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Study and Review of the modelling process of a PP polymerization

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ABSTRACT

Polypropylene(PP) is one of the most basic and useful olefin which have many diverse functions, cheaply produced and has a variety of applications. Many industries are using this product and constantly searching for improvement in the polymerization process. This paper will focus on the process, control of reactor using LIPP and modelling of PP polymers. For better utilization of raw materials a recycling system was introduced. EMSO software is used for the process and computer implementation of the process. If there is an increase in the material recycle resource then the efficiency of the process will also increase which will give smooth and better results.

Keywords: Polypropylene, LIPP, Polymers, EMSO.

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1. Introduction

Application versatility of polypropylene(pp) makes it a product of high economic value. Polypropylene is synthesized using numerous processes. These processes are prepared using Slurry, bulk or a gas phase(Simonazzi et al., 1989) .Using a liquid monomer for polymerization is considered as the best way of conducting this process in a bulk phase as it has a high rate of reaction and the process in conducted in less steps which further reduces the productional cost(Bai & Bai, 2019).

In the gas phase, the reaction takes place between the catalyst and the resin. There is no liquid phase in this process so it ceases any relation to viscosity or solubility of the liquid phase. Out of all three phases, the slurry phase is the costliest but it's feature makes it widely used in the industries(Zohuri et al., 2012).

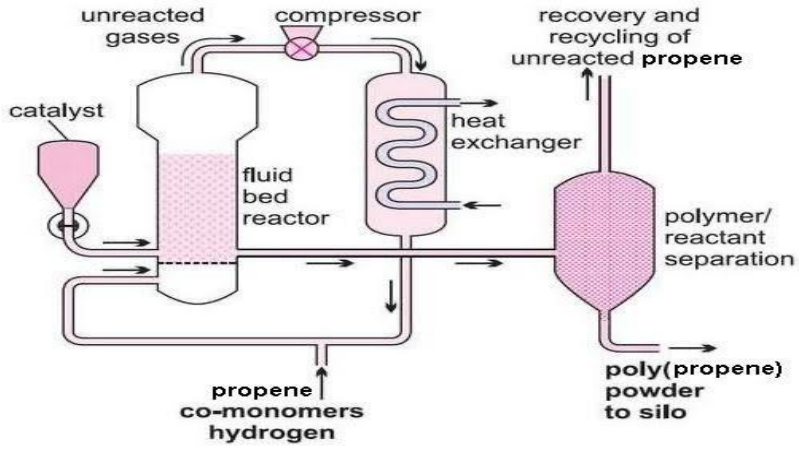

Figure 1: Diagram illustrating the process of PP polymerization

Simulators are valuable assets in these processes as they improve the production and keep a check on changes in the reactors without affecting the real operation thus lowering the time consumed in the operational phase.

2. Propylene Polymerization: Modelling

(Koerner & Koerner, 2018) proposed a model in 2018 in which a liquid monomer steam was continuously passes in a continuous stir tank reactor(CSTR) operating at a high pressure and having three catalysts. This process contains:

- Polymer particles which use propylene liquid as a suspension way.
- Deactivation of the catalyst.
- Additives like trimethyl-aluminum(TEA) and para-ethoxy ethyl benzoate(PEEB).
- A chain transfer agent in the form of hydrogen.

As the reaction is exothermic a top cool condenser is used to manage the temperature of the reactor. As a result three catalyst system was replaces by a single well type known as Ziegler- natta(ZN) which produces polymer with high molecular weight low stiffness(Crawford & Quinn, 2017).

3. Process Model of PP Polymerization

For the better utilization of raw materials a recycle stream was added to the reactor. Then the reactor output stream and unreacted monomer undergo liquid-vapor flash separator. Then the polymer is removed from the and products and Propylene returns to the chamber through recycle stream. This process is really fast so energy produced is not considered and the fresh monomer and recycle stream are at same temperature.

If some more recycling structures are added they may increase the response time, complexity and may make it difficult to find the error causing object. The disturbances not only affect the output of the project but also affect the raw material used in process. Snowball effect causes instabilities in the process(Guvendiren et al., 2012).

This process can be give in the form of equation: m rec= Wm. Ms

Where m rec is mass flow of recycled monomer, ms is slurry output stream And Ws is mass fraction of monomer left in reactor. To decouple the process and to prevent snowball effect from occuring the monomer can be inserted into reactor and thereby considering a lag for First order reaction. An unreacted propylene accumulation tank is used in this process. Reactor feed flow(m comb) can be measured by:

M comb (tk)= mm(tk)+ m rec(tk) .(1-e^-0.005tk)

In this tk is the time instant and mm is the fresh monomer feed rate.

A) Process Control

Control process consist of six controlling loops divided into two hierarchical layers: lower layer for providing stability and upper layer to minimize the effect of disturbances. The equation of this control is :

U(tk)= u(tk-1)+ kc[e(tk)-e(tk-1)+ Ts* e(tk)/Ti

In this equation U(tk) and U(tk-1) is initial variable for instants like K and K-1.Kc is the controller gain and ti is integral time constant. E(tk) and e(tk-1) are the error constants.

B) Emso Model of PP Polymerisation

An EMSO software developed at Federal University of Rio Grande Do Sul was used to simulate the process of PP polymerization. It is easy to handle and operate this software. It is featured by a dynamic simulator which has Dasslc numerical method to solve Algebraic equations and an optimizer. These two are used in simulation of the polymers in chemical and petrochemical processes. This software uses a high level language programming thus making it useful in the fields of research and teaching.

EMSO model does not allow equations to have multiple variables so modification of equation of controllers was required. As a result of which terms like u(tk)- u(tk-1) and e(tk)-e(tk-1) was implemented as first derivatives which were used to modify implementation controller(Vaughan et al., 2012).

4. Results

A) Reactor Feed Stream Control:

To check the effect of mass integration on fresh propylene the initial use of recycle stream was cancelled(m rec=0) making only fresh monomer to feed inside the reactor. So it was observed that 20,000 Kg/h fresh monomer is required to maintain rate of reaction(Shanmuganathan & Ellison, 2014).

Other case is if the fresh monomer is supplied to feed the process of mass recycling while keeping initial conditions same, it is observed that the rate of consumption of the monomer is reduced. So to maintain the rate of 20,000 Kg/h combined fresh and recycled monomer is used.

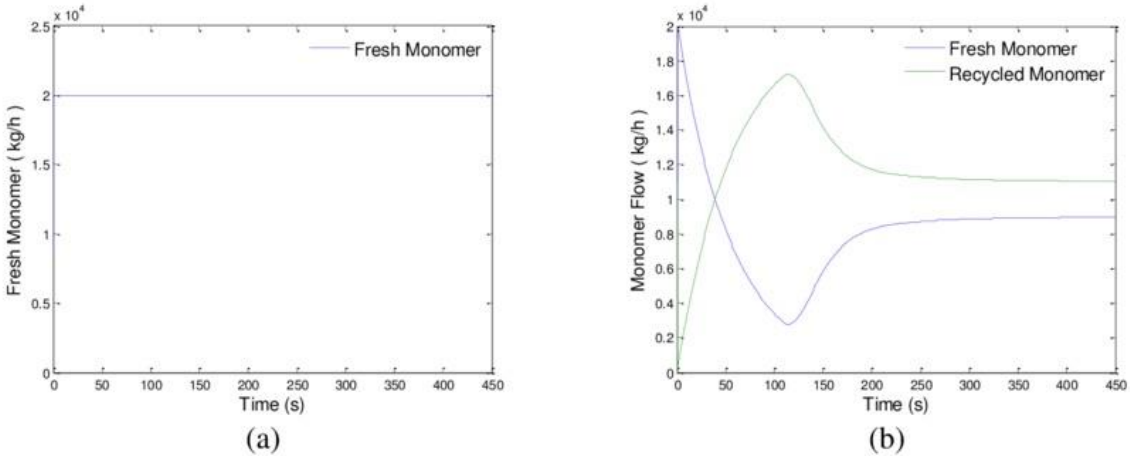

Figure 2: Graphs a depicting monomer stream profile without mass recycle. Graphs b depicting monomer stream profile with mass recycle.

5. Conclusion

In this paper we studied about the polymerization of a PP polymer in polypropylene liquid suspension. The catalyst provide a Kinetic of Ziegler- Natta type. To optimize the production rate and other factors a recycle stream was introduced in the process. To start recycle stream it's controller was tuned. An EMSO software was used for dynamic process.

The EMSO software is coded in high level languages like C++ , C and FORTRAN. When the process is started it is important to make some necessary adjustments so that there is smooth conduction of polymerization.

A recycling structure was proposed for the better utilization of raw materials. By adding a recycle stream the consumption rate of fresh monomer is reduced by 50%. The control of this loop was efficient and yielded better results. The pp polymerization is a step wise process and needs to be handled out carefully. The experiments and the observations conclude that mass integration does not affect the performance of PP polymerization.

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