound, $TiCl_4$, and an internal electron donor in a chlorinated organic solvent; $TiCl_4$ is dispersed in the precursor porous surface, forming $MgCl_2$ crystals and $TiCl_3.OR$. In the activation step, $TiCl_3.OR$ is removed by further addition of $TiCl_4$ and solvent. The formed catalyst is washed with a volatile organic solvent in the washing step. Finally, hot nitrogen is used in the drying step to evaporate the solvent, obtaining a free-flowing $TiCl_4/MgCl_2$ powder (Chang et al., 2006).

Electron donors control the $TiCl_4$ distribution on the (100) and (110) faces of the $MgCl_2$ surface, as illustrated in Figure 2-1. Ti_2Cl_8 species coordinate with the (100) faces through dinuclear bonds to form the isospecific polymerization sites, while the electron donor molecules tend to coordinate with the non-stereospecific and more acidic sites on the (110) faces. When aromatic monoesters and diesters are used as internal donors, the addition of alkylaluminums (alkylation) results in the partial removal of the internal donor; therefore, external donors are needed to maintain high stereoselectivity. During catalyst preparation, there is also a chance of the internal donor to coordinate with the (100) face, but it has been reported that, in the case of ethyl benzoate, $TiCl_4$ is able to remove the donor from the (100) stereospecific face during the titanation step (Busico *et al.*, 1985). However, when 1,3-diethers are used as internal donors, they coordinate strongly with the (110) faces and cannot be removed by alkylaluminums (Barino and Scordamaglia, 1998). As a consequence, Ziegler-Natta catalysts with excellent isospecificity are obtained with diether internal donors in the absence of external donors.

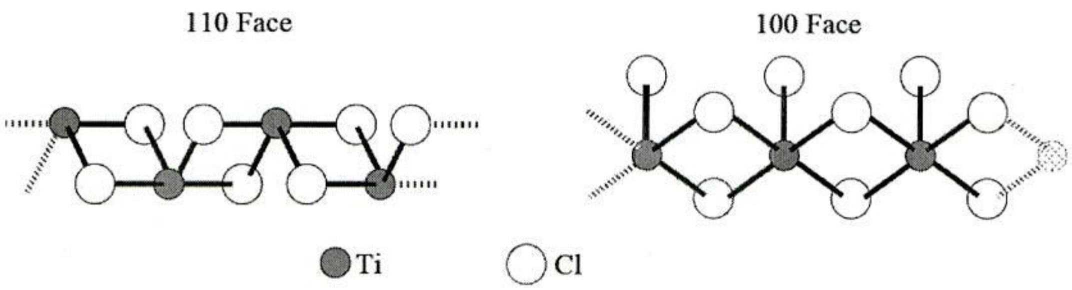


Figure 2-1. Lateral faces of a $TiCl_4/MgCl_2$ Ziegler-Natta catalyst (Busico *et al.*, 1985).

2.1.2. Polymerization Mechanism and Catalyst Geometry

According to the Cossee-Arlman's mechanism (Arlman and Cosee, 1964), propylene molecules require an activated catalyst site that has been alkylated by cocatalyst, as shown in Figure 2-2.

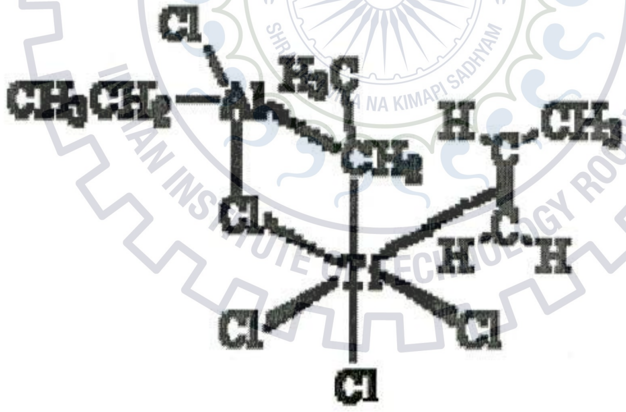


Figure 2-2. Catalyst, cocatalyst (alkylaluminum), and propylene complexation.

The π -bond electrons in the double bond of the incoming propylene are shared with the titanium atom during the coordination step. During the insertion step, the double bond breaks, forming a C-Ti bond between the monomer molecule and the Ti site, and a C-C bond between the monomer and the growing chain, restoring the vacant coordination site for further coordination and insertion steps, as illustrated in Figure 2-3.

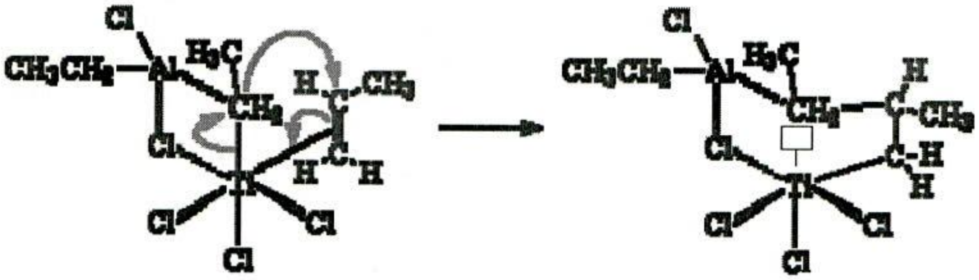


Figure 2-3. Transition state forming new vacant site.

Catalyst geometry is very important in propylene polymerization to ensure that the methyl group in the propylene molecule is aligned in the same plane, producing isotactic polypropylene chains. Figure 2-4 shows molecular structural models for γ-$TiCl_3$. Three site structures were postulated: highly isotactic, low isotactic, and atactic. The highly isotactic site has one coordination vacancy, and is bonded to the alkyl-polymer chain site (blue molecule, on top), and four Cl atoms. Due to site symmetry, stereo- and regioregular insertions are favored. The low isotactic site, despite of also having only one coordination vacancy, has two Cl atoms not bonded to Ti atoms; since the site occupied by the growing chain and the vacant site are not symmetrical, stereo- and/or regiodefects, may occur during insertion. Finally, the two coordination vacancies of the atactic site allow for the random coordination of propylene molecules and the formation of atactic polypropylene chains.

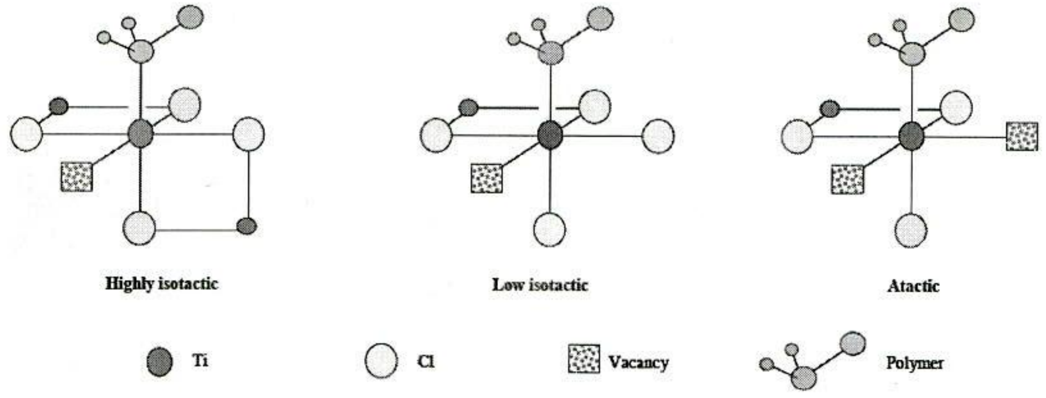


Figure 2-4. Active site models for γ-$TiCl_3$ (Kakugo *et al.,* 1988).

When $TiCl_4$ is supported on $MgCl_2$, the resulting structure is similar to that of β-$TiCl_3$ (Figure 2-5 and Figure 2-6). An electron donor molecule can complex with the Ti atom in the low isotactic site, blocking the coordination vacancy, and rendering the site inactive for polymerization, as illustrated in Figure 2-5. On the other hand, the atactic site has two vacancies to which an electron donor molecule may complex; if only one vacancy is occupied by the electron donor, as shown in Figure 2-6, the site is transformed into a highly isotactic site. In this case, the bulkiness of the electron donor provides steric hindrance, rendering the site isospecificity. It is interesting to notice that some donors may kill the catalyst or reduce its activity when used in excess. This phenomenon, called self extinction, is used in some commercial processes to shut down the polymerization. Chen reported that esters derived from aromatic carboxylic acids, such as para-ethoxy-ethyl-benzoate (PEEB), were good example of such donors. However, not all donors are able to reduce the polymerization activity, even if an excess amount is added to the polymerization reactor, such as alkoxysilanes (Chen, 2008).

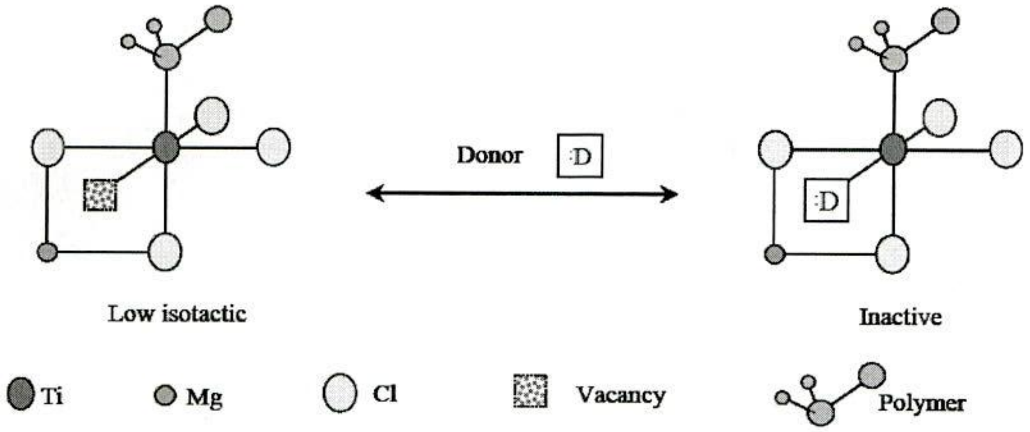


Figure 2-5. Donor addition to low isotactic site on $TiCl_4/MgCl_2$ (Kakugo *et al.*, 1988).

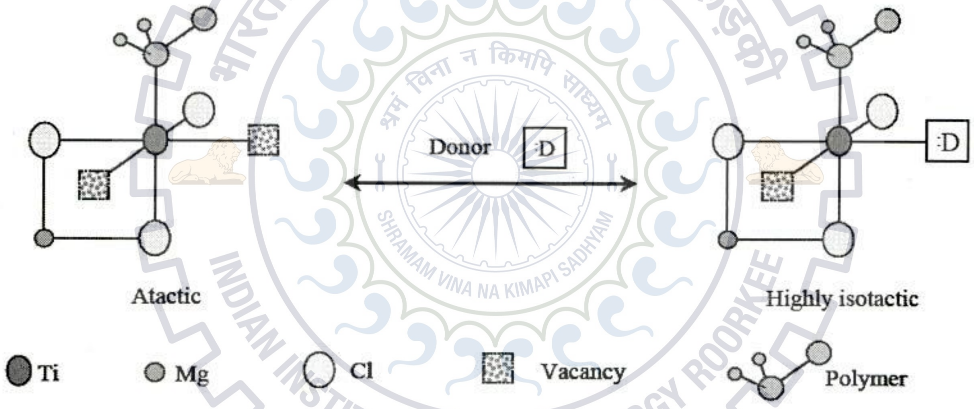


Figure 2-6. Donor addition to atactic site on $TiCl_4/MgCl_2$ (Kakugo *et al.*, 1988).

Busico *et al.* (1999) preferred to classify the catalyst sites according to the chains they produced as highly isotactic, poorly isotactic (or isotactoid), and syndiotactic, as shown in Figure 2-7. Atactic polypropylene is assumed to be produced in the isotactoid and syndiotactic sites. The highly isotactic site (a) has either two ligands (a chlorine or a donor atom), or one ligand with a strong steric hindrance to prevent the wrong insertion of monomer at position S2. The isotactoid site (b) has only one ligand. The syndiotactic propagation site (c) has two vacancies and no stereoselective control; it has been proposed that site (c) follows a chain end control mechanism rather than the most common site control mechanism for insertion. Busico *etal.* have proposed that losses of ligand L1 and/or L2 will result in a loss of the steric hindrance that may lead to the transformation of highly isotactic sites into isotactoid, and then to syndiotactic propagation sites.

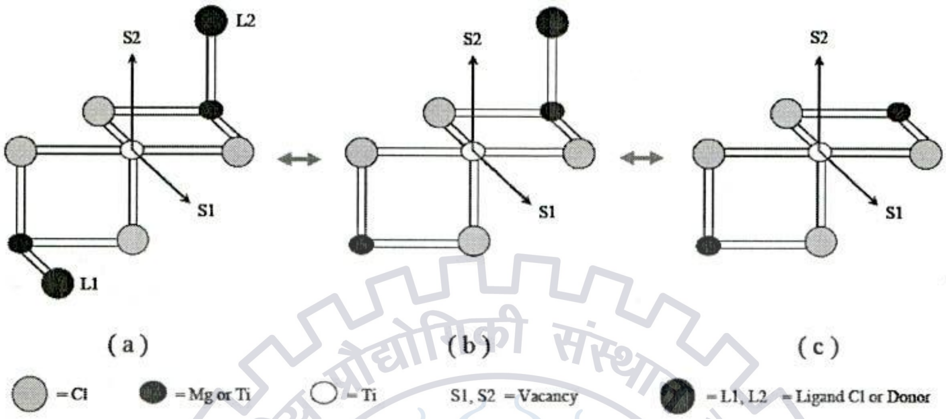


Figure 2-7. Active site models for $TiCl_4/MgCl_2$: (a) highly isotactic; (b) isotactoid; (c) syndiotactic (Busico *et al.*, 1999).

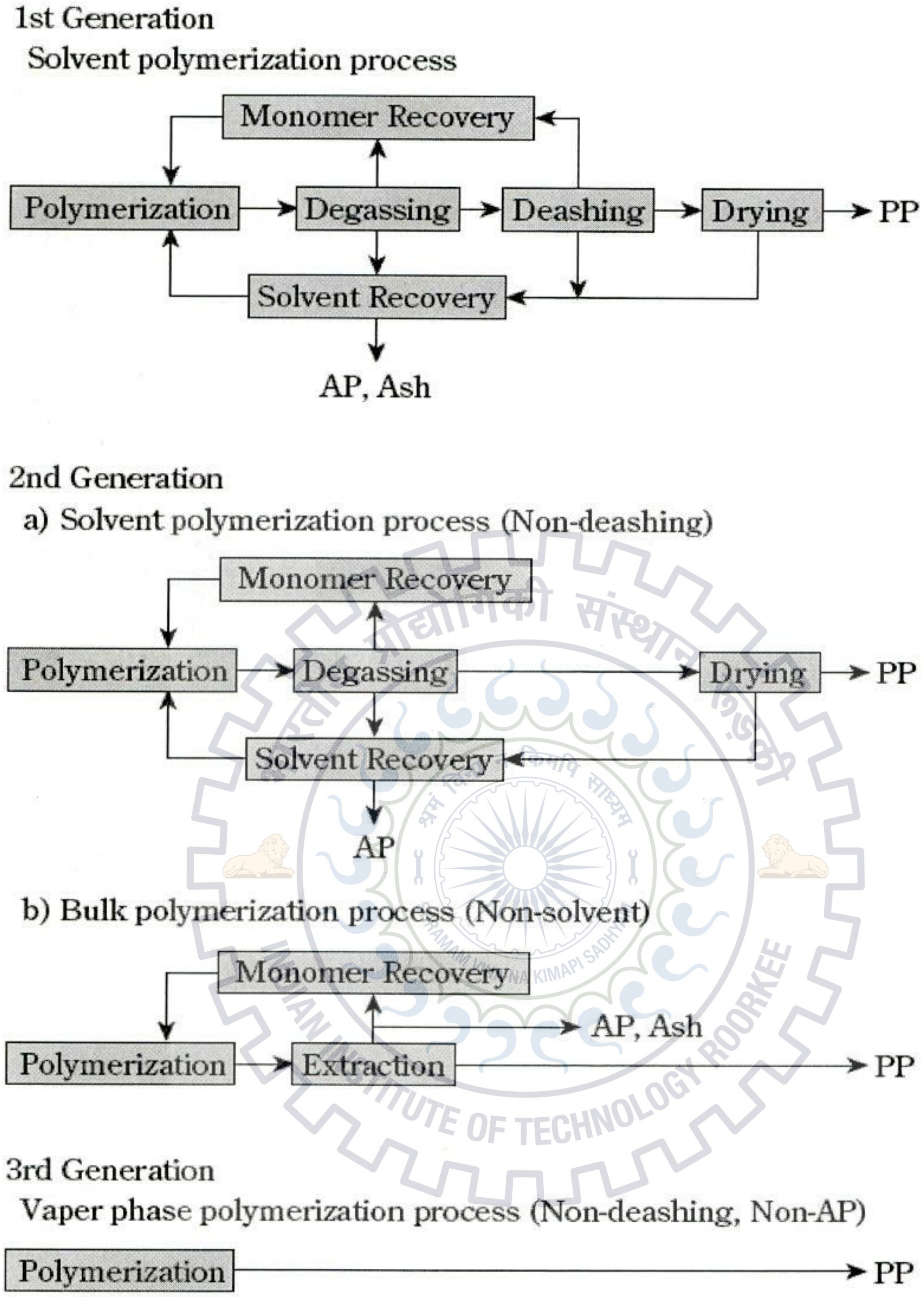
2.2. Changes in the Polypropylene Manufacturing Process

The Polypropylene manufacturing process is mainly made up of a raw material refining process, polymerization process, after-treatment process and granulation process. The raw material refining process is the furthest upstream process and is a process for eliminating minute amounts of impurities that affect the process, such as water, oxygen, carbon monoxide, carbon dioxide, carbonyl sulphide and the like, from the propylene and other monomers as well as the solvents and other raw materials and auxiliary materials used. Moreover, this process may be set up at a raw material manufacturing plant positioned upstream of the PP manufacturing plant, but in either case, it is a fundamentally necessary process for stabilization of the overall process. The polymerization process is a process for polymerization that brings the propylene and, if necessary, ethylene and other monomers into contact with a catalyst having polymerization activity. Most of the main industrial catalysts are in a granular shape. The main catalysts are mostly in the form of secondary or tertiary particles of several tens of μm that are aggregations of primary molecules having diameters of several hundred angstroms. The polymerization reaction occurs at the active points of the catalyst particles, and the PP that is formed precipitates out, and the catalyst splits into primary particles. However, there are few deviations in the shape of the catalyst, and this forms PP particles that resemble the original aggregated catalyst shape. The aftertreatment process is a process for eliminating catalyst residue, the solvent and atactic polymers (AP: noncrystalline polymers where the methyl groups of propylene units are arranged irregularly on the chain), which are components that are unnecessary, from the PP particles obtained in the polymerization process. Of these, the operation for eliminating the catalyst is known as deashing.

In addition, when a solvent is used in the polymerization process, a process for recovering and purifying it is included. The granulation process is the furthest downstream process, and it is a process for melting and kneading additives and fillers into the PP particles that have undergone the after-processing and forming pellets.

In recent years, there are cases where large diameter PP particles are shipped directly without granulation through improvements in the catalyst performance, methods of stabilizer distribution, etc. However, this is limited to a few examples still, and it has not come to the point of completely eliminating the granulation process. Moreover, storage, packaging and shipping, etc., are indispensable further downstream in commercial plants, but since they are not unique to PP manufacturing processes, we will not touch on them in this project.

Of these processes, there have been particularly large improvements in simplifications for the aftertreatment process, such that they can be cited as a representative example of advances in chemical manufacturing processes. The PP manufacturing process can be divided into three generations, the first generation (deashing and AP removal), second-generation (non-deashing or non-solvent) and third-generation (non-deashing and non-AP removal) according to these advances in technology. In addition, classification can be done according to the polymerization method into solvent processes, bulk polymerization processes and vapor phase polymerization processes. **Figure. 2-8** shows the changes in the PP manufacturing processes arranged according to the processes required for the representative polymerization process for each generation. Moreover, the furthest upstream raw material refining process and the downstream granulation process, which are fundamentally required in all of these processes, are omitted in **Figure. 2-8**.


1st Generation

Solvent polymerization process

2nd Generation

a) Solvent polymerization process (Non-deashing)

b) Bulk polymerization process (Non-solvent)

3rd Generation

Vaper phase polymerization process (Non-deashing, Non-AP)

Figure. 2-8. Polypropylene manufacturing process

2.2.1. Solvent polymerization process

Since the PP particles are dispersed in the form of a slurry in the solvent with the solvent polymerization process, this is also called the slurry polymerization process, and it was a representative manufacturing process that was the main current in the first generation.

Figure. 2-9 shows the first-generation solvent polymerization process. The Sumitomo Chemical solvent polymerization process was one that initially introduced technology from the Italian company Montecatini, which was the first in the world to industrialize PP, but subsequently Sumitomo Chemical made a large number of technical improvements of its own and licensed them to a number of companies.

Solvent polymerization used an autoclave provided with an agitator for the reactor, and the conditions are a temperature of 50 to 80°C and pressure of approximately 1 MPa. It is carried out in the presence of hexane, heptane or another inert hydrocarbon solvent where polymerization inhibitors have been eliminated. In the first generation, PP particles were obtained after going through separation and recovery of unreacted propylene, deashing (decomposition and elimination of the catalyst using alcohol), washing in water, centrifugal separation and drying for the aftertreatment processes. In addition, a process for separating the AP, which was produced as a secondary product at 10% of the amount polymerized was necessary at one time, and therefore, the AP was separated using its solubility in the polymerization solvent. Not only was this process complicated, but also the cost burden was large because of the separation and purification of the particularly large amount of alcohol and water used in deashing from the solvent that was recovered. Subsequently, in the second generation, the deashing process was omitted because of improvements in catalyst activity, and the large amounts of alcohol and water became unnecessary.

While the process was simplified in this manner, the omission of the process for eliminating secondary AP had to wait for the advent of superior catalysts that gave a high level of stereoregularity that made possible a reduction in the proportion of secondary AP generated in addition to increasing the polymerization activity.

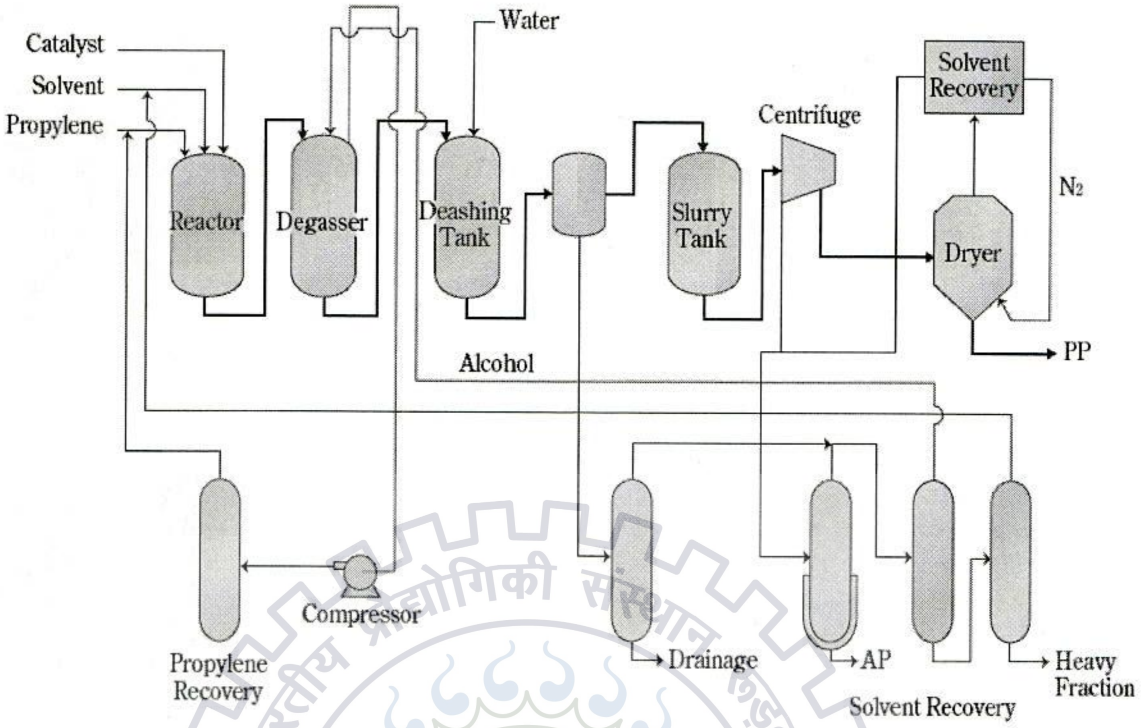


Figure 2-9. Schematic flow diagram of solvent polymerization process.

2.2.2 Bulk polymerization process

The bulk polymerization process is also called the mass polymerization process, and solvents such as hexane and heptane are not used. It carries out polymerization in liquefied propylene. It aims at simplifying the process by also using the propylene monomer, which is the raw material, as the solvent.

Since no solvent other than the liquefied propylene is used, the energy costs for the steam, electricity, etc., required for recovering the solvent may be greatly reduced. The bulk polymerization process is a process that is representative of the second generation, but it coexisted with the first generation, and even now when the third generation is the main current, there are times when it is advantageous for the manufacture of propylene homopolymers. It plays a part in a variety of commercial process groups **Figure. 2-10** shows the second generation bulk polymerization process, but if it is compared with the first generation solvent polymerization process (**Figure. 2-9**), we can see that it has been made much simpler.

It is characterized by the use of a continuous extraction tower and has a special internal structure. Furthermore, in addition to using a high performance catalyst, we were successful to greatly simplify deashing and the secondary AP elimination process by providing a counter current washing system that uses refined liquefied propylene. The typical operating conditions for the bulk polymerization process are a temperature of 50 to 80°C and a pressure that is roughly the vapor pressure of propylene. It changes according to the temperature, but is in a range of 2 to 4 MPa. Since liquefied propylene, which is a monomer, is used for the solvent, the polymerization reaction is rapid, and the retention time is shortened. Since the volumetric efficiency is greatly improved, the reactor size for obtaining the same production capacity can be smaller than it was conventionally. However, even though there is high productivity, the heat elimination surface area is insufficient for removing the polymerization heat if the size of the device is reduced. Therefore, in the case of a stirred tank reactor, a special external heat exchanger that implements measures for preventing adherence of the polymer is used. On the other hand, loop reactors where the surface area for heat elimination can be increased relative to the reaction volume have become practical.

The bulk polymerization process is a process with many advantages like these, but it is not suitable for the manufacture of the polymers known as impact copolymers. Impact copolymers are a mixture of a propylene homopolymer component with a comparatively low molecular weight and a rubber component, which is an ethylene-propylene copolymer with a comparatively high molecular weight. This has improved impact strength at low temperatures while at the same time maintaining the rigidity, which is one of the superior original characteristics of PP, as much as possible. It is mainly used in injection molding applications starting with automobile components. Industrially, it is obtained by polymerizing the latter following the polymerization of the former, and during continuous production, individual reactors are required for polymerization of each of the components. To polymerize the rubber component, the reaction composition must have a high ethylene concentration, but if ethylene is dissolved in the liquefied propylene to the point of obtaining the required ethylene concentration with bulk polymerization, the overall reaction pressure increases, so there have been almost no practical implementations. In addition, since the rubber component is dissolved in the liquefied propylene, there is a problem with the limitations for polymerization of the rubber component.

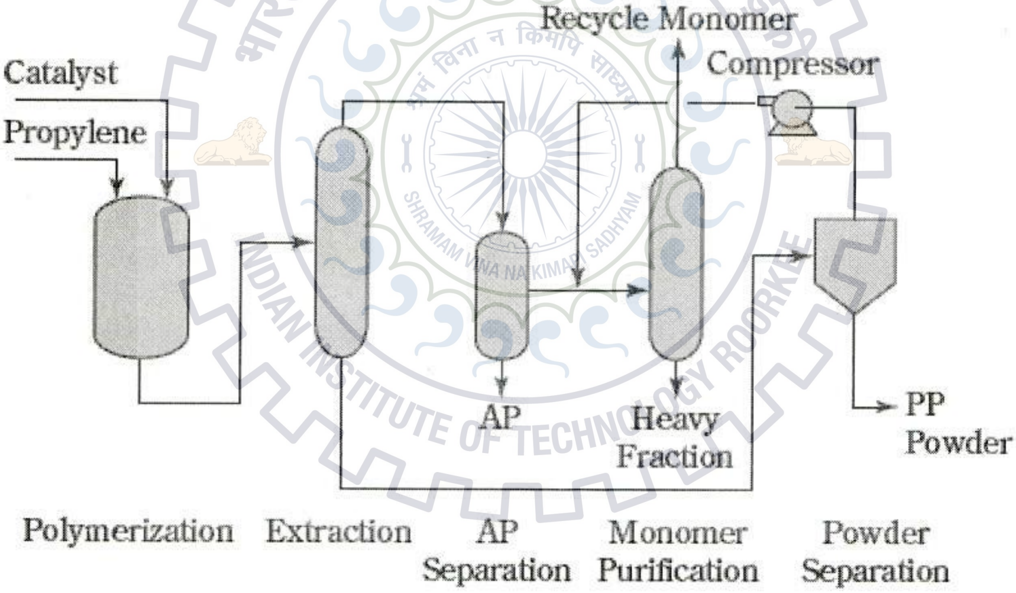


Figure 2-10. Schematic flow diagram of bulk polymerization process

2.2.3. Vapor phase polymerization process

The vapor phase polymerization process falls under the category of bulk (mass) polymerization processes carried out only with monomers in the broad sense, but since polymerization is carried out in propylene gas rather than in liquefied propylene, it is handled as a process different from conventional bulk polymerization. It is positioned as a third-generation process, but the history is longer than expected, and the technology already existed when first generation processes were the main current. The vapor phase polymerization at that time was inferior in terms of quality because there was no process for separating the very many AP secondary products, and products were limited to special applications. However, with the subsequent complete elimination of deashing and AP removal operations because of the rapid improvement in catalyst performance, further simplifications were achieved in the process, and it achieved a position as the third generation process capable of manufacturing high performance products with diverse levels of quality. **Figure 2-11.** shows the initial third generation vapor phase polymerization process for manufacturing impact copolymers. Manufacturing impact copolymers requires at least two reactors, and a supply line for ethylene, which is a comonomer, is installed for the second stage reactor so that the rubber component can be polymerized. Moreover, manufacturing is fundamentally possible with one reactor for polymers other than impact copolymers. The typical operating conditions are a temperature of 50 to 80°C and a pressure in the range of 1 to 2 MPa. Various types of reactors, such as stirred tanks and fluidized beds, have been developed by various companies, but while there are small differences in construction costs and variable costs, these are not determiners of the differences in the final product costs. The competition between makers can be said to be mainly in the area of product quality.

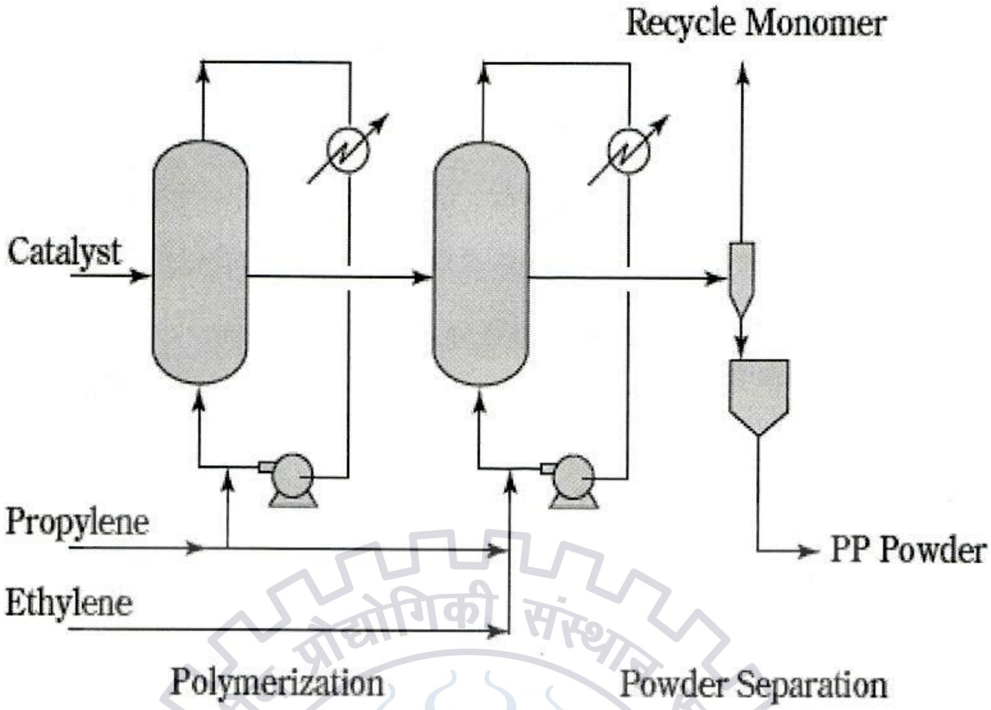


Figure 2-11. Schematic flow diagram of vapor phase polymerization process

2.3 PROCESS DESIGN BASICS

Process design is a very important aspect before any project implementation as a proper design during the initial stages can save costs to a great extent. The cost involved in designing a project is very less compared to the construction cost and it can be greatly helpful in maximizing profits of the plant as well as providing a safe environment. The plot shown in Figure. 2.13 gives a brief idea of how proper plant design can cut costs to a great extent.

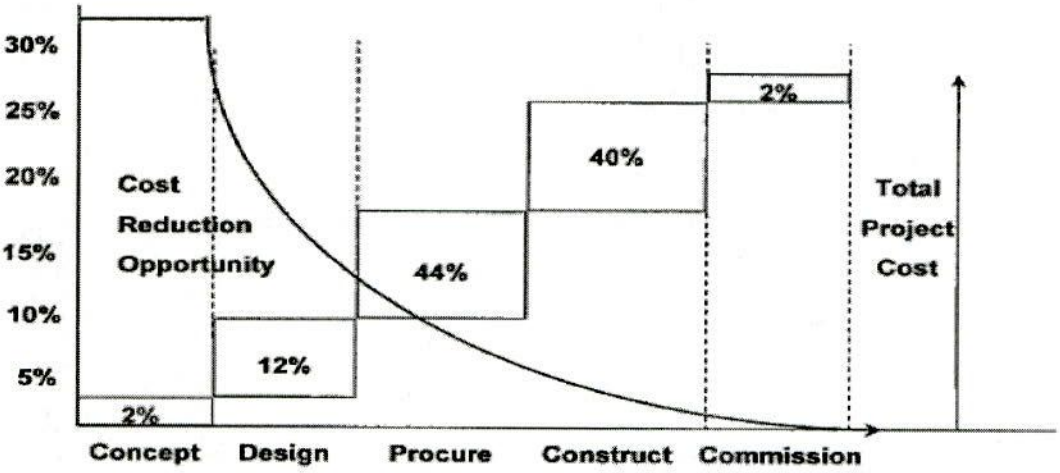


Figure 2.12 Cost reduction during project implementation

The following points need to be taken care for a proper process design.

1. *Raw material cost reduction.* Selectivity of reaction is increased by proper use of catalysts. Increasing selectivity can reduce separation and recycle costs.

2. *Capital-cost reduction.* Better flow sheeting can reduce capital costs effectively

3. *Energy use reduction.* Pinch point analysis is used for energy saving.

4. *Increased process flexibility.* Process plant should be able to handle a range of feed compositions.

5. *Increased process safety.* Nonlinear analysis can be done to make the process safer.

6. *Increased attention to quality.* Reduction of by products and the effective use of process control equipment can lead to process safety.

7. *Better environmental performance.* Minimization of harmful wastes to the environment.

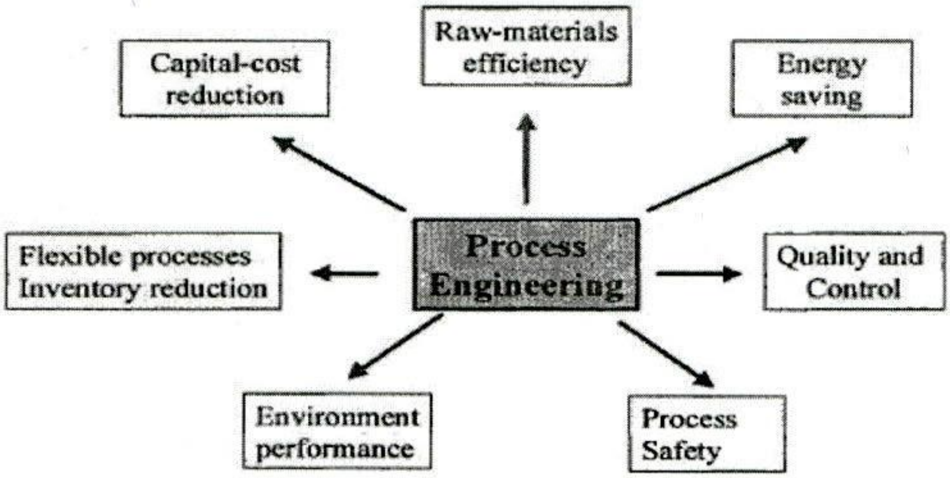


Figure 2.13 Factors to be considered during process design

The order in which designing should be done follows a systematic procedure as shown in Figure 2.14

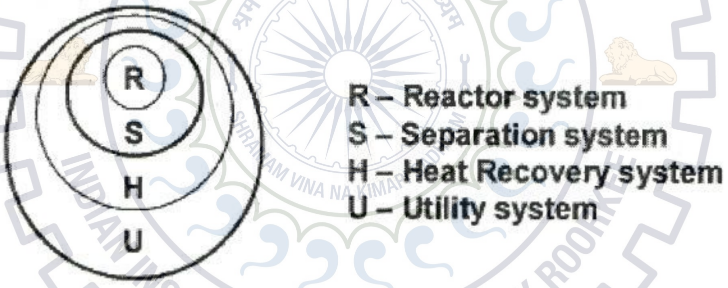


Figure 2.14 Onion Diagram (traditional process design hierarchy of phases)

A process simulation diagram is drawn from the process flow diagram. The chemical components are specified. The chemical component properties are generally available in a standard data base. The input streams are specified. Thermodynamic modelling is done. Series of simulations are run for convergence of a particular variable. Sensitivity analysis which consists of varying the sampled variables as a function of the manipulated variables is normally done. The major parts of a polypropylene production plant are reactor system, separation system and they are optimized.

CHAPTER 3

PROCESS FLOWSHEET DESIGN

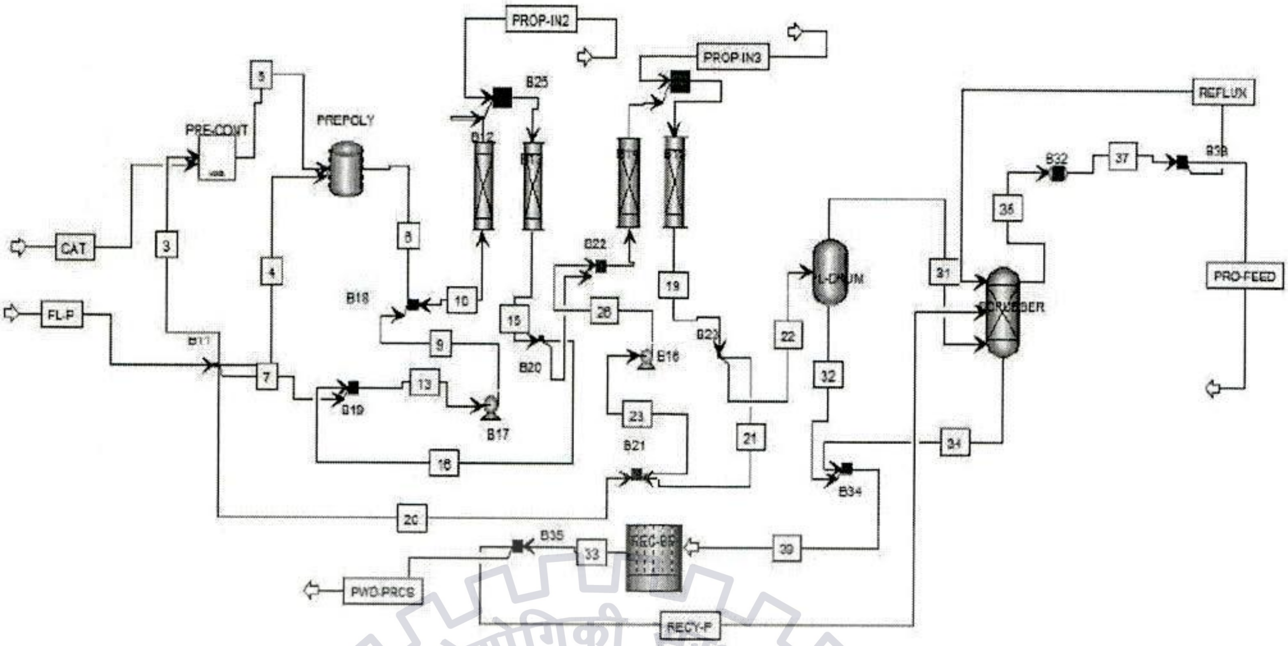


Figure 3.1. Flow sheet design in Aspen Plus 11.1

3.1 Process Description

3.1.1. Catalyst, Co-Catalyst, liquid additive and metering system

The catalyst system consist of three components:

Titanium catalyst supported on $MgCl_2$ (solid), Triethyl Aluminium (TEAL)(liquid), donor (liquid).TEAL is discharged into TEAL storage drum, wherefrom it is transferred to TEAL metering drum. From here it is fed to the Pre contacting pot. Donor is transferred into Donor Storage drum. Donor Metering Pump meters the donor solution to catalyst pre contacting units. Paraffinic Hydrocarbon (HC) oil and grease are discharged into Oil Drum and Grease Drum respectively and then transferred to Catalyst Dispersion Drum, where the solid catalyst component is fed from Catalyst Drum by hoist. The solid catalyst component is dispersed in the HC oil, and then adding grease, and then with continued agitation, cooled down to set the dispersion into a stable mud.

3.1.2 Precontacting, Prepolymerization & Bulk Polymerization

The Catalyst Paste is precontacted and activated with TEAL and Donor in the Precontacting pot is injected into a stream of cold propylene, which feeds the prepolymerizer reactor. Propylene, coming from Propylene Feed tank is cooled down , and then joins catalyst mixture in Catalyst inline Mixer. The slurry is fed to a Prepolymerizer reactor where reaction takes place at low kinetics. The main polymerization reaction takes place in two loop reactors in series. Circulation Pump maintains high velocity and very uniform mixing inside reactor. The prepolymer flows with propylene from Prepoly Reactor directly into first loop reactor and is dispersed into the slurry, which is kept circulating in the reactor. The slurry is transferred from 1st Loop Reator to 2nd LOOP Reactor. Hydrogen is used to control the Melt Flow rate of the polymer produced in the loop reactors. For random copolymer productions, the loop reators are separately fed with ethylene. Ethylene is added to the loop reactors in certain product types (random copolymer), Ethylene polymerizes with the propylene to form a copolymer.

For Terpolymer production , Butene-1 (coming from butene-1 battery limits) can be fed to the loop reactors together with the propylene main feed streams. The slurry is normally discharged from 2nd loop reactor to flash line. The heat of reaction of each loop and of gas phase reactor is removed with a centralized jacketed water circuit.

3.1.3. High pressure degassing and propylene recycle

The slurry from reactors is discharged to the flash pipe. After leaving the flash pipe, solid is separated from gas in the flash – drum. During homo-polymer and random copolymer runs the polymer collected from the bottom of Flash Drum is discharged to the Recycle Gas Filter, while during high impact copolymer runs, polymer from flash drum is routed to the Gas Phase Reactor.

All the monomers recovered from the degassing section are sent to the Recycle Propylene Scrubber. The bottom stream of the recycle Propylene Scrubber is lined up to Recycle gas filter. The vapor leaving the top of Propylene condenser is purged to the off-gas header. The recycle-condensed propylene is sent to the Propylene Feed Tank. In case of homo polymer or random & ter-polymer production, the polymer is routed from the Flash Drum to the Low Pressure Degassing Filter. During heterophasic copolymer runs, Recycle Gas Filter receives the polymer from gas phase reactor discharge. The filter gas is sent to washing and compression section. Gas stream leaving Recycle gas filter is washed in low Pressure Propylene Scrubber in order to remove any powder entrainment and minimize the aluminum alkyl content to the compressor. The delivery of Recycle Gas Compressor Unit is sent to Recycle Propylene Scrubber in case of homopolymer and random copolymer runs or to the Ethylene Stripper when producing heterophasic copolymers.

3.1.4. Gas phase co polymerization

In this section a rubber ethylene-propylene phase is added to the homo polymer matrix (coming from bulk polymerization inside loop reactors) to produce a high impact hetero plastic copolymer. The rubber phase is produced in a vertical cylindrical reactor fed with homo polymers matrix from Flash drum. Ethylene rich top gas is recycled to gas phase reactor while the propylene /propane bottom stream joins the recycle propylene scrubber top gas stream to Propylene condenser for condensation and liquid recycle to the feed tank.

3.1.5. Steaming

Recovery of monomers dissolved in the polymer and drying from Recycle Gas Filter the polymer powder is discharged by gravity to the steamer where steam is injected to complete removal of dissolved monomer and propane and to deactivate catalyst residual activity. Steam is condensed and discharged from the steamer to the sewer after passing through the steamer scrubber. Residual un reacted monomers and propane compressed by means of steamer Off gas compressor, can be sent to battery limits for propane purging of recycled the Recycle Gas Filter after water removal in Propylene Gas Drying Unit. The polymer is discharged from the steamer to the fluid bed dryer where removal of surface water is effected by means of hot nitrogen. Dry polymer is transferred to the finishing unit surge silos by nitrogen closed pneumatic conveyor.

3.1.6. Monomer Purification

Propylene makeup coming from Battery limit is sent to Light ends stripper after drying unit package. After drying propylene is sent to Phosphine, Sulphur and arsine removal column. Purified propylene is sent to propylene feed tank. Ethylene from battery limit OS sent to CO removal towers. Then Ethylene is sent to drying and CO2 removal unit. Purified and filtered ethylene is sent to drying and CO2 removal unit. Purified and filtered Ethylene is sent to polymerization in Gas phase reactor during impact copolymer production. Hydrogen from battery limit is sent to purification unit followed by hydrogen compression. After compression hydrogen is sent to polymerization areas. Butene-1 make up coming from battery limit is stored in Butene storage tank and pumped to propylene Feed tank.

3.1.7 PP polymer transport, storage and metering to extrusion and extrusion

PP polymer discharged from the dryer is sent to the intermediate surge silos. From the intermediate surge silos the polymer is discharged to the screw feeder, which also receives solid additives from the additive metering systems. The total system is then discharged to the polymer additives cont. mixer, where according to product recipes, also liquid additives can be fed. The solid additives metered to the screw feeder by means of Solid additive metering. For liquid additivation, solid additives are fed to additive melter. The melted additive is discharged to the metering pot. From where it is fed to the Polymer / Additives continuous mixer, a liquid peroxide metering station is provided for special polymer grades production. Additives and polymer mixture from Polymer cont. mixer are fed to the extruder through a feeding hopper. PP polymer powder and additives are homogenized , extruded and granulated by and under-water pelletizer in the extruder.

The melted polymer is pushed against a die-plate . As soon as polymer emerges as strands from the holes in the die-plate, is cut into pellets by a set of rotating knives . A water stream in which both the die plate and the knives are submerged then transports pellets. Pellets and water stream leaving the underwater pelletizer are normally conveyed to the Pellet centrifugal Dryer. Dried pellets leaving Pellet Centrifugal dryer are conveyed to the vibrating screen which separates fines and coarse from pellets. On-spec pellets are discharges in the Pneumatic Transport hopper. From Pneumatic Transport hopper the pellets are fed to the PP pellets pneumatic transport for the conveying to the homogenizing silos. Finished PP pellets from the extrusion unit are collected by means of PP pellets Pneumatic transport in Six blender silos.

3.2 Process Simluation

3.2.1 Executive Summary

The polypropylene gas-phase polymerization process model illustrates the use of PolymersPlus to model a gas-phase UNIPOL process for propylene homopolymerization using a four site Ziegler-Natta kinetic model. The atactic content, melt flow ratio and molecular weight averages are some of the polymer product properties and attributes predicted by the simulation.

3.2.2 About The Process in Simulation

There are three types of processes commonly employed for the manufacture of isotactic polypropylene (PP) homo- and co-polymers. These include liquid slurry processes, bulk or liquid pool processes, and gas-phase processes. Table below provides basic information on these processes and lists some of the companies that have commercialized the process technology. All of these processes use a Ziegler-Natta catalyst (usually TiCl4) in either asupported or nonsupported form together with an alkylaluminum or aluminum chlorides(e.g. triethlyaluminum) cocatalyst. Liquid slurry processes use an inert hydrocarbon diluent as the slurry medium or polymer suspending agent. This process is still the most widely used process for PP manufacture. Continuous stirred tank reactors are usually used and several reactor may be used in series or parallel arrangements. Typical reactor operating conditions and residence times are listed in Table 3.1 given below.

Process	Reactor	Diluent / Solvent	Catalyst	Tacticity (%)	Temp. (°C)	Press. (atm)	Residence Time (hr)	Company
Bulk (Liquid Pool)	loop reactor	Liquid monomer	supported Ti Catalyst	up tp 99%	60-80	30-40	1-2	Himont Mitsui
	CSTR	Liquid monomer	unsupported or supported Ti catalyst	up to 98%	60-75	30-40	2.0	Dart El Paso Montedison Sumitomo
Diluent Slurry	CSTR	n-hexane, n-heptane	unsupported or supported Ti catalyst	up to 98%	60-80	15-20	3-4	Amoco Montedison
Gas	fluidized bed	N2	supported Ti catalyst	up to 98%	60-80	20	3-5	Sumitomo Union Carbide
	vertical stirred bed	---	unsupported or supported Ti catalyst	up to 98%	70-90	20	4	BASF ICI USI
	horizontal compartmented stirred bed	---	unsupported or supported Ti catalyst	up to 98%	70-90	20	4	Amoco

Bulk or liquid pool processes are a special case of the slurry processes. They use liquid propylene instead of an inert diluent as the slurry medium to suspend the polymer. The increased monomer concentration leads to higher polymerization rates in liquid pool processes relative to slurry processes. Hence, shorter reactor residence times may be employed. Several reactor types, including stirred autoclaves with evaporative cooling and loop reactors, are used to attain good heat transfer rates. In gas-phase processes, gaseous propylene is contacted with solid catalyst/polymer powder in fluidized bed or mechanically stirred bed reactors. The reactor temperature is usually controlled by evaporative cooling of liquid propylene. The unreacted monomer is removed from the reactor headspace, condensed or cooled and recirculated to the reactor. Polymers Plus can be used with Aspen Plus for the simulation of steady-state operation of any of the PP processes described above. Polymers Plus can be used with Aspen Custom Modeler when dynamic simulation or detailed modeling of the flow patterns or heat transfer within the reactor is desired. This example describes a steady-state simulation of a gas-phase UNIPOL flowsheet.

3.2.3 Process Definition:

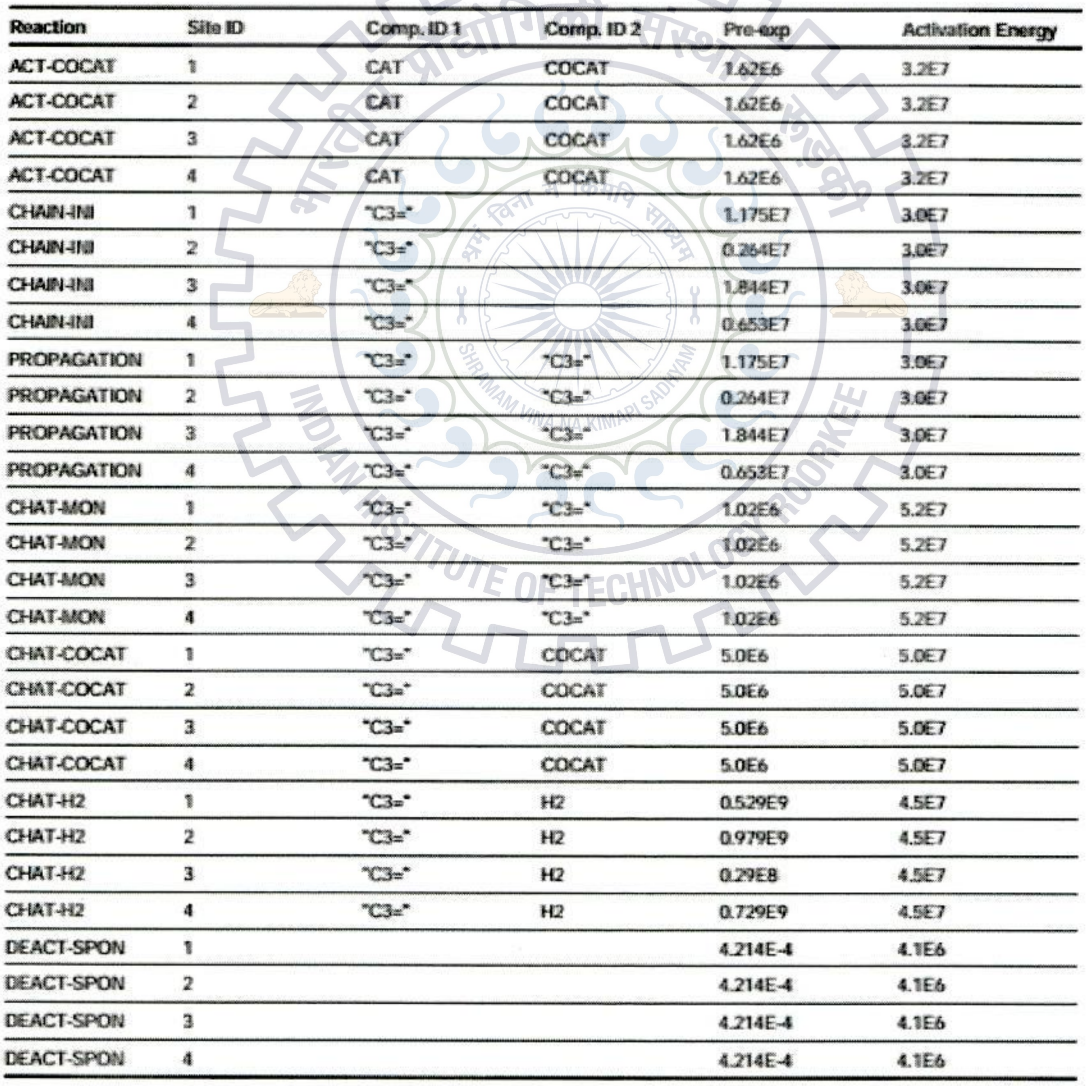
A Polymers Plus model is developed to simulate a PP gas-phase UNIPOL flowsheet. The flowsheet includes the fluidized bed reactor, the gas recycle/cooling loop, discharge and purge units as shown in Figure below. The fluidized bed reactor is modeled using the CSTR reactor in Aspen Plus with two phases; a gas phase and a polymer phase. The POLYNRTL thermodynamic model is used to relate the gas phase monomer, hydrogen, etc. composition to their concentrations in the polymer phase. The multisite Ziegler-Natta kinetic model is used to describe the polymerization reactions in the polymer phase. The kinetic model calculates the reaction rates for the components and polymer attributes at each site type. User-Property models are used to calculate polymer properties such as melt flow index (MFI), isotactic index (or atactic fraction) from the polymer attributes. Various components of the process are mentioned in the following Table 3.2. The polymer Non-Random Two liquid activity coefficient model (POLYNRTL) is used as physical property method.

Components	
Titanium Tetrachloride (CAT)	Catalyst
Triethyl-Aluminium (COCAT)	Co-catalyst
Propylene (C3=)	Monomer
Propane (C3)	Inert
Polypropylene (PP)	Polymer
H2	Chain transfer agent
N2	Inert
Water (H2O)	Cooling water
Propylene Segment (C3-SEG)	Polymer segment
Component	**Flow rate (Kg/Hr)**
Catalyst	3.0
Co-catalyst	10.0
Propylene	17462.0
Propane	162.29
H2	1.38
N2	1.45
Operating Conditions	
Temperature	69 °C
Pressure drop	200 KPa
Total volume	90 m^3
Polymer Phase volume	60 m^3

Table 3.2 Various components and Operating conditions of the process

3.2.4 Reactor Kinetics

The Ziegler-Natta kinetic scheme used in the model includes site activation by co-catalyst, chain initiation, propagation, chain transfer to hydrogen, monomer and co-catalyst, and spontaneous site deactivation. Four site types are used in this example to represent the broad molecular weight distributions that are typically observed for Ziegler-Natta polymers. The actual number of site types necessary to model a given catalyst-polymerization system is determined by deconvolution of the polymer molecular weight distribution curve obtained from a GPC analysis. The rate parameters used in the model are displayed in the Table 3.3.



Reaction	Site ID	Comp. ID 1	Comp. ID 2	Pre-exp	Activation Energy
ACT-COCAT	1	CAT	COCAT	1.62E6	3.2E7
ACT-COCAT	2	CAT	COCAT	1.62E6	3.2E7
ACT-COCAT	3	CAT	COCAT	1.62E6	3.2E7
ACT-COCAT	4	CAT	COCAT	1.62E6	3.2E7
CHAIN-INI	1	"C3="		1.175E7	3.0E7
CHAIN-INI	2	"C3="		0.264E7	3.0E7
CHAIN-INI	3	"C3="		1.844E7	3.0E7
CHAIN-INI	4	"C3="		0.653E7	3.0E7
PROPAGATION	1	"C3="	"C3="	1.175E7	3.0E7
PROPAGATION	2	"C3="	"C3="	0.264E7	3.0E7
PROPAGATION	3	"C3="	"C3="	1.844E7	3.0E7
PROPAGATION	4	"C3="	"C3="	0.653E7	3.0E7
CHAT-MON	1	"C3="	"C3="	1.02E6	5.2E7
CHAT-MON	2	"C3="	"C3="	1.02E6	5.2E7
CHAT-MON	3	"C3="	"C3="	1.02E6	5.2E7
CHAT-MON	4	"C3="	"C3="	1.02E6	5.2E7
CHAT-COCAT	1	"C3="	COCAT	5.0E6	5.0E7
CHAT-COCAT	2	"C3="	COCAT	5.0E6	5.0E7
CHAT-COCAT	3	"C3="	COCAT	5.0E6	5.0E7
CHAT-COCAT	4	"C3="	COCAT	5.0E6	5.0E7
CHAT-H2	1	"C3="	H2	0.529E9	4.5E7
CHAT-H2	2	"C3="	H2	0.979E9	4.5E7
CHAT-H2	3	"C3="	H2	0.29E8	4.5E7
CHAT-H2	4	"C3="	H2	0.729E9	4.5E7
DEACT-SPON	1			4.214E-4	4.1E6
DEACT-SPON	2			4.214E-4	4.1E6
DEACT-SPON	3			4.214E-4	4.1E6
DEACT-SPON	4			4.214E-4	4.1E6

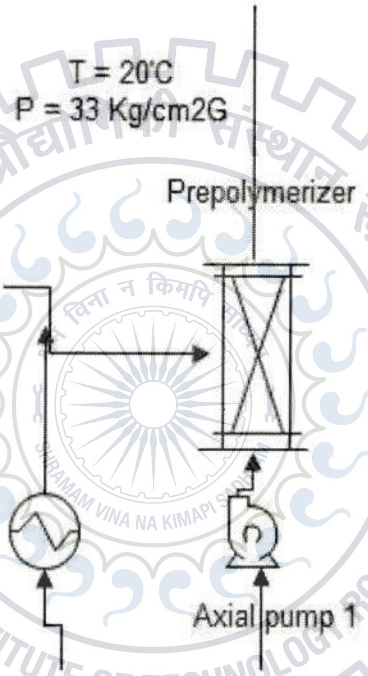
CHAPTER 4

RESULTS OF SIMULATION

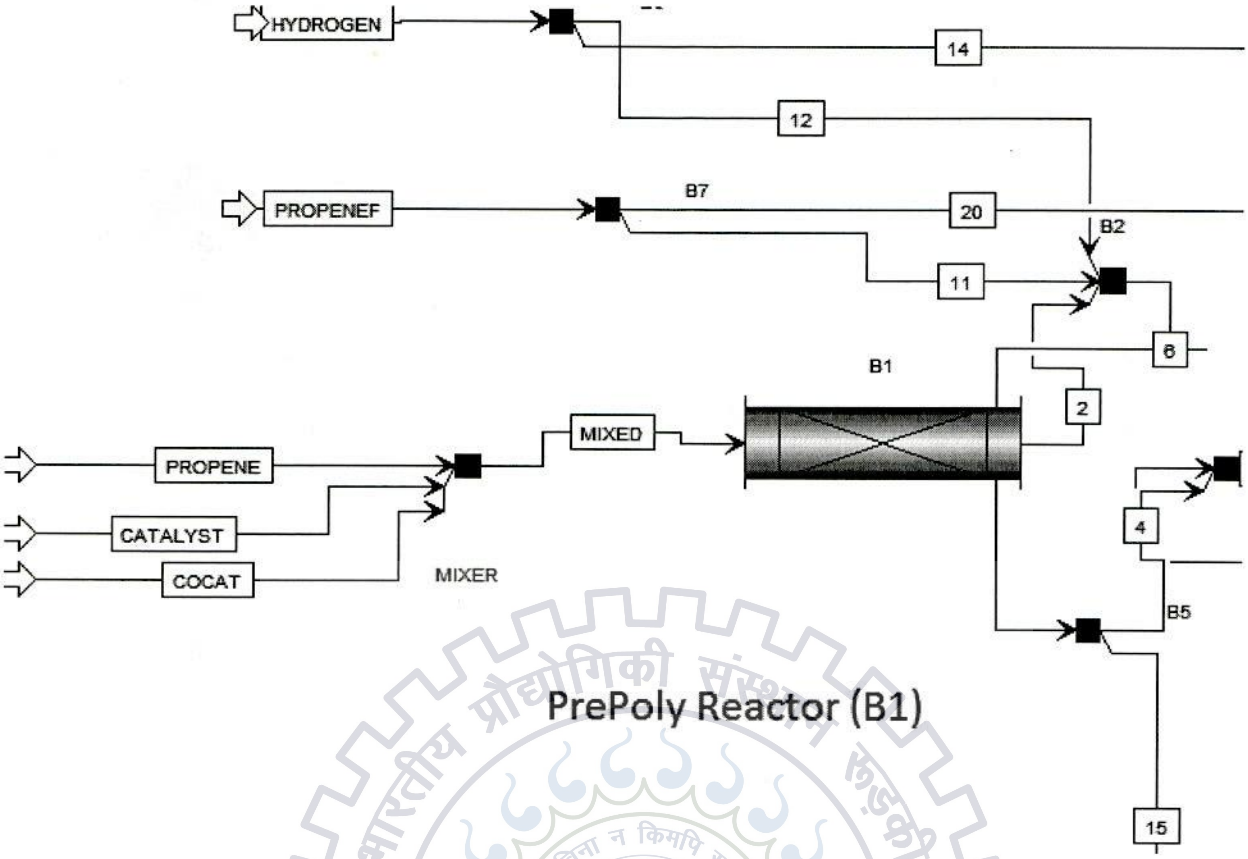
4.1 Reactor Data obtained by Simulation and Equipment details.

4.1.1. Pre-polymerization Reactor:

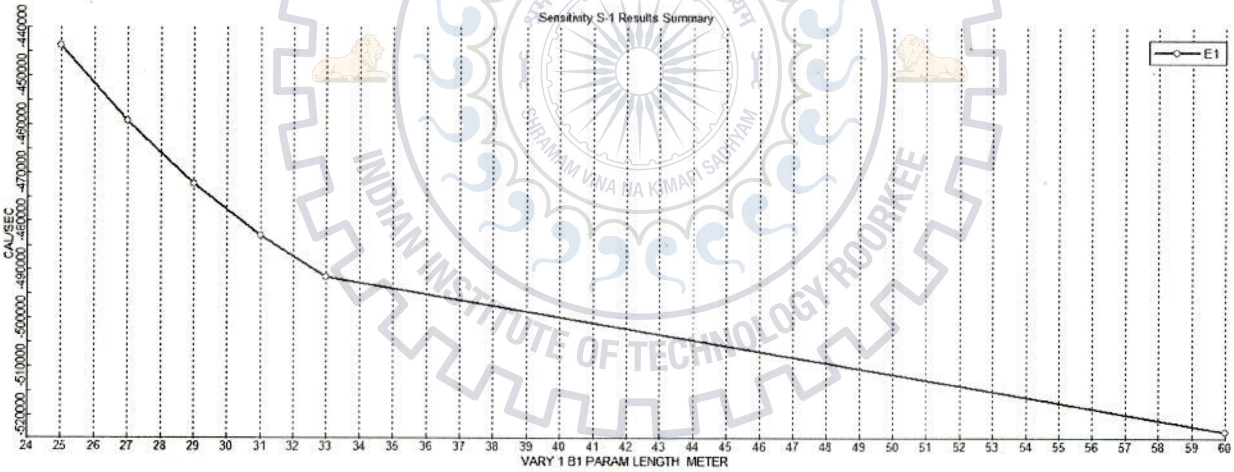
The reaction part of process is initiated in prepolymerzation reactor at low temperature and high pressure. Ziegler-Natta kinetic scheme is used in the model, which includes site activation by co-catalyst, chain initiation, propagation, chain transfer to hydrogen, monomer and co-catalyst, and spontaneous site deactivation. Four site types are used in this example to represent the broad molecular weight distributions that are typically observed for Ziegler-Natta polymers.



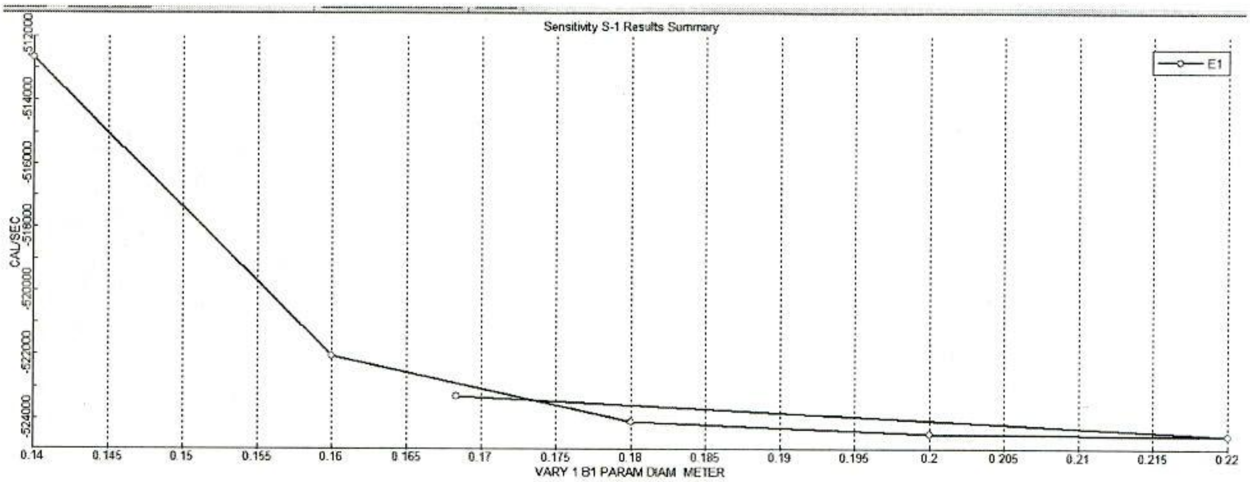
```
BLOCK:  PREPOLYREACTOR MODEL: RPLUG
   -----------------------------
   INLET STREAM:          MIXED
   OUTLET STREAM:          2
   PROPERTY OPTION SET:   POLYNRTL  / REDLICH-KWONG

               ***  MASS AND ENERGY BALANCE  ***
                    IN          OUT       GENERATION   RELATIVE DIFF.
   TOTAL BALANCE
   MOLE(KMOL/HR )        95.2558       95.2574      0.159875E-02 -0.110820E-15
   MASS(KG/HR   )       4026.43       4026.43                  0.101647E-14
   ENTHALPY(CAL/SEC )     26799.1      -496507.                     1.05398
```



PrePoly Reactor (B1)



Graph 4.1. Heat of reaction v/s length of reactor



Graph 4.2. Heat of reaction v/s diameter of reactor

```
                 ***  INPUT DATA  ***

REACTOR TYPE:
  SPECIFIED TEMPERATURE
  LIQUID FLUID PHASE
REACTOR TUBE LENGTH              METER          60.000
           DIAMETER           METER          0.16830
NUMBER OF REACTOR TUBES                          1
REACTOR VOLUME               L              1334.8
ERROR TOLERANCE                              0.10000E-03
INTEGRATION METHOD                             GEAR
CORRECTOR METHOD                              NEWTON
INITIAL STEP SIZE FACTOR                      0.10000E-01
CORRECTOR TOLERANCE FACTOR                          0.10000
MAXIMUM NUMBER OF STEPS                          1000

TEMPERATURE PROFILES:

 RELATIVE LOCATION         TEMPERATURE
     0.00000E+00         293.15    K


                 *** REACTION DATA ***

MODEL: ZIEGLER-NAT   BLOCK: Z-N

RATE PARAMETERS:

  REACTION     SITE CID1     CID2      K0        EACT       ORD
  ACT-COCAT     1  TITAN-01 TRIET-01  0.1620E+07  0.3200E+08   1.000
  ACT-COCAT     2  TITAN-01 TRIET-01  0.1620E+07  0.3200E+08   1.000
  ACT-COCAT     3  TITAN-01 TRIET-01  0.1620E+07  0.3200E+08   1.000
  ACT-COCAT     4  TITAN-01 TRIET-01  0.1620E+07  0.3200E+08   1.000
```

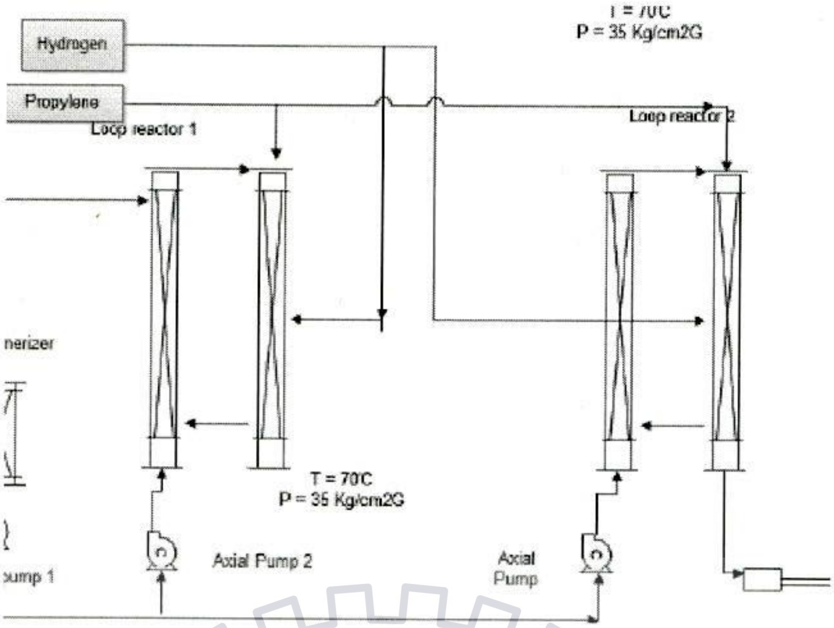
```
CHAIN-INI     1 PROPY-01          0.1175E+08  0.3000E+08  1.000
CHAIN-INI     2 PROPY-01          0.2600E+07  0.3000E+08  1.000
CHAIN-INI     3 PROPY-01          0.1844E+08  0.3000E+08  1.000
CHAIN-INI     4 PROPY-01          0.6530E+07  0.3000E+08  1.000
PROPAGATION   1 PROPY-01 PROPY-01 0.1175E+08  0.3000E+08  1.000
PROPAGATION   2 PROPY-01 PROPY-01 0.2640E+07  0.3000E+08  1.000
PROPAGATION   3 PROPY-01 PROPY-01 0.1844E+08  0.3000E+08  1.000
PROPAGATION   4 PROPY-01 PROPY-01 0.6530E+07  0.3000E+08  1.000
CHAT-MON      1 PROPY-01 PROPY-01 0.1020E+07  0.5200E+08  1.000
CHAT-MON      2 PROPY-01 PROPY-01 0.1020E+07  0.5200E+08  1.000
CHAT-MON      3 PROPY-01 PROPY-01 0.1020E+07  0.5200E+08  1.000
CHAT-MON      4 PROPY-01 PROPY-01 0.1020E+07  0.5200E+08  1.000
CHAT-COCAT    1 PROPY-01 TRIET-01 0.5000E+07  0.5000E+08  1.000
CHAT-COCAT    2 PROPY-01 TRIET-01 0.5000E+07  0.5000E+08  1.000
CHAT-COCAT    3 PROPY-01 TRIET-01 0.5000E+07  0.5000E+08  1.000
CHAT-COCAT    4 PROPY-01 TRIET-01 0.5000E+07  0.5000E+08  1.000
DEACT-SPON    1                   0.4214E-03  0.4100E+07  1.000
DEACT-SPON    2                   0.4214E-03  0.4100E+07  1.000
DEACT-SPON    3                   0.4214E-03  0.4100E+07  1.000
DEACT-SPON    4                   0.4214E-03  0.4100E+07  1.000
ATACT-PROP    1 PROPY-01 PROPY-01 0.5000E+06  0.3000E+08  1.000
ATACT-PROP    2 PROPY-01 PROPY-01 0.1200E+07  0.3000E+08  1.000
ATACT-PROP    3 PROPY-01 PROPY-01 0.3000E+06  0.3000E+08  1.000
ATACT-PROP    4 PROPY-01 PROPY-01 0.7000E+06  0.3000E+08  1.000
```

```
                 ***  RESULTS  ***



REACTOR DUTY            CAL/SEC              -0.52331E+06
RESIDENCE TIME          HR                0.25297
REACTOR MINIMUM TEMPERATURE K                      293.15
REACTOR MAXIMUM TEMPERATURE K                       293.15


     *** RESULTS PROFILE (PROCESS STREAM) ***

  LENGTH       PRESSURE     TEMPERATURE   VAPOR FRAC    RES-TIME
  METER       ATM        K                  HR
```

```
0.00000E+00   33.907      293.15      0.00000E+00  0.00000E+00
 6.0000      33.907     293.15     0.00000E+00  0.18059E-01
 12.000      33.907     293.15     0.00000E+00  0.38327E-01
 18.000      33.907     293.15     0.00000E+00  0.60932E-01
 24.000      33.907     293.15     0.00000E+00  0.85683E-01
 30.000      33.907     293.15     0.00000E+00  0.11208
 36.000      33.907     293.15     0.00000E+00  0.13954
 42.000      33.907     293.15     0.00000E+00  0.16759
 48.000      33.907     293.15     0.00000E+00  0.19593
 54.000      33.907     293.15     0.00000E+00  0.22442
 60.000      33.907     293.15     0.00000E+00  0.25297
```

4.1.2 Loop reactors:

This process is carried out in two large reactors connected in series of equal capacity, each consisting of an axial pump to maintain a uniform flow rates of slurry present in reactors. Ziegler-Natta reactions is carried out at controlled high pressures and moderated temperatures and high pressure of 70-75'c and 32-35 atm. Hydrogen used for controlling melt flow rate in first reactor is almost double of second reactor. Slurry density for the operating melt flow rate is 560-565 Kg/m3. The production split between the two reactors is claimed to be 65% for the first reactor and remaining 35% for the second reactor, assuming no loss in catalytic activity. The net amount of conversion obtained is approximated to 53%, which is reliable and matching with the concerned plant results. An alternate way would be use of two CSTR reactors in series with optimum recycle ratio for each one.

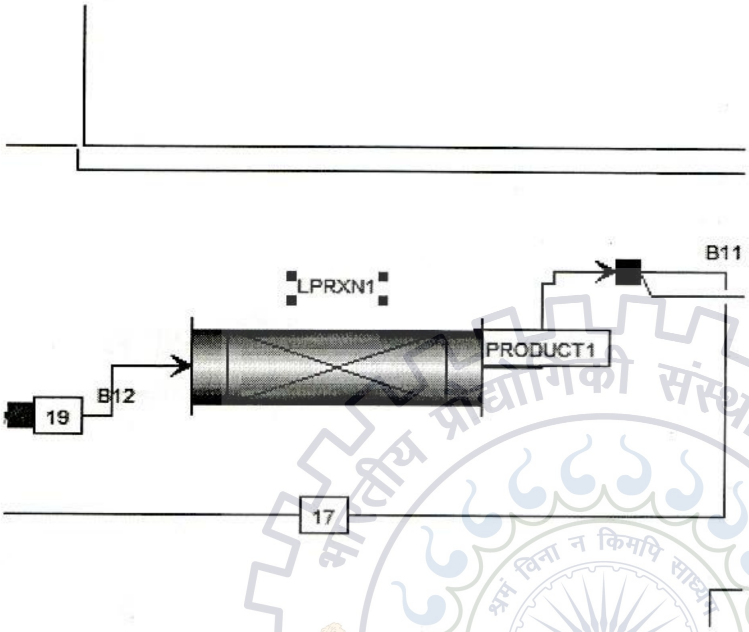


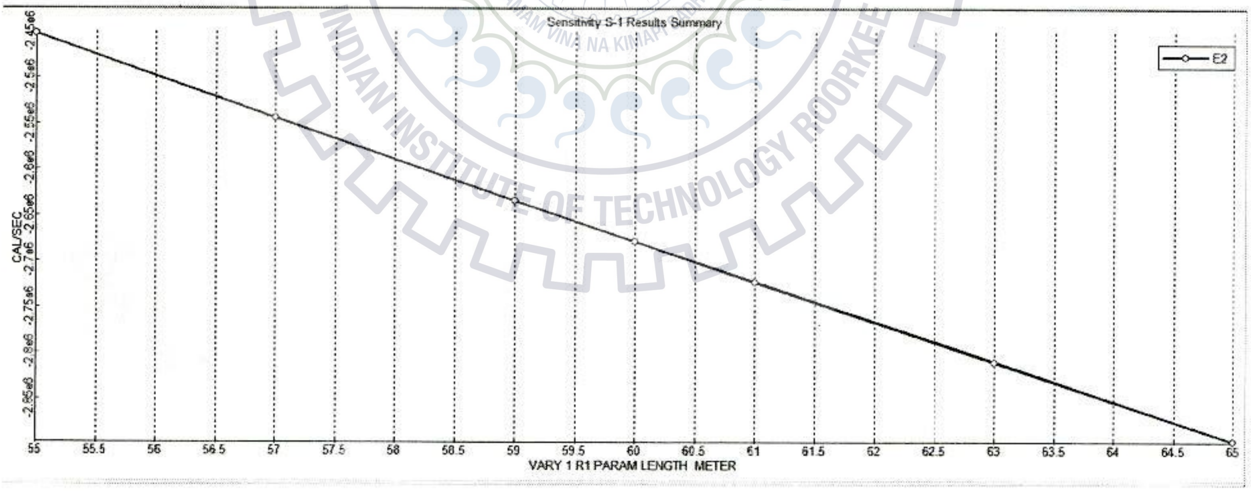
a. Data obtained from Reactor (Loop Reactor) :

```
BLOCK:  Reactor1     MODEL: RPLUG
 -----------------------------
  INLET STREAM:          19
  OUTLET STREAM:         PRODUCT1
  PROPERTY OPTION SET:   POLYNRTL  / REDLICH-KWONG

              ***  MASS AND ENERGY BALANCE  ***
                   IN        OUT       GENERATION   RELATIVE DIFF.
  TOTAL BALANCE
  MOLE(KMOL/HR )        1048.40      1048.40      0.515127E-04  0.361826E-16
  MASS(KG/HR   )      44115.5     44115.5                 -0.834545E-13
  ENTHALPY(CAL/SEC )    85087.7    -0.259382E+07              1.03280

                ***  INPUT DATA  ***

  REACTOR TYPE:
   SPECIFIED TEMPERATURE
   LIQUID FLUID PHASE
  REACTOR TUBE LENGTH              METER            60.000
          DIAMETER              METER            0.60960
  NUMBER OF REACTOR TUBES                             1
  REACTOR VOLUME                L               17512.
  ERROR TOLERANCE                                0.10000E-03
  INTEGRATION METHOD                               GEAR
  CORRECTOR METHOD                                NEWTON
  INITIAL STEP SIZE FACTOR                        0.10000E-01
  CORRECTOR TOLERANCE FACTOR                           0.10000
  MAXIMUM NUMBER OF STEPS                            1000
```

TEMPERATURE PROFILES:

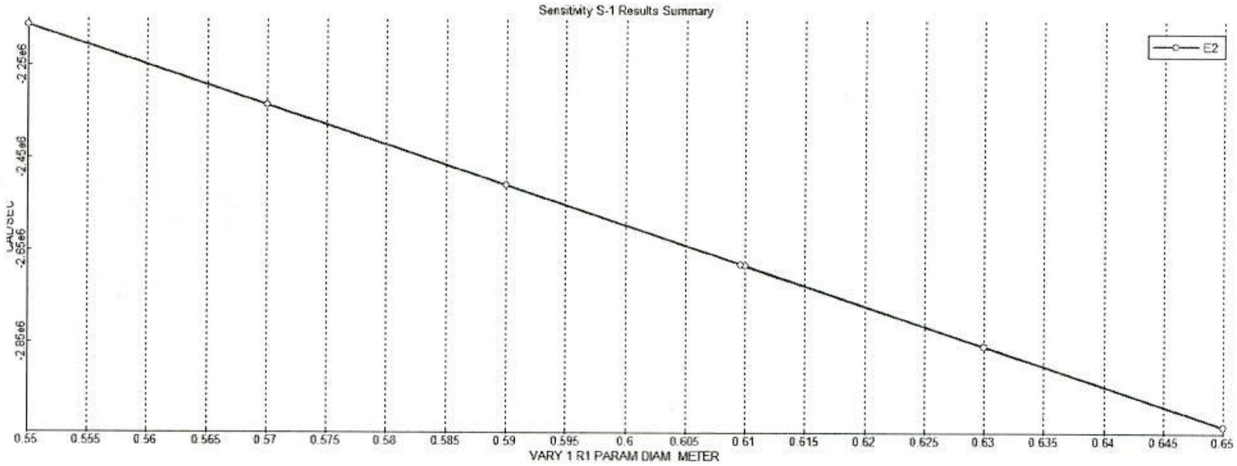
RELATIVE LOCATION	TEMPERATURE
0.00000E+00	346.15 K





Heat of reaction v/s Length of reactor

Graph 4.3



Graph 4.4. Heat of reaction v/s Diameter of reactor

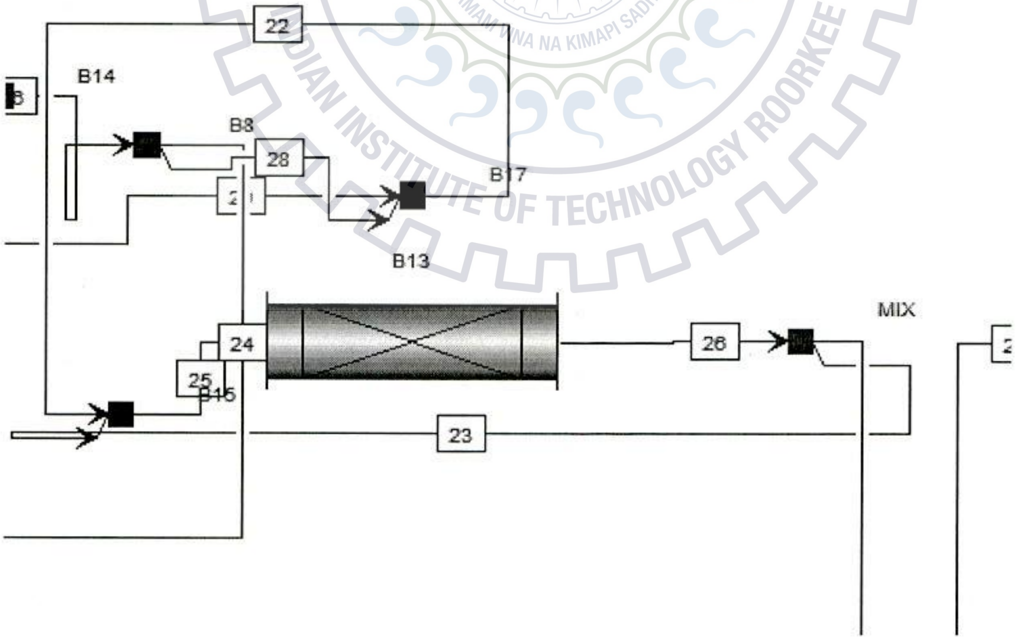
```
          *** REACTION DATA ***

MODEL: ZIEGLER-NAT   BLOCK: Z-N

RATE PARAMETERS:

 REACTION     SITE CID1     CID2        K0          EACT       ORD
 ACT-COCAT     1  TITAN-01 TRIET-01  0.1620E+07  0.3200E+08   1.000
 ACT-COCAT     2  TITAN-01 TRIET-01  0.1620E+07  0.3200E+08   1.000
 ACT-COCAT     3  TITAN-01 TRIET-01  0.1620E+07  0.3200E+08   1.000
 ACT-COCAT     4  TITAN-01 TRIET-01  0.1620E+07  0.3200E+08   1.000
 CHAIN-INI    1  PROPY-01            0.1175E+08  0.3000E+08   1.000
 CHAIN-INI    2  PROPY-01            0.2600E+07  0.3000E+08   1.000
 CHAIN-INI    3  PROPY-01            0.1844E+08  0.3000E+08   1.000
 CHAIN-INI    4  PROPY-01            0.6530E+07  0.3000E+08   1.000
 PROPAGATION    1  PROPY-01 PROPY-01  0.1175E+08  0.3000E+08   1.000
 PROPAGATION    2  PROPY-01 PROPY-01  0.2640E+07  0.3000E+08   1.000
 PROPAGATION    3  PROPY-01 PROPY-01  0.1844E+08  0.3000E+08   1.000
 PROPAGATION    4  PROPY-01 PROPY-01  0.6530E+07  0.3000E+08   1.000
 CHAT-MON      1  PROPY-01 PROPY-01  0.1020E+07  0.5200E+08   1.000
 CHAT-MON      2  PROPY-01 PROPY-01  0.1020E+07  0.5200E+08   1.000
 CHAT-MON      3  PROPY-01 PROPY-01  0.1020E+07  0.5200E+08   1.000
 CHAT-MON      4  PROPY-01 PROPY-01  0.1020E+07  0.5200E+08   1.000
 CHAT-COCAT     1  PROPY-01 TRIET-01  0.5000E+07  0.5000E+08   1.000
 CHAT-COCAT     2  PROPY-01 TRIET-01  0.5000E+07  0.5000E+08   1.000
 CHAT-COCAT     3  PROPY-01 TRIET-01  0.5000E+07  0.5000E+08   1.000
 CHAT-COCAT     4  PROPY-01 TRIET-01  0.5000E+07  0.5000E+08   1.000
 DEACT-SPON    1              0.4214E-03  0.4100E+07   1.000
 DEACT-SPON    2              0.4214E-03  0.4100E+07   1.000
 DEACT-SPON    3              0.4214E-03  0.4100E+07   1.000
 DEACT-SPON    4              0.4214E-03  0.4100E+07   1.000
 ATACT-PROP    1  PROPY-01 PROPY-01  0.5000E+06  0.3000E+08   1.000
 ATACT-PROP    2  PROPY-01 PROPY-01  0.1200E+07  0.3000E+08   1.000
 ATACT-PROP    3  PROPY-01 PROPY-01  0.3000E+06  0.3000E+08   1.000
 ATACT-PROP    4  PROPY-01 PROPY-01  0.7000E+06  0.3000E+08   1.00
```

```
                    ***  RESULTS  ***

REACTOR DUTY             CAL/SEC              -0.26789E+07
RESIDENCE TIME           HR               0.19112
REACTOR MINIMUM TEMPERATURE K                     346.15
REACTOR MAXIMUM TEMPERATURE K                      346.15


   *** RESULTS PROFILE (PROCESS STREAM) ***

 LENGTH      PRESSURE    TEMPERATURE  VAPOR FRAC   RES-TIME
 METER       ATM         K                 HR

 0.00000E+00  34.053      346.15      0.00000E+00  0.00000E+00
  6.0000       34.053      346.15    0.00000E+00  0.16439E-01
  12.000       34.053      346.15    0.00000E+00  0.33394E-01
  18.000       34.053      346.15    0.00000E+00  0.50892E-01
  24.000       34.053      346.15    0.00000E+00  0.68964E-01
  30.000       34.053      346.15    0.00000E+00  0.87640E-01
  36.000       34.053      346.15    0.00000E+00  0.10695
  42.000       34.053      346.15    0.00000E+00  0.12693
  48.000       34.053      346.15    0.00000E+00  0.14760
  54.000       34.053      346.15    0.00000E+00  0.16899
  60.000       34.053      346.15    0.00000E+00  0.19112
```

b. Data obtained from Loop Reactor 2:

```
BLOCK:  REACTOR 2    MODEL: RPLUG
 ------------------------------
  INLET STREAM:         25
  OUTLET STREAM:        26
  PROPERTY OPTION SET:   POLYNRTL  / REDLICH-KWONG

            ***  MASS AND ENERGY BALANCE  ***
                   IN         OUT      GENERATION   RELATIVE DIFF.
  TOTAL BALANCE
  MOLE(KMOL/HR )        1639.44       1639.44     0.235802E-04 -0.266444E-16
  MASS(KG/HR   )      68980.4      68980.4                 0.189862E-14
  ENTHALPY(CAL/SEC )  -0.239696E+07 -0.395315E+07              0.393659
```

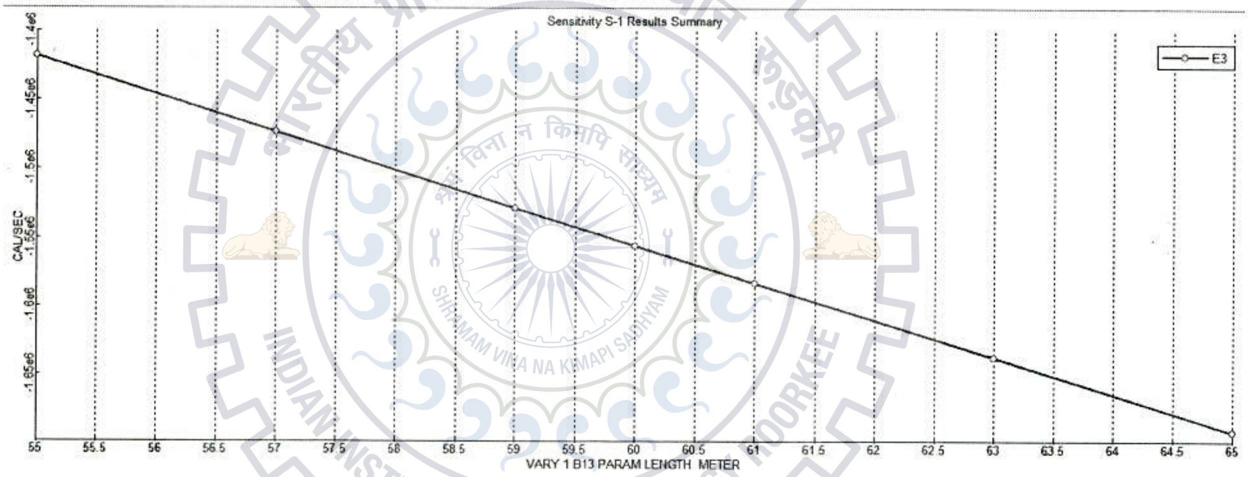
```
              ***  INPUT DATA  ***

REACTOR TYPE:
 SPECIFIED TEMPERATURE
 LIQUID FLUID PHASE
REACTOR TUBE LENGTH               METER          60.000
        DIAMETER            METER          0.60960
NUMBER OF REACTOR TUBES                           1
REACTOR VOLUME              L              17512.
ERROR TOLERANCE                            0.10000E-03
INTEGRATION METHOD                          GEAR
CORRECTOR METHOD                           NEWTON
INITIAL STEP SIZE FACTOR                    0.10000E-01
CORRECTOR TOLERANCE FACTOR                         0.10000
MAXIMUM NUMBER OF STEPS                          1000

TEMPERATURE PROFILES:

 RELATIVE LOCATION      TEMPERATURE
    0.00000E+00      346.15   K
```



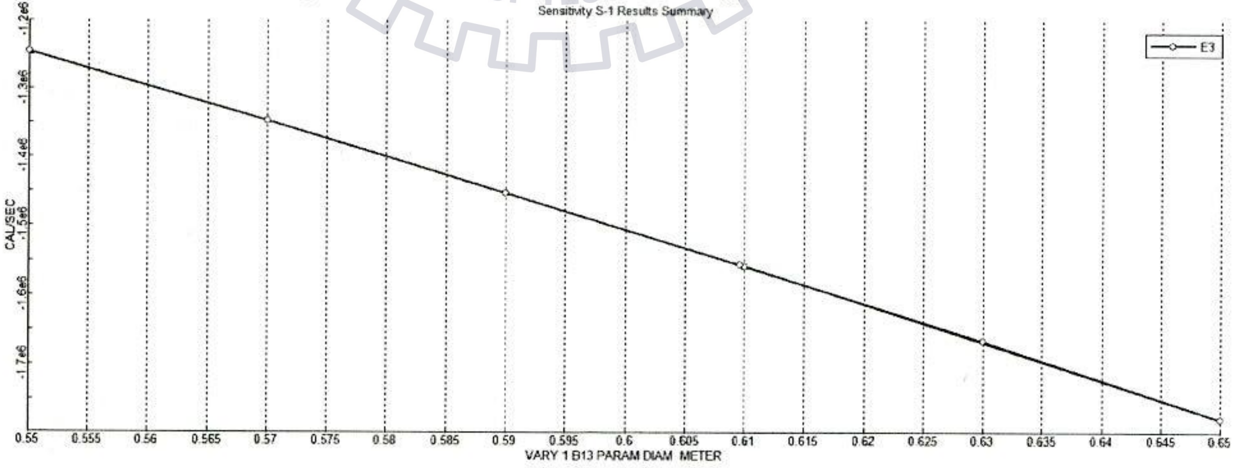
```
             *** REACTION DATA ***

MODEL: ZIEGLER-NAT   BLOCK: Z-N

RATE PARAMETERS:
```

```
REACTION     SITE CID1    CID2       K0        EACT       ORD
ACT-COCAT     1  TITAN-01 TRIET-01  0.1620E+07  0.3200E+08   1.000
ACT-COCAT     2  TITAN-01 TRIET-01  0.1620E+07  0.3200E+08   1.000
ACT-COCAT     3  TITAN-01 TRIET-01  0.1620E+07  0.3200E+08   1.000
ACT-COCAT     4  TITAN-01 TRIET-01  0.1620E+07  0.3200E+08   1.000
CHAIN-INI    1  PROPY-01           0.1175E+08  0.3000E+08   1.000
CHAIN-INI    2  PROPY-01           0.2600E+07  0.3000E+08   1.000
CHAIN-INI    3  PROPY-01           0.1844E+08  0.3000E+08   1.000
CHAIN-INI    4  PROPY-01           0.6530E+07  0.3000E+08   1.000
PROPAGATION    1  PROPY-01 PROPY-01  0.1175E+08  0.3000E+08   1.000
PROPAGATION    2  PROPY-01 PROPY-01  0.2640E+07  0.3000E+08   1.000
PROPAGATION    3  PROPY-01 PROPY-01  0.1844E+08  0.3000E+08   1.000
PROPAGATION    4  PROPY-01 PROPY-01  0.6530E+07  0.3000E+08   1.000
CHAT-MON      1  PROPY-01 PROPY-01  0.1020E+07  0.5200E+08   1.000
CHAT-MON      2  PROPY-01  *** RESULTS PROFILE (PROCESS STREAM) ***

LENGTH      PRESSURE    TEMPERATURE  VAPOR FRAC   RES-TIME
METER       ATM          K                   HR

0.00000E+00   36.422     346.15     0.00000E+00  0.00000E+00
 6.0000       36.422     346.15     0.00000E+00  0.12571E-01
 12.000       36.422     346.15     0.00000E+00  0.25311E-01
 18.000       36.422     346.15     0.00000E+00  0.38224E-01
 24.000       36.422     346.15     0.00000E+00  0.51313E-01
 30.000       36.422     346.15     0.00000E+00  0.64578E-01
 36.000       36.422     346.15     0.00000E+00  0.78023E-01
 42.000       36.422     346.15     0.00000E+00  0.91650E-01
 48.000       36.422     346.15     0.00000E+00  0.10546
 54.000       36.422     346.15     0.00000E+00  0.11946
 60.000       36.422     346.15     0.00000E+00  0.13364


  ***  TOTAL MOLE FRACTION PROFILE (PROCESS STREAM) ***

LENGTH       TITAN-01     TRIET-01     PROPY-01     POLY(-01
METER

0.00000E+00  0.14004E-04  0.47034E-04  0.63458      0.36489
 6.0000      0.14004E-04  0.47033E-04  0.61392      0.38554
 12.000      0.14004E-04  0.47032E-04  0.59350      0.40597
 18.000      0.14004E-04  0.47032E-04  0.57332      0.42615
 24.000      0.14004E-04  0.47031E-04  0.55339      0.44608
 30.000      0.14004E-04  0.47030E-04  0.53373      0.46573
 36.000      0.14004E-04  0.47029E-04  0.51436      0.48510
 42.000      0.14004E-04  0.47028E-04  0.49529      0.50418
 48.000      0.14004E-04  0.47027E-04  0.47652      0.52294
 54.000      0.14004E-04  0.47026E-04  0.45808      0.54139
 60.000      0.14004E-04  0.47025E-04  0.43998      0.55949
```

```
LENGTH      PROPANE
HYDROGEN METER

0.00000E+00   0.19967E-03   0.27232E-03
 6.0000       0.19967E-03   0.27232E-03
 12.000       0.19967E-03   0.27232E-03
 18.000       0.19967E-03   0.27232E-03
 24.000       0.19967E-03   0.27232E-03
 30.000       0.19967E-03   0.27232E-03
 36.000       0.19967E-03   0.27232E-03
 42.000       0.19967E-03   0.27232E-03
 48.000       0.19967E-03   0.27232E-03
 54.000       0.19967E-03   0.27232E-03
 60.000       0.19967E-03   0.27232E-03
```



Graph 4.5. Heat of reaction v/s Length of reactor



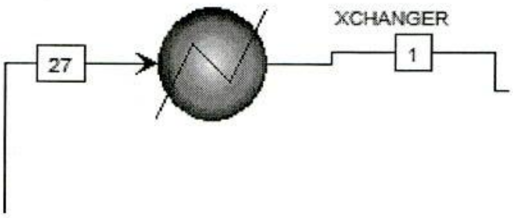
Graph 4.6. Heat of reaction v/s Diameter of reactor2

4.1.3 Flash drum:

The slurry from reactors is discharged to the flash pipe. After leaving the flash pipe, solid is separated from gas in the flash drum. During homo-polymer and random copolymer runs the polymer collected from the bottom of Flash Drum is discharged to the Recycle Gas Filter, while during high impact copolymer runs, polymer from flash drum is routed to the Gas Phase Reactor.

a. Heat exchanger before Flash Drum:

```
BLOCK:  XCHANGER MODEL: HEATER
 ------------------------------
   INLET STREAM:          27
   OUTLET STREAM:          1
   PROPERTY OPTION SET:   POLYNRTL  / REDLICH-KWONG

                *** MASS AND ENERGY BALANCE ***
                          IN          OUT       RELATIVE DIFF.
    TOTAL BALANCE
      MOLE(KMOL/HR )          1639.44       1639.44       0.000000E+00
      MASS(KG/HR   )       68980.4       68980.4       0.000000E+00
      ENTHALPY(CAL/SEC )    -0.395315E+07  -0.348550E+07  -0.118297

                 *** INPUT DATA ***
   TWO   PHASE  TP  FLASH
   SPECIFIED TEMPERATURE             K                363.150
   SPECIFIED PRESSURE              ATM               18.4211
   MAXIMUM NO. ITERATIONS                            30
   CONVERGENCE TOLERANCE                               0.000100000
```

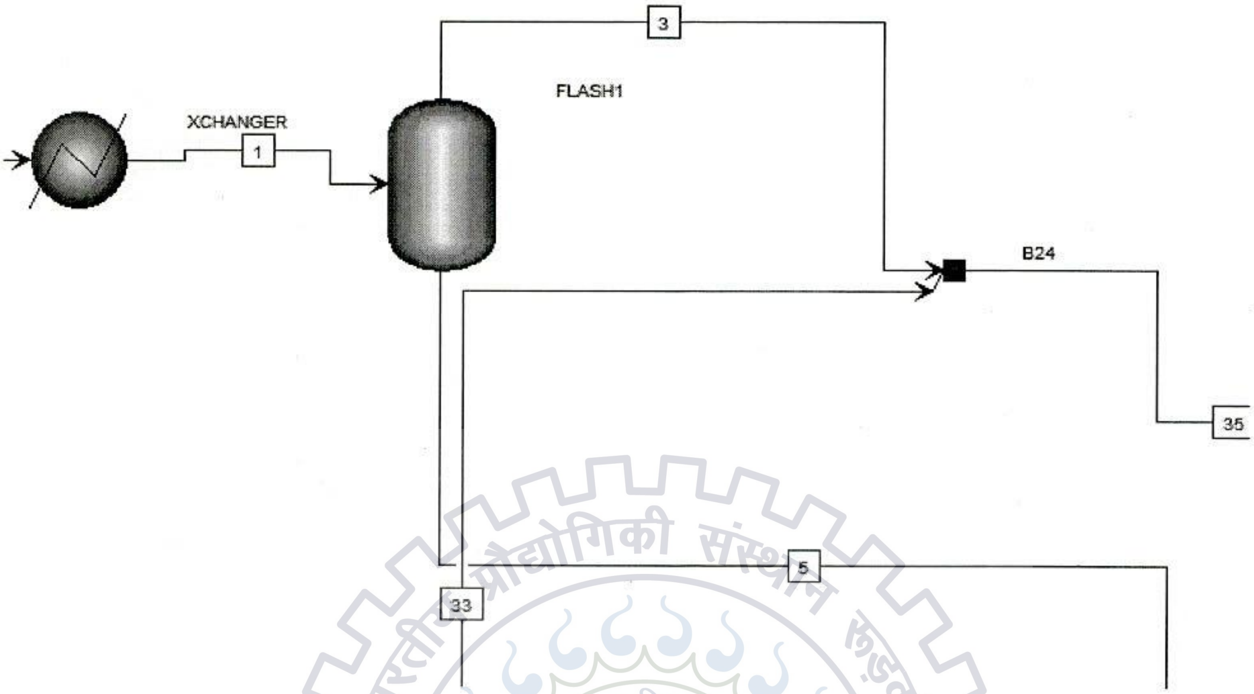


```
                 *** RESULTS ***
   OUTLET TEMPERATURE    K                         363.15
   OUTLET PRESSURE       ATM                      18.421
   HEAT DUTY             CAL/SEC                0.46765E+06
   OUTLET VAPOR FRACTION                           0.19883
   PRESSURE-DROP CORRELATION PARAMETER                         0.93690E+06
```

```
V-L PHASE EQUILIBRIUM :

      COMP          F(I)         X(I)         Y(I)         K(I)
    TITAN-01    0.14004E-04  0.17260E-04  0.88196E-06  0.51098E-01
    TRIET-01    0.47025E-04  0.58672E-04  0.95316E-07  0.16245E-02
    PROPY-01    0.43998      0.30144      0.99820      3.3114
    POLY(-01    0.55949      0.69834      0.28841-187  0.41299-187
    PROPANE     0.19967E-03  0.14234E-03  0.43067E-03  3.0257
    HYDROGEN    0.27232E-03  0.24624E-09  0.13696E-02  0.55620E+07
```

b. Flash Drum

```
BLOCK:  FLASH1   MODEL: FLASH2
------------------------------
  INLET STREAM:           1
  OUTLET VAPOR STREAM:    3
  OUTLET LIQUID STREAM:   5
  PROPERTY OPTION SET:   POLYNRTL  / REDLICH-KWONG

                 ***  MASS AND ENERGY BALANCE  ***
                        IN          OUT       RELATIVE DIFF.
  TOTAL BALANCE
    MOLE(KMOL/HR )          1639.44       1639.44      -0.138690E-15
    MASS(KG/HR   )          68980.4       68980.4      -0.421914E-15
    ENTHALPY(CAL/SEC )   -0.348550E+07  -0.317756E+07  -0.883507E-01

                   ***  INPUT DATA  ***
  TWO    PHASE  TP  FLASH
  SPECIFIED TEMPERATURE K                        375.150
  SPECIFIED PRESSURE    ATM                      7.77489
  MAXIMUM NO. ITERATIONS                           30
  CONVERGENCE TOLERANCE                            0.000100000
  LIQUID ENTRAINMENT                             0.25000E-02
```



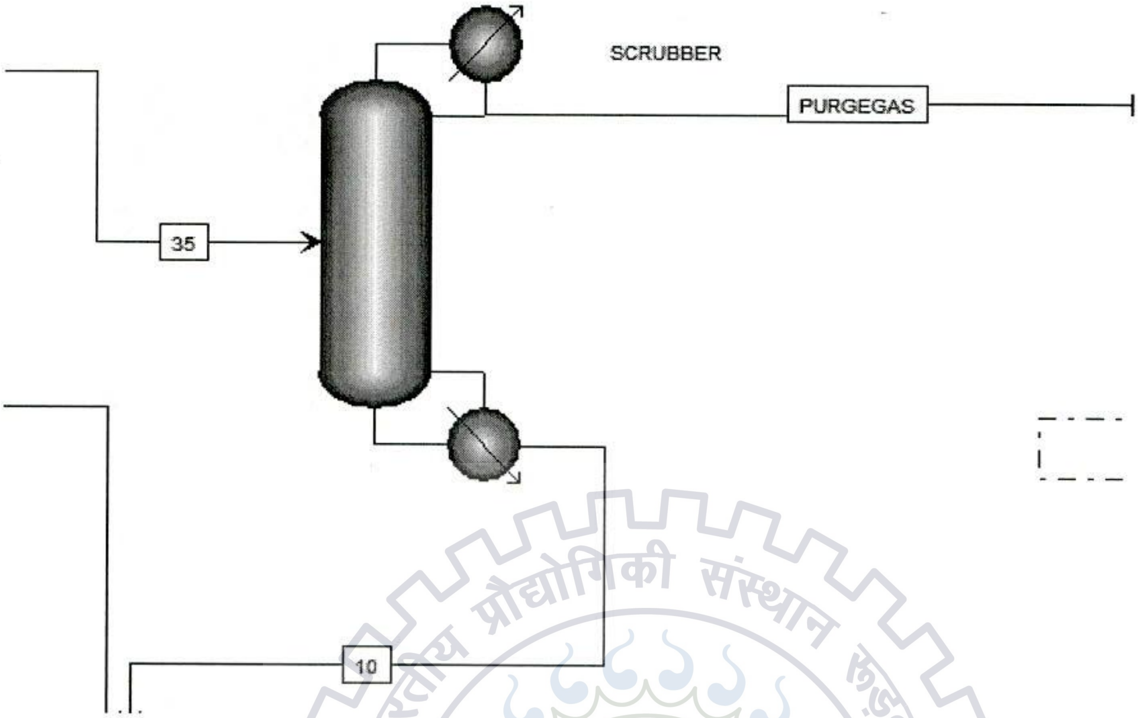
```
          *** RESULTS ***
OUTLET TEMPERATURE   K                    375.15
OUTLET PRESSURE      ATM                  7.7749
HEAT DUTY            CAL/SEC              0.30795E+06
VAPOR FRACTION                            0.36751


V-L PHASE EQUILIBRIUM :

  COMP          F(I)          X(I)          Y(I)          K(I)
  TITAN-01      0.14004E-04   0.20396E-04   0.30020E-05   0.14718
  TRIET-01      0.47025E-04   0.74052E-04   0.51159E-06   0.69086E-02
  PROPY-01      0.43998       0.11527       0.99881       8.6647
  POLY(-01      0.55949       0.88458       0.12831-187   0.14505-187
  PROPANE       0.19967E-03   0.56769E-04   0.44560E-03   7.8495
  HYDROGEN      0.27232E-03   0.54997E-10   0.74100E-03   0.13474E+08
```

4.1.4. Recycle gas filter:

All the monomers recovered from the degassing section are sent to the Recycle Propylene Scrubber. The bottom stream of the recycle Propylene Scrubber is lined up to Recycle gas filter. The vapor leaving the top of Propylene condenser is purged to the off-gas header. The recycle-condensed propylene is sent to the Propylene Feed Tank.

In case of homo polymer or random & ter-polymer production, the polymer is routed from the Flash Drum to the Low Pressure Degassing Filter. During heterophasic copolymer runs ,Recycle Gas Filter receives the polymer from gas phase reactor discharge. The filter gas is sent to washing and compression section. Gas stream leaving Recycle gas filter is washed in low Pressure Propylene Scrubber in order to remove any powder entrainment and minimize the aluminum alkyl content to the compressor. The delivery of Recycle Gas Compressor Unit is sent to Recycle Propylene Scrubber in case of homopolymer and random copolymer runs or to the Ethylene Stripper when producing heterophasic copolymers.

```
          BLOCK:  SCRUBBER MODEL: DISTL
                  -----------------
  -----------     INLET
  STREAM:         35
  CONDENSER OUTLET:      PURGEGAS
  REBOILER OUTLET:       10
  PROPERTY OPTION SET:   POLYNRTL  / REDLICH-KWONG


             ***  MASS AND ENERGY BALANCE  ***
                       IN          OUT       RELATIVE DIFF. TOTAL
  BALANCE
     MOLE(KMOL/HR )          733.607      733.607      0.577728E-06
     MASS(KG/HR   )         30854.1      30854.1      0.577696E-06
     ENTHALPY(CAL/SEC )      996689.      767928.      0.229521

         ***  INPUT DATA  *** THEORETICAL STAGES   12

           FEED STAGE NO. FROM TOP                       11
           REFLUX RATIO                                 0.30260
           TOP STAGE PRESSURE (ATM     )                 18.9051
           BOTTOM STAGE PRESSURE (ATM     )              8.74273
           DISTILLATE TO FEED RATIO                      0.94863
           CONDENSER TYPE: PARTIAL CONDENSER
```



```
        *** RESULTS ***
FEED-QUALITY                                    0.95120
FEED STAGE TEMPERATURE (K      )                     296.634
TOP STAGE TEMPERATURE (K      )                     319.632
BOTTOM STAGE TEMPERATURE (K      )                      465.991
CONDENSER COOLING REQUIRED (CAL/SEC )                   243,981.
NET CONDENSER DUTY (CAL/SEC )                    -243,981.
REBOILER HEATING REQUIRED (CAL/SEC )                15,219.2
NET REBOILER DUTY (CAL/SEC )                    15,219.2
```

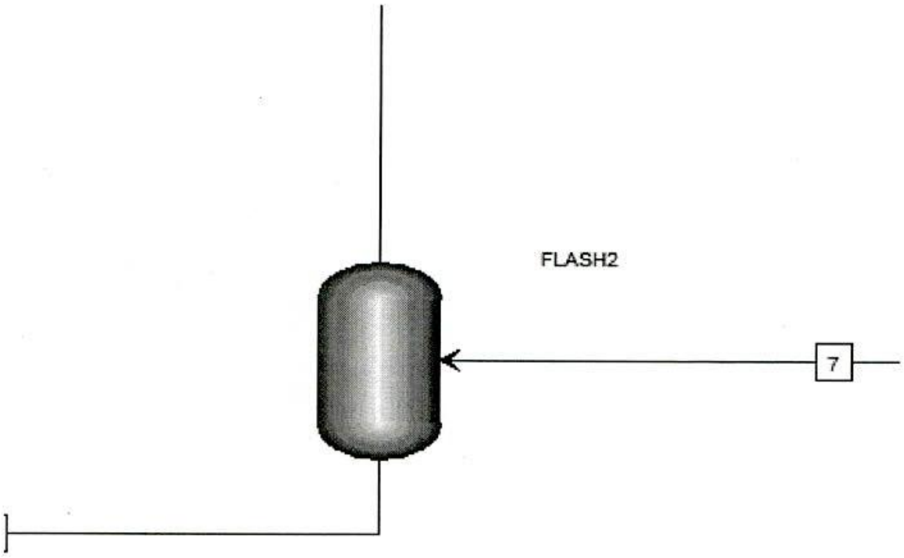
4.1.5 Steamer:

Recovery of monomers dissolved in the polymer and drying from Recycle Gas Filter the polymer powder is discharged by gravity to the steamer where steam is injected to complete removal of dissolved monomer and propane and to deactivate catalyst residual activity. Steam is condensed and discharged from the steamer to the sewer after passing through the steamer scrubber. Residual un reacted monomers and propane compressed by means of steamer Off gas compressor, can be sent to battery limits for propane purging of recycled the Recycle Gas Filter after water removal in Propylene Gas Drying Unit.

The polymer is discharged from the steamer to the fluid bed dryer where removal of surface water is effected by means of hot nitrogen. Dry polymer is transferred to the finishing unit surge silos by nitrogen closed pneumatic conveyor.

a. Bag Filter:

```
BLOCK:  Bag Filter   MODEL: FLASH2
 ------------------------------ INLET
   STREAM:        7
   OUTLET VAPOR STREAM:   33
   OUTLET LIQUID STREAM:  PRODUCT
   PROPERTY OPTION SET:   POLYNRTL  / REDLICH-KWONG

                     ***  MASS AND ENERGY BALANCE  ***
                          IN          OUT        RELATIVE DIFF. TOTAL
    BALANCE
      MOLE(KMOL/HR )          1072.03       1072.03       0.000000E+00
      MASS(KG/HR   )        45121.2      45121.2      -0.341174E-10
      ENTHALPY(CAL/SEC )     -0.426354E+07  -0.431883E+07   0.128028E-01

                   ***  INPUT DATA  *** TWO
   PHASE  TP  FLASH
   SPECIFIED TEMPERATURE K                              363.150
   SPECIFIED PRESSURE    ATM                            1.80000
   MAXIMUM NO. ITERATIONS                                30
   CONVERGENCE TOLERANCE                                  0.000100000
   LIQUID ENTRAINMENT                                  0.30000E-01
```

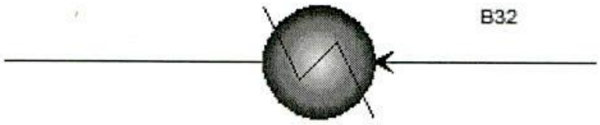


```
             ***  RESULTS  ***

OUTLET TEMPERATURE    K                        363.15
OUTLET PRESSURE       ATM                      1.8000
HEAT DUTY             CAL/SEC              -55291. VAPOR
FRACTION                       0.92656E-01


V-L PHASE EQUILIBRIUM :

  COMP          F(I)         X(I)         Y(I)         K(I)
  TITAN-01     0.22983E-04  0.24333E-04  0.97665E-05  0.40137
  TRIET-01     0.74248E-04  0.81711E-04  0.11695E-05  0.14313E-01
  PROPY-01     0.11776      0.27720E-01  0.99950      36.057
  POLY(-01     0.88208      0.97216      0.27260-187  0.28041-187
  PROPANE      0.58796E-04  0.15008E-04  0.48759E-03  32.489
  HYDROGEN     0.53063E-10  0.66681E-17  0.57269E-09  0.85886E+08
```

b. Heat Exchanger after Recycle gas Fileter:

```
BLOCK:  B32     MODEL: HEATER
 ------------------------------
  INLET STREAM:          PRODUCT
  OUTLET STREAM:         36
  PROPERTY OPTION SET:   POLYNRTL   / REDLICH-KWONG

                 ***  MASS AND ENERGY BALANCE  ***
                         IN            OUT        RELATIVE DIFF. TOTAL
 BALANCE
   MOLE(KMOL/HR )         943.518       943.518      0.000000E+00
   MASS(KG/HR   )        39712.8       39712.8       0.000000E+00
```

```
   ENTHALPY(CAL/SEC )     -0.434313E+07  -0.470659E+07   0.772247E-01

              ***  INPUT DATA  ***
 ONE   PHASE  TP  FLASH   SPECIFIED PHASE IS  LIQUID
 SPECIFIED TEMPERATURE            K              301.150
 SPECIFIED PRESSURE            ATM               1.50000
 MAXIMUM NO. ITERATIONS                           30
 CONVERGENCE TOLERANCE                             0.000100000
```



```
              ***  RESULTS  ***
 OUTLET TEMPERATURE   K                   301.15
 OUTLET PRESSURE        ATM              1.5000
 HEAT DUTY              CAL/SEC         -0.36346E+06

PRESSURE-DROP CORRELATION PARAMETER              0.20342E+06
```

4.2 Material and Energy balance obtained through simulation:

Stream Results	CATALYST	COCAT	HYDROGEN	MIXED	PROPENE	PROPENE
Temperature K	303.15	303.15	303.15	303.15	303.15	
Pressure atm	15.51762	15.51762	15.5176166	15.5176166	15.5176166	15.5
Vapor Frac	0	0	1	0	0	
Mole Flow kmol/hr	0.045917	0.155212	0.89291029	95.255848	95.0547194	3182
Mass Flow kg/hr	8.71	17.72	1.8	4026.43	4000	133
Volume Flow l/min	0.086144	0.253292	24.0801865	134.098248	133.954081	4485
Enthalpy MMBtu/hr	-0.03482	-0.03486	0.00013546	0.3828511	0.45253633	15.1
Mole Flow kmol/hr						
TITAN-01	0.045917	0	0	0.04591682	0	
TRIET-01	0	0.155212	0	0.15521172	0	
PROPY-01	0	0	0	95.0365774	95.0365774	3182
POLY(-01	0	0	0	0	0	
PROPANE	0	0	0	0.01814202	0.01814202	0.63
C3H6-R	0	0	0	0	0	
NITRO-01	0	0	0	0	0	
HYDROGEN	0	0	0.89291029	0	0	
WATER	0	0	0	0	0	

Continued….

Stream Results	R1OUT	R2IN	R2OUT	FLASHIN	FLASHOUT	SCRUBIN

Temperature K	346.15	329.9061	346.15	363.15	375.15	374.023626
Pressure atm	34.87444	35	34.8744387	18.4211399	7.77488774	7.77
Vapor Frac	0	0	0	0.19883704	0.99571582	0.95270653
Mole Flow kmol/hr	1048.403	1639.44	1639.44003	1639.44003	605.096178	733.606971
Mass Flow kg/hr	44115.49	68980.41	68980.405	68980.405	25445.7997	30854.1429
Volume Flow l/min	1296.362	2145.857	2044.14846	9099.85054	37549.0024	43465.2564
Enthalpy MMBtu/hr	-37.0552	-34.2428	-56.474481	-49.793657	13.8915846	14.2386525
Mole Flow kmol/hr						
TITAN-01	0.022958	0.022958	0.02295841	0.02295841	0.0018616	0.00354176
TRIET-01	0.077109	0.077109	0.07709538	0.07709538	0.0005002	0.00300076
PROPY-01	449.6014	1040.357	721.317387	721.317387	602.085613	702.17483
POLY(-01	598.2092	598.2092	917.248793	917.248793	2.29312198	30.661648
PROPANE	0.209169	0.327344	0.32734397	0.32734397	0.26862556	0.31749576
C3H6-R	0	0	0	0	0	0
NITRO-01	0	0	0	0	0	0
HYDROGEN	0.282753	0.446455	0.44645515	0.44645515	0.44645509	0.44645515
WATER	0	0	0	0	0	0

Continued..

Stream Results	SCRUBOUT	RESCRUB	BAGIN	PURGEGAS	PRODUCT
Temperature K	465.9903	363.15	374.77398	319.632023	363.15
Pressure atm	8.742729	1.8	5	18.9050604	1.8
Vapor Frac	0	0.77293	0.0473596	1	0
Mole Flow kmol/hr	37.68494	128.5108	1072.0287	695.921581	943.51799
Mass Flow kg/hr	1586.554	5408.343	45121.159	29267.5697	39712.816
Volume Flow l/min	21.42784	27053.52	6038.2384	11953.4334	837.83604
Enthalpy MMBtu/hr	-1.62272	0.347068	-60.908712	12.5933029	-62.045687
Mole Flow kmol/hr					
TITAN-01	0.003542	0.00168	0.0246385	0	0.0229584
TRIET-01	0.003001	0.002501	0.0795959	0	0.0770953
PROPY-01	7.012434	100.0892	126.24420	695.162364	26.154778
POLY(-01	30.66165	28.36853	945.617319	0	917.249007

			0.0630307		0.0141604
C3H6-R	0	0	0	0	0
NITRO-01	0	0	0	0	0
HYDROGEN	0	5.69E-08	5.69E-08	0.44645515	0
WATER	0	0	0	0	0

4.3. Sensitive analysis of polypropylene plant:

The data below represent the sensitive analysis of polypropylene plant, temperature of both the reactors T1 and T2 were varied with their diameters also. Length of reactor 1 is varied while keeping the length of second reactor constant 60m.

With the variation of this variables polypropylene production obtained and energy of reactions is calculated, various graphs were plotted to show the variations in energy and production.

338K < T1< 358K

338K < T1< 358K

55m < L1 < 65m

0.55m < D1 < 0.65m

0.55m < D1 < 0.65m

T1	T2	L1	D1	D2	Polymer	Heat of Reaction
338	338	55	0.55	0.57	672.1124	-2981339.35
338	338	55	0.55	0.59	689.5447	-3078038.83
338	338	55	0.55	0.61	707.4809	-3177533.01
338	338	55	0.55	0.63	725.7601	-3278930.46
338	338	55	0.55	0.65	744.5514	-3383167.96
338	338	55	0.57	0.55	678.2114	-3015171.22
338	338	55	0.57	0.57	694.9511	-3108028.81
338	338	55	0.57	0.59	712.1842	-3203622.78
338	338	55	0.57	0.61	729.9236	-3302025.6
338	338	55	0.57	0.63	747.9918	-3402252.38
338	338	55	0.57	0.65	766.5553	-3505226.58
338	338	55	0.59	0.55	701.5732	-3144762.51
338	338	55	0.59	0.57	718.1507	-3236719.63
338	338	55	0.59	0.59	735.1813	-3331190.77
338	338	55	0.59	0.61	752.718	-3428469.33
338	338	55	0.59	0.63	770.6049	-3527690.14
338	338	55	0.59	0.65	788.8853	-3629093.66
338	338	55	0.61	0.55	725.255	-3276128.51
338	338	55	0.61	0.57	741.6268	-3366944.99
338	338	55	0.61	0.59	758.461	-3460326
338	338	55	0.61	0.61	775.697	-3555936.75
338	338	55	0.61	0.63	793.3479	-3653848.21
338	338	55	0.61	0.65	811.4322	-3754164.05
338	338	55	0.63	0.55	749.1751	-3408816.1
338	338	55	0.63	0.57	765.3093	-3498314.51

338	338	55	0.63	0.59	781.8977	-3590332.49
338	338	55	0.63	0.61	798.9089	-3684695.68

338	338	55	0.63	0.63	816.3479	-3781432.17
338	338	55	0.63	0.65	834.1187	-3880009.36
338	338	55	0.65	0.55	773.1661	-3541897.3
338	338	55	0.65	0.57	789.077	-3630157.23
338	338	55	0.65	0.59	805.432	-3720880.11
338	338	55	0.65	0.61	822.2283	-3814051.68
338	338	55	0.65	0.63	839.3097	-3908804.5
338	338	55	0.65	0.65	856.8636	-4006178.25
338	338	57.5	0.55	0.55	669.3297	-2965903.32
338	338	57.5	0.55	0.57	686.1779	-3059362.82
338	338	57.5	0.55	0.59	703.4863	-3155374.73
338	338	57.5	0.55	0.61	721.3057	-3254221.05
338	338	57.5	0.55	0.63	739.4544	-3354894.21
338	338	57.5	0.55	0.65	758.1077	-3458366.23
338	338	57.5	0.57	0.55	693.1731	-3098166.15
338	338	57.5	0.57	0.57	709.7791	-3190281.32
338	338	57.5	0.57	0.59	726.8815	-3285150.64
338	338	57.5	0.57	0.61	744.4966	-3382863.99
338	338	57.5	0.57	0.63	762.4658	-3482541.36
338	338	57.5	0.57	0.65	780.8339	-3584431.47
338	338	57.5	0.59	0.55	717.2439	-3231689.71
338	338	57.5	0.59	0.57	733.6862	-3322897.34
338	338	57.5	0.59	0.59	750.5934	-3416683.47
338	338	57.5	0.59	0.61	767.9055	-3512716.35
338	338	57.5	0.59	0.63	785.6441	-3611114.15
338	338	57.5	0.59	0.65	803.8108	-3711887.6
338	338	57.5	0.61	0.55	741.6469	-3367056.42
338	338	57.5	0.61	0.57	757.8492	-3456932.73
338	338	57.5	0.61	0.59	774.5099	-3549351.34
338	338	57.5	0.61	0.61	791.5913	-3644104.45
338	338	57.5	0.61	0.63	809.1168	-3741320.52
338	338	57.5	0.61	0.65	826.9711	-3840360.31
338	338	57.5	0.63	0.55	766.1593	-3503029.7
338	338	57.5	0.63	0.57	782.1364	-3591656.79
338	338	57.5	0.63	0.59	798.5588	-3682753.68
338	338	57.5	0.63	0.61	815.3906	-3776121.95
338	338	57.5	0.63	0.63	832.6473	-3871847.23
338	338	57.5	0.63	0.65	850.2262	-3969359.24
338	338	57.5	0.65	0.55	790.6923	-3639117.15
338	338	57.5	0.65	0.57	806.5039	-3726826.13
338	338	57.5	0.65	0.59	822.6507	-3816394.92
338	338	57.5	0.65	0.61	839.2542	-3908496.31
338	338	57.5	0.65	0.63	856.1405	-4002166.69
338	338	57.5	0.65	0.65	873.4209	-4098023.22
338	338	60	0.55	0.55	683.41	-3044008.76
338	338	60	0.55	0.57	700.0969	-3136573.12

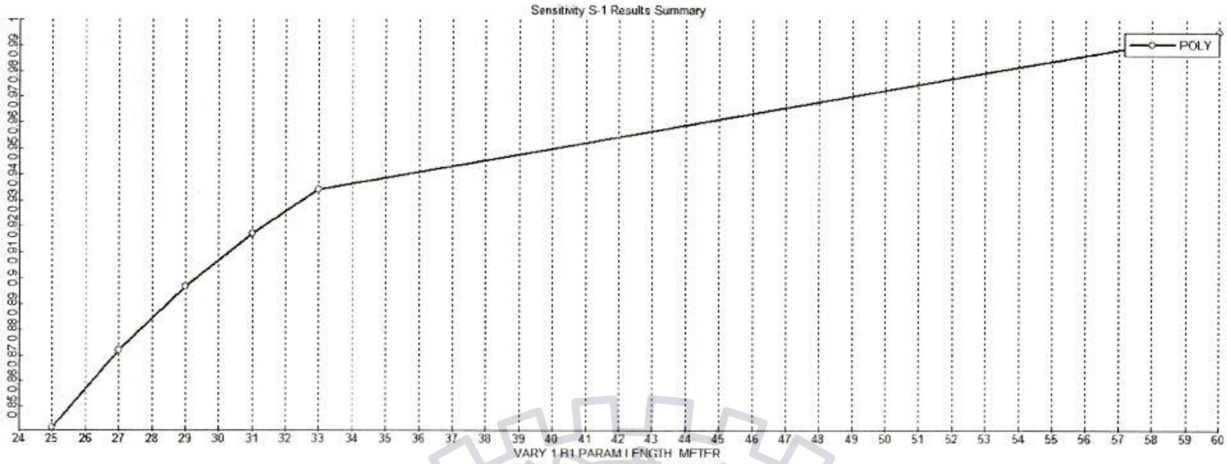
338	338	60	0.55	0.59	717.2965	-3231981.27
338	338	60	0.55	0.61	734.9883	-3330120.46
338	338	60	0.55	0.63	753.0516	-3430319.72
338	338	60	0.55	0.65	771.4556	-3532409.02
338	338	60	0.57	0.55	707.8768	-3179729.36
338	338	60	0.57	0.57	724.4004	-3271387.55
338	338	60	0.57	0.59	741.3747	-3365546.21
338	338	60	0.57	0.61	758.8522	-3462496.16
338	338	60	0.57	0.63	776.6162	-3561035.58
338	338	60	0.57	0.65	794.8917	-3662412.05
338	338	60	0.59	0.55	732.7271	-3317576.86
338	338	60	0.59	0.57	749.009	-3407894.54
338	338	60	0.59	0.59	765.754	-3500781.28
338	338	60	0.59	0.61	782.9182	-3595993.69
338	338	60	0.59	0.63	800.5443	-3693767.91
338	338	60	0.59	0.65	818.4945	-3793339.49
338	338	60	0.61	0.55	757.7153	-3456189.61
338	338	60	0.61	0.57	773.7711	-3545253.22
338	338	60	0.61	0.59	790.2764	-3636810.18
338	338	60	0.61	0.61	807.1971	-3730671.34
338	338	60	0.61	0.63	824.5463	-3826909.8
338	338	60	0.61	0.65	842.2213	-3924955.15
338	338	60	0.63	0.55	782.7543	-3595084.32
338	338	60	0.63	0.57	798.6571	-3683298.96
338	338	60	0.63	0.59	814.8872	-3773329.65
338	338	60	0.63	0.61	831.5746	-3865896.51
338	338	60	0.63	0.63	848.55	-3960061.24
338	338	60	0.63	0.65	865.9243	-4056438.93
338	338	60	0.65	0.55	807.853	-3734310.08
338	338	60	0.65	0.57	823.4901	-3821050.65
338	338	60	0.65	0.59	839.4883	-3909795.08
338	338	60	0.65	0.61	855.824	-4000411.03
338	338	60	0.65	0.63	872.5589	-4093241.68
338	338	60	0.65	0.65	889.6312	-4187943.84
338	338	62.5	0.55	0.55	697.2266	-3120651.04
338	338	62.5	0.55	0.57	713.8408	-3212812.11
338	338	62.5	0.55	0.59	730.9099	-3307497.01
338	338	62.5	0.55	0.61	748.4871	-3404999.72
338	338	62.5	0.55	0.63	766.4165	-3504456.34
338	338	62.5	0.55	0.65	784.7419	-3606109.95
338	338	62.5	0.57	0.55	722.4222	-3260414.33
338	338	62.5	0.57	0.57	738.819	-3351369.58
338	338	62.5	0.57	0.59	755.6792	-3444894.96
338	338	62.5	0.57	0.61	772.9424	-3540656.47
338	338	62.5	0.57	0.63	790.6246	-3638741.66
338	338	62.5	0.57	0.65	808.7375	-3739216.55

338	338	62.5	0.59	0.55	747.9081	-3401787.94
338	338	62.5	0.59	0.57	764.0538	-3491350.35
338	338	62.5	0.59	0.59	780.6545	-3583436.11
338	338	62.5	0.59	0.61	797.6781	-3677868.72
338	338	62.5	0.59	0.63	815.1312	-3774682.91
338	338	62.5	0.59	0.65	832.9161	-3873338.37
338	338	62.5	0.61	0.55	773.4288	-3543354.72
338	338	62.5	0.61	0.57	789.3898	-3631892.43
338	338	62.5	0.61	0.59	805.7419	-3722599.37
338	338	62.5	0.61	0.61	822.5346	-3815750.75
338	338	62.5	0.61	0.63	839.6127	-3910484.96
338	338	62.5	0.61	0.65	857.1628	-4007837.88
338	338	62.5	0.63	0.55	799.0671	-3685573.31
338	338	62.5	0.63	0.57	814.7942	-3772813.71
338	338	62.5	0.63	0.59	830.8538	-3861898.3
338	338	62.5	0.63	0.61	847.319	-3953232.96
338	338	62.5	0.63	0.63	864.1558	-4046628.71
338	338	62.5	0.63	0.65	881.3355	-4141926.86
338	338	62.5	0.65	0.55	824.6422	-3827441.66
338	338	62.5	0.65	0.57	840.0667	-3913003.21
338	338	62.5	0.65	0.59	855.8827	-4000736.58
338	338	62.5	0.65	0.61	872.0292	-4090303.56
338	338	62.5	0.65	0.63	888.563	-4182018.63
338	338	62.5	0.65	0.65	905.427	-4275565.27
338	338	65	0.55	0.55	710.9111	-3196560.91
338	338	65	0.55	0.57	727.4085	-3288074
338	338	65	0.55	0.59	744.3726	-3382175.92
338	338	65	0.55	0.61	761.8042	-3478871.55
338	338	65	0.55	0.63	779.5425	-3577267.96
338	338	65	0.55	0.65	797.7817	-3678443.12
338	338	65	0.57	0.55	736.8094	-3340222.02
338	338	65	0.57	0.57	753.055	-3430338.7
338	338	65	0.57	0.59	769.7616	-3523012.13
338	338	65	0.57	0.61	786.8869	-3618008.58
338	338	65	0.57	0.63	804.4683	-3715534.42
338	338	65	0.57	0.65	822.3756	-3814868.83
338	338	65	0.59	0.55	762.843	-3484633.77
338	338	65	0.59	0.57	778.8512	-3573433.14
338	338	65	0.59	0.59	795.306	-3664710.02
338	338	65	0.59	0.61	812.1729	-3758272.89
338	338	65	0.59	0.63	829.4663	-3854201.91
338	338	65	0.59	0.65	847.0831	-3951924.28
338	338	65	0.61	0.55	788.9067	-3629212.31
338	338	65	0.61	0.57	804.7488	-3717090.74
338	338	65	0.61	0.59	820.9142	-3806762.27
338	338	65	0.61	0.61	837.5362	-3898966.25

338	338	65	0.61	0.63	854.4432	-3992751.48
338	338	65	0.61	0.65	871.7447	-4088725.56
338	338	65	0.63	0.55	815.0056	-3773986.51
338	338	65	0.63	0.57	830.5683	-3860314.3
338	338	65	0.63	0.59	846.4897	-3948632.58
338	338	65	0.63	0.61	862.7449	-4038802.51
338	338	65	0.63	0.63	879.3952	-4131163.47
338	338	65	0.63	0.65	896.3788	-4225373.64
338	338	65	0.65	0.55	840.9728	-3918029.44
338	338	65	0.65	0.57	856.2219	-4002618.53
338	338	65	0.65	0.59	871.8537	-4089329.78
338	338	65	0.65	0.61	887.8199	-4177896.44
338	338	65	0.65	0.63	904.1442	-4268449.73
338	338	65	0.65	0.65	920.7978	-4360828.99
338	343	55	0.55	0.55	679.4633	-2953448.51
338	343	55	0.55	0.57	698.1354	-3057382.16
338	343	55	0.55	0.59	717.3206	-3164171.55
338	343	55	0.55	0.61	736.9982	-3273702.03
338	343	55	0.55	0.63	757.1462	-3385850.74
338	343	55	0.55	0.65	777.741	-3500486.31
338	343	55	0.57	0.55	702.3964	-3081099.75
338	343	55	0.57	0.57	720.872	-3183939.42
338	343	55	0.57	0.59	739.8489	-3289569.93
338	343	55	0.57	0.61	759.305	-3397867.1
338	343	55	0.57	0.63	779.2198	-3508718.07
338	343	55	0.57	0.65	799.5687	-3621984.67
338	343	55	0.59	0.55	725.7019	-3210823.94
338	343	55	0.59	0.57	743.9688	-3312502.2
338	343	55	0.59	0.59	762.7249	-3416903.32
338	343	55	0.59	0.61	781.9487	-3523907.79
338	343	55	0.59	0.63	801.6164	-3633382.98
338	343	55	0.59	0.65	821.7046	-3745198.68
338	343	55	0.61	0.55	749.2668	-3341992.31
338	343	55	0.61	0.57	767.3131	-3442442.09
338	343	55	0.61	0.59	785.8364	-3545547.27
338	343	55	0.61	0.61	804.8136	-3651179.42
338	343	55	0.61	0.63	824.2218	-3759210.22
338	343	55	0.61	0.65	843.9511	-3869028.33
338	343	55	0.63	0.55	773.0121	-3474164.3
338	343	55	0.63	0.57	790.8257	-3573319.15
338	343	55	0.63	0.59	809.0591	-3674810.73
338	343	55	0.63	0.61	827.8209	-3779243.32
338	343	55	0.63	0.63	846.9559	-3885753.75
338	343	55	0.63	0.65	866.4093	-3994036.17
338	343	55	0.65	0.55	796.8571	-3606891.49
338	343	55	0.65	0.57	814.4262	-3704685.14

338	343	55	0.65	0.59	832.3996	-3804729.68
338	343	55	0.65	0.61	850.8911	-3907658.11
338	343	55	0.65	0.63	869.7405	-4012578.18
338	343	55	0.65	0.65	888.9658	-4119591.23
338	343	57.5	0.55	0.55	693.5887	-3032074.03
338	343	57.5	0.55	0.57	712.1408	-3135339.51
338	343	57.5	0.55	0.59	731.1341	-3241060.91
338	343	57.5	0.55	0.61	750.7404	-3350194.46
338	343	57.5	0.55	0.63	770.7458	-3461549.41
338	343	57.5	0.55	0.65	791.1902	-3575348.09
338	343	57.5	0.57	0.55	717.2946	-3164026.88
338	343	57.5	0.57	0.57	735.6379	-3266130.13
338	343	57.5	0.57	0.59	754.4748	-3370981.05
338	343	57.5	0.57	0.61	773.7111	-3478055.16
338	343	57.5	0.57	0.63	793.4616	-3587990.99
338	343	57.5	0.57	0.65	813.7252	-3700783.66
338	343	57.5	0.59	0.55	741.2966	-3297628.23
338	343	57.5	0.59	0.57	759.4191	-3398502.19
338	343	57.5	0.59	0.59	778.022	-3502050.45
338	343	57.5	0.59	0.61	797.0838	-3608153.23
338	343	57.5	0.59	0.63	816.581	-3716679.41
338	343	57.5	0.59	0.65	836.4022	-3827009.44
338	343	57.5	0.61	0.55	765.5266	-3432498.05
338	343	57.5	0.61	0.57	783.4147	-3532067.55
338	343	57.5	0.61	0.59	801.7704	-3634239.8
338	343	57.5	0.61	0.61	820.5715	-3738891.42
338	343	57.5	0.61	0.63	839.7939	-3845888.02
338	343	57.5	0.61	0.65	859.4126	-3955090.94
338	343	57.5	0.63	0.55	789.8946	-3568136.3
338	343	57.5	0.63	0.57	807.5362	-3666333.96
338	343	57.5	0.63	0.59	825.5866	-3766806.92
338	343	57.5	0.63	0.61	844.1584	-3870182.3
338	343	57.5	0.63	0.63	863.0269	-3975208.6
338	343	57.5	0.63	0.65	882.4056	-4083075.62
338	343	57.5	0.65	0.55	814.306	-3704016.42
338	343	57.5	0.65	0.57	831.6888	-3800773.28
338	343	57.5	0.65	0.59	849.5111	-3899976.43
338	343	57.5	0.65	0.61	867.7502	-4001499.87
338	343	57.5	0.65	0.63	886.3824	-4105211.21
338	343	57.5	0.65	0.65	905.3794	-4210953.44
338	343	60	0.55	0.55	707.5735	-3109916.94
338	343	60	0.55	0.57	726.0036	-3212503.14
338	343	60	0.55	0.59	744.9323	-3317865.3
338	343	60	0.55	0.61	764.2639	-3425469.81
338	343	60	0.55	0.63	784.1984	-3536430.21
338	343	60	0.55	0.65	804.4904	-3649380.39

338	343	60	0.57	0.55	731.9753	-3245743.5



Graph 4.7. Polypropylene produced v/s Length of reactor (Prepoly Reactor)

358	348	62.5	0.55	0.55	854.7125	-3860230.68
358	348	62.5	0.55	0.57	873.9222	-3967599.85
358	348	62.5	0.55	0.59	893.5968	-4077566.94
358	348	62.5	0.55	0.61	913.7103	-4189987.58
358	348	62.5	0.55	0.63	934.2278	-4304666.31
358	348	62.5	0.55	0.65	955.1163	-4421418.71
358	348	62.5	0.57	0.55	886.7971	-4039561.32
358	348	62.5	0.57	0.57	905.6472	-4144920.54
358	348	62.5	0.57	0.59	924.9416	-4252762.66
358	348	62.5	0.57	0.61	944.5682	-4362462.03
358	348	62.5	0.57	0.63	964.7366	-4475189.33
358	348	62.5	0.57	0.65	985.1698	-4589397.07
358	348	62.5	0.59	0.55	918.8316	-4218612.17
358	348	62.5	0.59	0.57	937.2974	-4321823.49
358	348	62.5	0.59	0.59	956.183	-4427380.85
358	348	62.5	0.59	0.61	975.4582	-4535115.83
358	348	62.5	0.59	0.63	995.0927	-4644858.81
358	348	62.5	0.59	0.65	1015.037	-4756334.5
358	348	62.5	0.61	0.55	950.5333	-4395802.86
358	348	62.5	0.61	0.57	968.5908	-4496731.8
358	348	62.5	0.61	0.59	987.0428	-4599865.57
358	348	62.5	0.61	0.61	1005.861	-4705043.61
358	348	62.5	0.61	0.63	1025.007	-4812057.23
358	348	62.5	0.61	0.65	1044.447	-4920712.75
358	348	62.5	0.63	0.55	981.5972	-4569428.36
358	348	62.5	0.63	0.57	999.2245	-4667952.98
358	348	62.5	0.63	0.59	1017.222	-4768545.05

358	348	62.5	0.63	0.61	1035.56	-4871044.06
358	348	62.5	0.63	0.63	1054.201	-4975234.41
358	348	62.5	0.63	0.65	1073.109	-5080918.75
358	348	62.5	0.65	0.55	1011.582	-4737022.82
358	348	62.5	0.65	0.57	1028.764	-4833058.78
358	348	62.5	0.65	0.59	1046.291	-4931020.39
358	348	62.5	0.65	0.61	1064.134	-5030754.41
358	348	62.5	0.65	0.63	1082.256	-5132039.32
358	348	62.5	0.65	0.65	1100.618	-5234670.03
358	348	65	0.55	0.55	872.1869	-3957900.56
358	348	65	0.55	0.57	891.2041	-4064193.7
358	348	65	0.55	0.59	910.6749	-4173021.96
358	348	65	0.55	0.61	930.4891	-4283769.89
358	348	65	0.55	0.63	950.8573	-4397613.61
358	348	65	0.55	0.65	971.5014	-4512999.99
358	348	65	0.57	0.55	904.9073	-4140784.75
358	348	65	0.57	0.57	923.5435	-4244948.55
358	348	65	0.57	0.59	942.6103	-4351518.64
358	348	65	0.57	0.61	962.077	-4460324.28
358	348	65	0.57	0.63	981.9131	-4571194.16
358	348	65	0.57	0.65	1002.073	-4683872.25
358	348	65	0.59	0.55	937.4111	-4322458.75
358	348	65	0.59	0.57	955.6412	-4424352.2
358	348	65	0.59	0.59	993.9699	-4524352.2
358	348	65	0.59	0.61	993.2871	-4634766.82
358	348	65	0.59	0.63	1012.637	-4742920.05
358	348	65	0.59	0.65	1032.292	-4852775.42
358	348	65	0.61	0.55	969.3921	-4501210.48
358	348	65	0.61	0.57	987.1921	-4600699.88
358	348	65	0.61	0.59	1005.372	-4702311.94
358	348	65	0.61	0.61	1023.902	-4805884.9
358	348	65	0.61	0.63	1042.746	-4911206.56
358	348	65	0.61	0.65	1061.867	-5018079.26
358	348	65	0.63	0.55	1000.523	-4675213.26
358	348	65	0.63	0.57	1017.873	-4772186.71
358	348	65	0.63	0.59	1035.577	-4871140.84
358	348	65	0.63	0.61	1053.608	-4971917.28
358	348	65	0.63	0.63	1071.924	-5074295.5
358	348	65	0.63	0.65	1090.492	-5178075.97
358	348	65	0.65	0.55	1030.411	-4842262.5
358	348	65	0.65	0.57	1047.297	-4936643.66
358	348	65	0.65	0.59	1064.511	-5032861.22
358	348	65	0.65	0.61	1082.027	-5130761.02
358	348	65	0.65	0.63	1099.806	-5230131.71
358	348	65	0.65	0.65	1117.808	-5330751.19
358	353	55	0.55	0.55	819.8163	-3590106.01

358	353	55	0.55	0.57	840.9938	-3709099.23
358	353	55	0.55	0.59	862.7192	-3831170.2
358	353	55	0.55	0.61	884.9429	-3956041.52
358	353	55	0.55	0.63	907.6461	-4083606.78
358	353	55	0.55	0.65	930.7864	-4213628.48
358	353	55	0.57	0.55	849.6182	-3757558.12
358	353	55	0.57	0.57	870.4964	-3874869.05
358	353	55	0.57	0.59	891.8997	-3995130.48
358	353	55	0.57	0.61	913.7796	-4118069.85
358	353	55	0.57	0.63	936.1134	-4243559.69
358	353	55	0.57	0.65	958.8559	-4371346.27
358	353	55	0.59	0.55	879.8284	-3927303.98
358	353	55	0.59	0.57	900.3815	-4042788.37
358	353	55	0.59	0.59	921.4355	-4161087.12
358	353	55	0.59	0.61	942.9414	-4281924.97
358	353	55	0.59	0.63	964.8768	-4405176.4
358	353	55	0.59	0.65	987.199	-4530601.3
358	353	55	0.61	0.55	910.0242	-4096969.13
358	353	55	0.61	0.57	930.2247	-4210472.34
358	353	55	0.61	0.59	950.8991	-4326637.85
358	353	55	0.61	0.61	972.0117	-4445266.35
358	353	55	0.61	0.63	993.5183	-4566108.19
358	353	55	0.61	0.65	1015.385	-4688972.15
358	353	55	0.63	0.55	940.0954	-4265933.68
358	353	55	0.63	0.57	959.925	-4377352.86
358	353	55	0.63	0.59	980.1963	-4491253.92
358	353	55	0.63	0.61	1000.878	-4607462
358	353	55	0.63	0.63	1021.932	-4725757.21
358	353	55	0.63	0.65	1043.312	-4845890.19
358	353	55	0.65	0.55	969.8496	-4433117.73
358	353	55	0.65	0.57	989.1889	-4541781.77
358	353	55	0.65	0.59	1009.125	-4653799.71
358	353	55	0.65	0.61	1029.354	-4767460.76
358	353	55	0.65	0.63	1049.924	-4883041.74
358	353	55	0.65	0.65	1070.793	-5000299.56
358	353	57.5	0.55	0.55	838.2682	-3693784.43
358	353	57.5	0.55	0.57	859.2637	-3811754.46
358	353	57.5	0.55	0.59	880.7924	-3932720.86
358	353	57.5	0.55	0.61	902.8063	-4056413.17
358	353	57.5	0.55	0.63	925.2838	-4182710.38
358	353	57.5	0.55	0.65	948.1828	-4311375.9
358	353	57.5	0.57	0.55	868.9829	-3866364.93
358	353	57.5	0.57	0.57	889.656	-3982523.69
358	353	57.5	0.57	0.59	910.8382	-4101543.06
358	353	57.5	0.57	0.61	932.4815	-4223152.76
358	353	57.5	0.57	0.63	954.5627	-4347223.3

358	353	57.5	0.57	0.65	977.0385	-4473511.25
358	353	57.5	0.59	0.55	899.8447	-4039772.1
358	353	57.5	0.59	0.57	920.1692	-4153972.11
358	353	57.5	0.59	0.59	940.9728	-4270864.14
358	353	57.5	0.59	0.61	962.2241	-4390271.19
358	353	57.5	0.59	0.63	983.8786	-4511944.12
358	353	57.5	0.59	0.65	1005.899	-4635670.51
358	353	57.5	0.61	0.55	930.6662	-4212952.92
358	353	57.5	0.61	0.57	950.49	-4324339.27
358	353	57.5	0.61	0.59	971.0165	-4439674.55
358	353	57.5	0.61	0.61	991.838	-4556666.89
358	353	57.5	0.61	0.63	1013.035	-4675771.74
358	353	57.5	0.61	0.65	1034.572	-4796779.64
358	353	57.5	0.63	0.55	961.2127	-4384588.32
358	353	57.5	0.63	0.57	980.7599	-4494420.65
358	353	57.5	0.63	0.59	1000.734	-4606651.42
358	353	57.5	0.63	0.61	1021.097	-4721069.94
358	353	57.5	0.63	0.63	1041.812	-4837460.1
358	353	57.5	0.63	0.65	1062.832	-4955568.84
358	353	57.5	0.65	0.55	991.2264	-4553230.45
358	353	57.5	0.65	0.57	1010.259	-4660169.91
358	353	57.5	0.65	0.59	1029.87	-4770362.94
358	353	57.5	0.65	0.61	1049.754	-4882085.96
358	353	57.5	0.65	0.63	1069.957	-4995604.28
358	353	57.5	0.65	0.65	1090.435	-5110668.85
358	353	60	0.55	0.55	856.4061	-3795697.91
358	353	60	0.55	0.57	877.214	-3912614.28
358	353	60	0.55	0.59	898.5411	-4032447.33
358	353	60	0.55	0.61	920.3396	-4154929.37
358	353	60	0.55	0.63	942.5861	-4279928.93
358	353	60	0.55	0.65	965.2355	-4407191.91
358	353	60	0.57	0.55	887.8738	-3972509.99
358	353	60	0.57	0.57	908.3367	-4087487.44
358	353	60	0.57	0.59	929.2879	-4205208.23
358	353	60	0.57	0.61	950.6981	-4325508.67
358	353	60	0.57	0.63	972.5217	-4448131.94
358	353	60	0.57	0.65	994.7219	-4572871.23
358	353	60	0.59	0.55	919.4219	-4149772.84
358	353	60	0.59	0.57	939.5104	-4262647.1
358	353	60	0.59	0.59	960.0627	-4378126.75
358	353	60	0.59	0.61	981.0442	-4496018.28
358	353	60	0.59	0.63	1002.412	-4616078.74
358	353	60	0.59	0.65	1024.13	-4738108.27
358	353	60	0.61	0.55	950.7487	-4325792.86
358	353	60	0.61	0.57	970.4367	-4436416.68
358	353	60	0.61	0.59	990.5609	-4549490.75

358	353	60	0.61	0.61	1011.084	-4664806.9
358	353	60	0.61	0.63	1031.968	-4782152.25
358	353	60	0.61	0.65	1053.169	-4901275.45
358	353	60	0.63	0.55	981.6195	-4499250.82
358	353	60	0.63	0.57	1000.792	-4606976.52
358	353	60	0.63	0.59	1020.551	-4718000.99
358	353	60	0.63	0.61	1040.592	-4830607.47
358	353	60	0.63	0.63	1060.962	-4945062.29
358	353	60	0.63	0.65	1081.619	-5061131.36
358	353	60	0.65	0.55	1011.743	-4668508.15
358	353	60	0.65	0.57	1030.465	-4773707.53
358	353	60	0.65	0.59	1049.749	-4882057.18
358	353	60	0.65	0.61	1069.286	-4991833.85
358	353	60	0.65	0.63	1089.12	-5103275.14
358	353	60	0.65	0.65	1109.216	-5216193.25
358	353	62.5	0.55	0.55	874.2484	-3895951.16
358	353	62.5	0.55	0.57	894.8634	-4011782.85
358	353	62.5	0.55	0.59	915.9836	-4130453.67
358	353	62.5	0.55	0.61	937.5607	-4251692.05
358	353	62.5	0.55	0.63	959.5759	-4375391.74
358	353	62.5	0.55	0.65	981.9756	-4501251.7
358	353	62.5	0.57	0.55	906.422	-4076729.11
358	353	62.5	0.57	0.57	926.6656	-4190474.1
358	353	62.5	0.57	0.59	947.386	-4306898.61
358	353	62.5	0.57	0.61	968.5481	-4425804.59
358	353	62.5	0.57	0.63	990.1071	-4546941.16
358	353	62.5	0.57	0.65	1012.03	-4670120.26
358	353	62.5	0.59	0.55	938.5117	-4257035.6
358	353	62.5	0.59	0.57	958.3595	-4368556.8
358	353	62.5	0.59	0.59	978.6549	-4482593.45
358	353	62.5	0.59	0.61	999.3601	-4598932.26
358	353	62.5	0.59	0.63	1020.438	-4717366.76
358	353	62.5	0.59	0.65	1041.845	-4837647.88
358	353	62.5	0.61	0.55	970.2376	-4435297.69
358	353	62.5	0.61	0.57	989.5714	-4543931.26
358	353	62.5	0.61	0.59	1009.502	-4655916.99
358	353	62.5	0.61	0.61	1029.724	-4769543.67
358	353	62.5	0.61	0.63	1050.288	-4885088.21
358	353	62.5	0.61	0.65	1071.15	-5002307.21
358	353	62.5	0.63	0.55	1001.289	-4609767.57
358	353	62.5	0.63	0.57	1020.171	-4715863.3
358	353	62.5	0.63	0.59	1039.623	-4825164.01
358	353	62.5	0.63	0.61	1059.34	-4935948.12
358	353	62.5	0.63	0.63	1079.363	-5048455.78
358	353	62.5	0.63	0.65	1099.652	-5162453.31
358	353	62.5	0.65	0.55	1031.221	-4777951.85

358	353	62.5	0.65	0.57	1049.634	-4881410.71
358	353	62.5	0.65	0.59	1068.589	-4987917.71
358	353	62.5	0.65	0.61	1087.78	-5095746.9
358	353	62.5	0.65	0.63	1107.247	-5205130.29
358	353	62.5	0.65	0.65	1126.952	-5315849.75
358	353	65	0.55	0.55	891.6649	-3993811.24
358	353	65	0.55	0.57	912.191	-4109143.77
358	353	65	0.55	0.59	933.0948	-4226599.07
358	353	65	0.55	0.61	954.4539	-4346611.71
358	353	65	0.55	0.63	976.2229	-4468928.44
358	353	65	0.55	0.65	998.365	-4593340.9
358	353	65	0.57	0.55	924.5663	-4178678.48
358	353	65	0.57	0.57	944.5911	-4291194.45
358	353	65	0.57	0.59	964.9343	-4405499.34
358	353	65	0.57	0.61	985.9839	-4523773.89
358	353	65	0.57	0.63	1007.274	-4643400.03
358	353	65	0.57	0.65	1028.908	-4764959.46
358	353	65	0.59	0.55	957.1097	-4361534.11
358	353	65	0.59	0.57	976.7125	-4471679.2
358	353	65	0.59	0.59	996.7458	-4584243.1
358	353	65	0.59	0.61	1017.172	-4699016.14
358	353	65	0.59	0.63	1037.954	-4815783.46
358	353	65	0.59	0.65	1059.045	-4934292.66
358	353	65	0.61	0.55	989.0932	-4541244.1
358	353	65	0.61	0.57	1008.157	-4648359.74
358	353	65	0.61	0.59	1027.801	-4758739.08
358	353	65	0.61	0.61	1047.72	-4870659.98
358	353	65	0.61	0.63	1067.961	-4984387.97
358	353	65	0.61	0.65	1088.481	-5099687.84
358	353	65	0.63	0.55	1020.186	-4715950.68
358	353	65	0.63	0.57	1038.777	-4820407.06
358	353	65	0.63	0.59	1057.92	-4927970.16
358	353	65	0.63	0.61	1077.309	-5036914.74
358	353	65	0.63	0.63	1096.986	-5147476.23
358	353	65	0.63	0.65	1116.917	-5259466.95
358	353	65	0.65	0.55	1049.994	-4883437.45
358	353	65	0.65	0.57	1068.079	-4985053.21
358	353	65	0.65	0.59	1086.719	-5089784.37
358	353	65	0.65	0.61	1105.56	-5195652.56
358	353	65	0.65	0.63	1124.659	-5302967.28
358	353	65	0.65	0.65	1143.977	-5411507.21
358	358	55	0.55	0.55	830.2768	-3563497.95
358	358	55	0.55	0.57	852.3906	-3688686.84
358	358	55	0.55	0.59	875.0863	-3817169.94
358	358	55	0.55	0.61	898.3014	-3948593.72
358	358	55	0.55	0.63	922.066	-4083128.27

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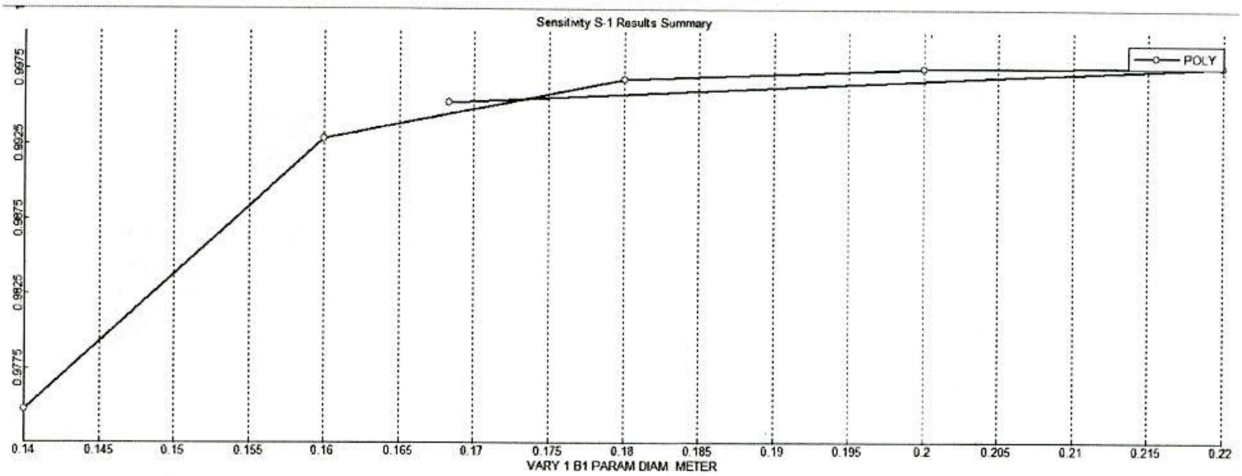
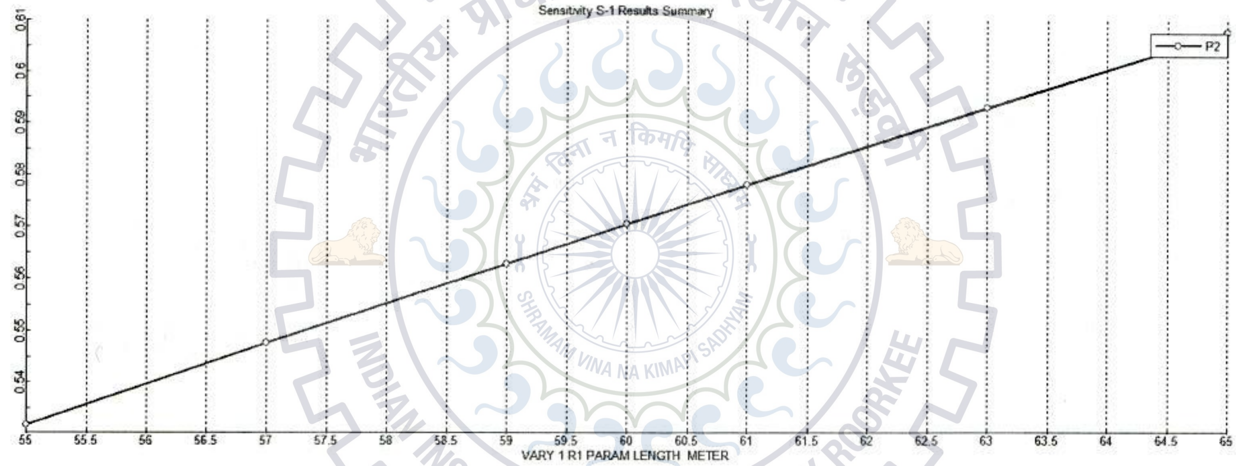
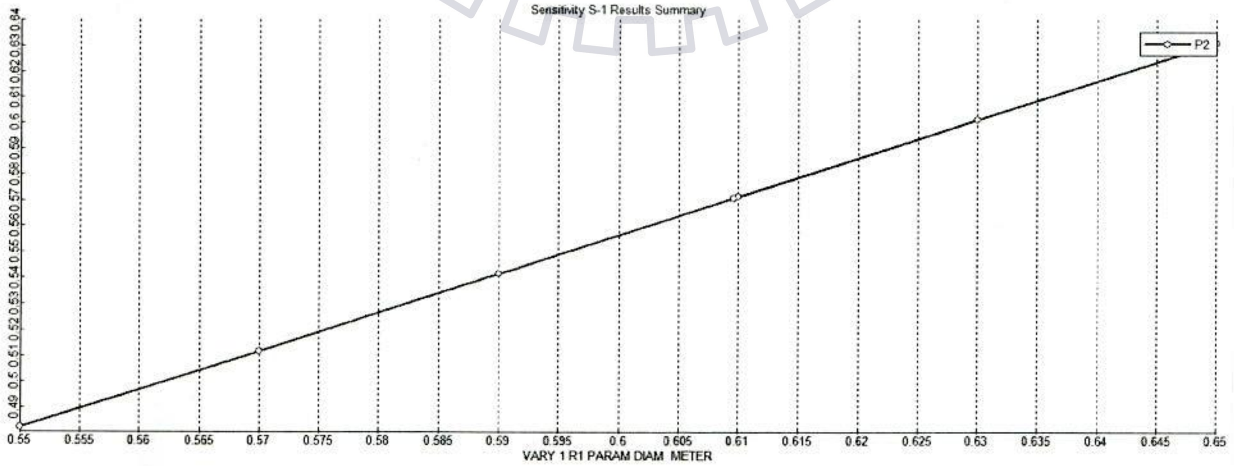


Graph 4.8. Polymer produced in prepolyreactor v/s diameter of reactor (Prepoly Reactor)

2. Loop Reactor 1:

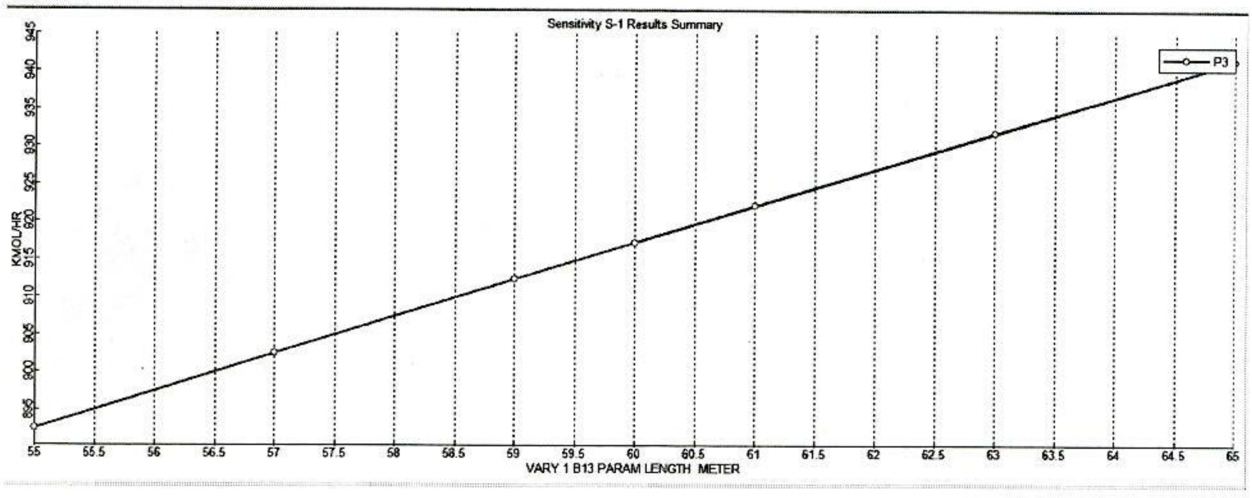


Graph 4.9. Polypropylene produced v/s length of reactor (Loop Reactor 1)

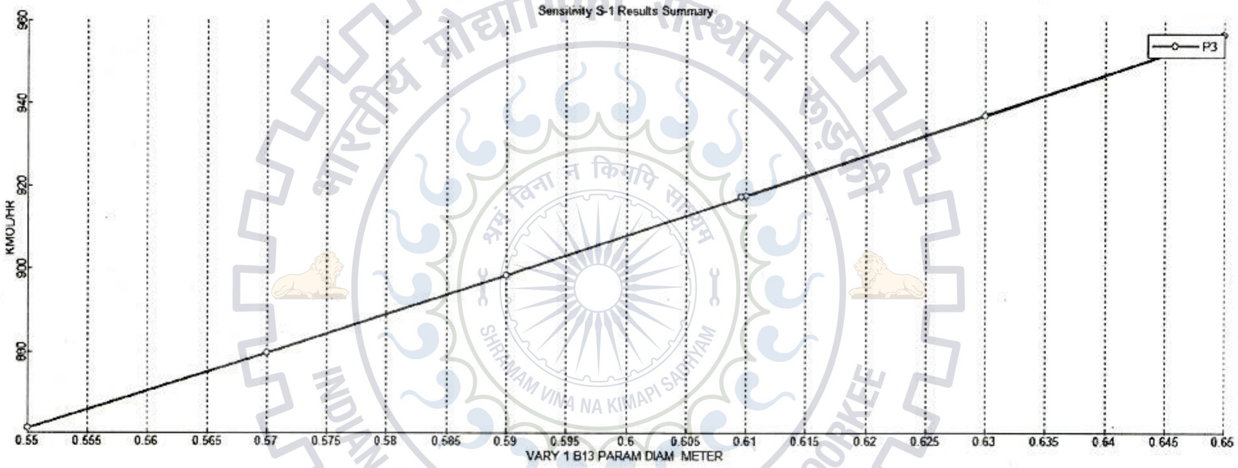


Graph 4.10. Polypropylene produced v/s diameter of reactor(Loop Reactor 1)

Loop Reactor 2:



Graph 4.11. Polypropylene produced v/s length of reactor (Loop Reactor 2)



Graph 4.12. Polymer produced v/s diameter of reactor2 (Loop Reactor 2)

CHAPTER 5

CONCLUSION

The ASPEN PLUS does an excellent job of describing the physical and thermodynamic properties for the UNIPOL polypropylene process. A Polymers Plus model is developed to simulate a Polypropylene gas-phase UNIPOL flowsheet. The flowsheet includes the fluidized bed reactor, the gas recycle/cooling loop, discharge and purge units. The fluidized bed reactor is modelled using the CSTR reactor in Aspen Plus with two phases; a gas phase and a polymer phase. The POLYNRTL thermodynamic model is used to relate the gas phase monomer, hydrogen, etc. composition to their concentrations in the polymer phase. The multisite Ziegler-Natta kinetic model is used to describe the polymerization reactions in the polymer phase. The kinetic model calculates the reaction rates for the components and polymer attributes at each site type. User-Property models are used to calculate polymer properties such as melt flow index (MFI), isotactic index (or atactic fraction) from the polymer attributes. The steady-state model accurately predicts the major polymer properties and key process variables for polymer. The model reliability is generally limited to systems whose feed compositions and process conditions are close to those used in model validation. There is always a desire to model everything in the plant. However, modeling is an art of simplifying the complexity while still capturing the essential details. A validated model, such as the one presented here, generates value for companies. It permits the exploration of different feed rates and operating conditions without wasting raw material or manpower. One can use the model to debottleneck the process, test new catalysts and products, and design new polymer grades. Polymers Plus can be used with Aspen Plus for the simulation of steady-state operation of any of the Polypropylene processes as described in this project.

Finally, I would like to explore more about integration of the POLYMER PLUS with the ASPEN dynamic model to explore various grade-change strategies, to minimize the transition time and the production of off-specification polymer. Polymers Plus can be used with Aspen Custom Modeler when dynamic simulation or detailed modelling of the flow patterns or heat transfer within the reactor is desired

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Corrigendum: (Only corrections indicated by evaluation committee during final Presentation)

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