Investigation of operational parameters effect on quality of HDPE in Ziegler-Natta solution polymerization of ethylene

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In this project, simulation of high-density polyethylene production process was performed using Aspen Polymer software and after comparing the simulation data with experimental values, sensitivity analysis was conducted on operational parameters and the effects of these parameters on system performance were analyzed. PC-SAFT or POLYPCSF thermodynamic model was used for the thermodynamic expression of the system. Comparing the experimental values with simulation data demonstrated that the simulated process can properly show the system's actual behavior. To carry out the sensitivity analysis of the flow rate of the input feed into the first reactor, flow rate of the input feed into the second reactor, temperature and pressure of the first reactor and temperature and pressure of the second reactor were considered as variable and the impact of these changes on the conversion rate in the reactor, the amount of the polymer produced, PDI and Mn of the produced polymer were examined. Studies revealed that increased flow rate reduces the conversion rate and increases the amount of the produced polymer. Further, increased pressure and decreased temperature lead to enhanced conversion rate and thus an increase in the amount of the polymer produced.

Keywords: High-density polyethylene, Aspen polymer, PDI, Mn, conversion rate

INTRODUCTION

Polyethylene (polyethene) is the simplest polymer because two carbon atoms are connected to all carbons of the main chain. This polyethylene is of a thermoplastic type and the reason is that the bonds between nonpolar chains in this polymer are weak. Hence, polyethylene chains can slide over each other by heating and break the London bonds while the strong covalent bonds in the polymer are still maintained. Lateral branchless polyethylene chains can become so close to each other that they make high-density polyethylene. This polyethylene has more strength and flexibility compared to the ordinary polyethylene. Polyethylene is a chain polymer with 104 units or more of ethene. This polymer was accidentally formed in the 1930s when oxygen entered the container of ethene. Initially, the created wax-like white substance was not considered seriously. Subsequent tests showed that this substance has high stability and is a good electricity insulator. This substance was first used as the cable insulator and cover for the radar areas in World War II. Also, it was first applied as an electrical insulator in 1939. Various types of polyethylene have different applications including pipes, packaging fibers, production of plastic materials used in the kitchen, components of chemical plants, toys, bulletproof vests and electrical insulation.

Due to its greater tensile strength and hardness, high-density polyethylene is used in the manufacture of pipes, production of liquids and milk containers and plastic kitchen appliances and many other utensils and containers [1, 2].

Different scholars have worked in the field of polymer processing simulation and have provided various reports in this regard.

Hakim, et al. [3, 4] have carried out the simulation of ethylene polymerization in the slurry phase in steady state with Ziegler–Natta catalyst to produce high-density polyethylene. The results obtained from this simulation have been compared with the data related to the first reactor in High-Density Polyethylene Unit of Arak Petrochemical Complex. The desired model has the ability to predict the production rate, average molecular weight, dispersion index and concentration of monomer, co-monomer and hydrogen inside the reactor. Ethylene polymerization reactors can be placed alongside each other in a sequential or parallel form. For one of the HDPE extrusion grades in Arak Petrochemical Complex, there are two stirred tank reactors in series and the contents of the first reactor go to the second reactor. Since the contents of the second reactor go to the final reactor and the polymerization reaction gets complete in it, hydrogen, monomer, catalyst, co-catalyst and hexane solvent are fed into the first reactor and co-monomer (1 - butene), monomer and solvent are fed

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into the the second reactor. In this way, homopolymer chains with not much molecular mass are produced in the first reactor and turn into copolymer in the second reactor in combination with co-monomer and increase molecular mass. For micro-scale modeling, differential equations were written for all the components inside the reactor and zeroth, first and second moments of growing and dead polymer chains, using kinetic rate constants.

Neeraj et al. [5] also investigated the static and dynamic modeling of the high-density polyethylene process. Experimental data was obtained from two industrial units with a capacity of 144000 ton / year and 240000 ton / year, which reactors of the first unit were placed in series and reactors of the second unit were placed in parallel. In their simulation, they initially determined the parameters of the state equation using the physical properties of pure substances existing in the process. Then, they implemented the processes intended for the simulation using Poymer Plus software. Kinetic constants were calculated using the experimental data provided.

Hakim et al. [8] examined the modeling and simulation of ethylene polymerization process in the slurry phase in three series stirred tank reactors for the production of HDPE, using the Ziegler-Natta catalyst. The catalyst model with several active centers was used for modeling. By analysis of the distribution chart, the molecular weight of the polymer sample was specified and it was concluded that at least six active centers are needed to simulate the wide distribution of molecular weight of the produced polymer. In the adopted method, only the distribution chart of molecular weight of the first reactor was analyzed to optimize the kinetic parameters. After setting the kinetic parameters and optimizing them, it was shown that the obtained model is able to predict the experimental data associated with average molecular weight, molecular weight distribution, production rate and the residence time of the polymer product in the reactors. Using the model, the effect of changes in the flow rate of hydrogen, monomer, co-monomer and flow of impurities on the rate of production and molecular weight distribution was evaluated. An overview of the polymerization process used has been displayed in Fig 8.2.

2. SIMULATION PROCESS

In this paper, simulation of high-density polyethylene production process has been provided using the Ziegler Natta method. To this end, the production process has been initially presented by drawing flow diagrams and expressing the operating conditions of the equipment.

2.1 Production process

In different resources, high-density polyethylene production process from the polymerization of ethylene has been stated [6, 3, 5, 7]. The intended process in this project for the solution polymerization of ethylene has been shown in Fig 3.1. In this process, the feed flow with the specified properties initially enters into the reactor of CSTR type. This reactor acts at a temperature of 160 ºC and pressure of 200 atm. In the reactor, sufficient retention time is given to the materials so that the polymerization operation is performed in the presence of Ziegler-Natta catalyst which is $TiCl_4$ in this project. Next, the output current is sent from the first reactor to the second reactor to complete the polymerization operation and increase the conversion rate. Along with this flow, another feed flow with specific percent composition enters into the second reactor. Operating conditions and performance of this reactor are similar to the first reactor. The output current from the second reactor contains polymer, solvent, unreacted gases and used catalyst. This flow is sent to the separator drum so that the produced polymer is separated from other materials existing in the stream. Separation in this drum is done by reducing the pressure, which by doing this, unreacted gases are separated from the produced polymer and are removed from the top of the drum and are returned to the beginning of the process. The polymer produced as the final product is sent from the bottom of the tower to packaging and storage.
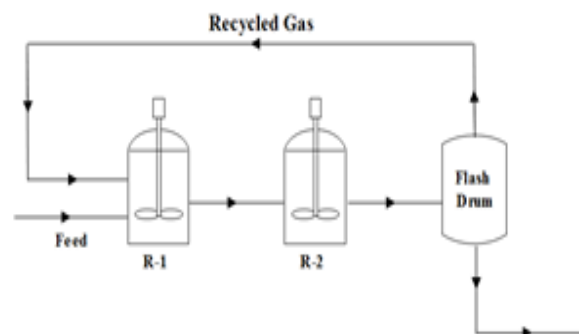

Fig 1: Flow diagram of HDPE production process

2.2 Ziegler-Natta processes

These are the processes in which the catalysts first discovered by two people named Ziegler and Natta are used. Processes of producing high-density polyethylene, linear low-density polyethylene and polypropylene use this kind of catalyst. Operating conditions of production in these processes are lower compared to the operating conditions of low-density

polyethylene production. Operating pressure in these processes is in the range of 10-80 atm and operating temperature ranges from 80-110° C. However, in some cases of solution polymerization, the pressure may increase up to about 200 atm and the temperature may rise up to about 250° C.

2.3 Process simulation in Aspen Plus software

This software is a set of software from Aspen tech-company. This company has offered several software programs to the market in the field of simulation and modeling of processes, their economic evaluation, engineering designs and so on for different uses. Aspen Polymer module is among the subset of process simulation software of this company. Different versions of this software are available in the market. In this project, Aspen Polymer 7.2 has been applied. For process simulation using this software, the process flow diagram should be first determined and after entering the necessary data for simulation and running the program, the results will be visible. To carry out simulation in the mentioned software, the steps below should be followed:

2.3.1 Definition of components

The first step in simulation using this software is the definition of the components existing in the simulation. The list of the materials defined in this simulation to evaluate the process is as follows:

Table 1: Software-defined materials list

Component ID	Type	Component name	Formula
TICL4	CONV	TITANIUM-TETRACHLORIDE	TICL4
TEA	CONV	TRIETHYL-ALUMINUM	C6H15AL
C2H4	CONV	ETHYLENE	C2H4
H2	CONV	HYDROGEN	H2
HEXANE	CONV	N-HEXANE	C6H14-1
HDPE	POLYMER	HIGH-DENSITY-POLY(ETHYLENE)	HDPE
C2H4-R	SEGMENT	ETHYLENE-R	C2H4-R

In the software applied, additional information should be included for the substances whose type is not selected as conventional so that the substance can be identified by the software. In this project, this information should be entered for the two substances which have been defined as the ethylene and polymer segment of HDPE. For the segment, its type should be entered, which the Repeat type was chosen for this segment. For HDPE, the type of polymer production should be selected, which in this project, Ziegler-Natta method was chosen.

2.3.2 Thermodynamic model

Selection of the appropriate thermodynamic model to calculate physical properties is essential. Thermodynamic behavior and physical properties of polymeric systems are much more complex than conventional systems. Relationships of this section are generally divided into equations of state and activity coefficient models. Equations of state are the relations that provide the system pressure equation as a function of solution volume and temperature and activity coefficient models are the relations used to calculate the correction factor of Raoult's law which has been provided assuming the solution as ideal [8].

In this project, PC-SAFT or POLYPCSF equation of state has been used for the thermodynamic expression of the system [9, 10]. This equation of state has been presented based on the perturbation theory of chain molecules. Gross and Sadowski argued that PC-SAFT equation of state better predicts the thermodynamic properties of pure substances and mixtures compared to the SAFT equation itself [11, 12].

PC-SAFT equation of state like SAFT equation of state and other chain state equations which are based on the perturbation theory is expressed based on the total of the reference mode and perturbation distribution of Helmholtz free energy. This expression is provided as the following equation:

$$\frac{A^{res}}{NkT} = \frac{A}{NkT} - \frac{A^{ig}}{NkT} = \frac{A^{ref}}{NkT} + \frac{A^{pert}}{NkT} \qquad (1)$$

In the above equation, A is the total Helmholtz free energy; N is the total number of molecules; K is Boltzmann's constant and T is the absolute temperature. Overall, the reference term existing in the equation states the distribution of repulsive forces and perturbation term is due to the existence of forces of attraction. In PC-SAFT equation, chain

fluid with hard pellets has been selected as the reference fluid. Thus, the reference term in equation 1 states the characteristics of chain fluid with hard pellets, which this section is similar to SAFT equation of state. These parameters include the number of segments (m), diameter of segments (σ) and the energy of each segment (ε /k). According to PC-SAFT theory, the number of segments (m) is directly proportional to the size of molecules (molecular weight). Values of these three parameters are usually available in data bank of the software. But if they do not exist or it is necessary to carry out the simulation more accurately, the values of the parameters of the intended state equation are determined using the regression of physical properties of each material. In the present project, given that ethylene, high-density polyethylene and $TiCl_4$ and TEA catalysts are the main substances in simulation, the values of these three parameters were determined using the regression of physical properties. The values specified for these three parameters have been reported in Table 2. The determined values should be entered by the user into the desired section in simulation so that the software can use these values in its calculations.

Table 2. Included values of the parameters of PC-SAFT state equation.

	$TiCl_4$	TEA	Ethylene	HDPE
r	0.0333	0.0333	0.0544	0.0535
$\epsilon/k(K)$	236.770	236.770	181.331	245.342
$\sigma(A°)$	3.798	3.798	3.488	3.782

2.3.3 Definition of reaction

The next step is the definition of the reactions performed in the system. The model that states the reactions occurred in Ziegler-Natta systems has been reported in various articles [12]. Although a lot of mechanisms have been stated for this purpose, the mechanism that accurately expresses the kinetic behavior of Ziegler-Natta systems has not been reported so far.

Rate of each reaction is equal to the product of the concentrations of reactants and reaction rate constant. To calculate the constant of each reaction, modified Arrhenius equation which considers the dependence of temperature and pressure is used.

$$k^k = k_o^k exp\left[-\frac{Ea^k}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right]$$

In the above equation, K_0 is the reaction constant whose unit is equal to 1/sec for the first order reactions and m3/kmol-sec for the second order reactions. Ea is the activation energy; P is the reaction pressure, R is the universal gas constant and T_{ref} is the reference temperature. Types of reactions defined in this process have been presented in the table below. The number of these reactions is 8. On the other hand, 4 types of active sites were considered for each catalyst and all of these reactions occur on each of the active sites of the catalyst and each has its own special kinetic speed. Therefore, 32 reactions were totally defined for this system. Type of the reactions defined for each active site has been provided in Table 3.

Table 3: Types of the reactions defined in the software for HDPE production process

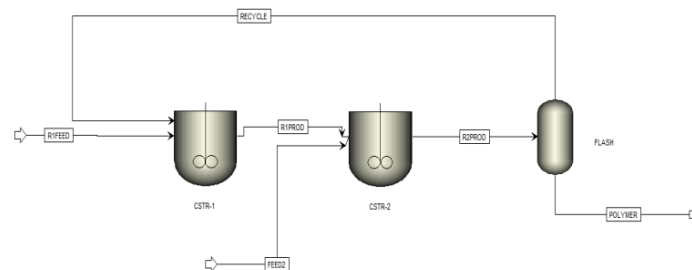| Reaction type	Reaction
Site Activation by cocatalyst	$C_{ps} + A_m \rightarrow P_0^k$
Spontaneous site activation	$C_{ps} \rightarrow P_0^k$
Chain initiation	$P_0^k + M_i \rightarrow P_{\delta_i}i$
Propgation	$P_{n,j}^k + M_i \rightarrow P_n + \delta_i i$
Chain transfer to hydrogen	$P_{n,j}^k + H_2 \rightarrow D_n^k + P_0^k$
Chain transfer to monomer	$P_{n,j}^k + M_i \rightarrow D_{n-}^k + P_0^k$
Spontaneous chain transfer	$P_{n,j}^k \rightarrow D_{n-}^k + P_0^k$
Spontaneous site deactivation	$P_0^k \rightarrow C_{ds}$
	$P_{n,j}^k \rightarrow C_{ds} + D_n^k$

Fig 2. Flow diagram drawn in the software for the process simulation.

2.3.4 Drawing flow diagram

The next step includes the drawing of flow diagram and step by step simulation of the process. The general flow diagram drawn has been displayed in Fig 2. In this Fig, CSTR-1 and CSTR-2 reactors are polymerization reactors in which the reactions mentioned in the previous section are performed. Flash block is used at the end of the process to separate the produced polymer from unreacted gases and solvents. Calculations of this block in the software are based on the phase equilibrium. Unreacted gases along with the solvent are returned to the beginning of the process.

3. SIMULATION RESULTS

In this paper, the results obtained from simulation have been discussed in two sections. First, the results of simulation have been compared with the experimental data. Then, sensitivity analysis was conducted based on the simulation carried out and the influence of different parameters on the production rate and quality of the produced polymer was examined.

3.1 Comparing the experimental data with simulation

In this section, the results obtained from the initial simulation carried out have been compared with different experimental data. Experimental data has been obtained from various articles in this regard [1, 3, 5, 7]. The comparisons made have been displayed in Fig 3 and 4. In Fig 3, the amount of production of various grades has been compared with the data obtained from simulation. With respect to the chart of Fig 3, it can be observed that the simulation conducted provides an accurate prediction of the amount of the produced polymer in different modes. The rate of relative error calculated for different modes is between 1% and 2%, which is acceptable. In Fig 4, the experimental data related to the amount of average molecular weight has been compared with the data obtained from simulation. By studying the chart of this Fig, it can be concluded that the investigated simulation has had a relatively accurate prediction of the amount of this parameter. The average relative error calculated in this mode is between 2% and 3% for various modes, which is acceptable. Hence, it can be generally concluded that the simulation carried out has provided a relatively accurate prediction of the behavior of actual processes and can be used with great accuracy for engineering applications.

3.2 Sensitivity analysis

According to the simulation conducted, the sensitivity analysis was performed for different parameters in simulation. The results of different examinations are as follows.

3.2.1 Investigating the effect of flow rate of the input feed into the first reactor

In an industrial unit, it is possible that changes take place in the flow rate of the input feed into the unit for various reasons. Thus, the flow rate of the input feed into the first reactor was initially changed in a predetermined range and impacts of this change on the conversion rate in the first reactor, conversion rate in the second reactor, the overall conversion rate of the unit, the final amount of the produced polymer, PDI and M_n of the produced polymer were assessed. The results of the studies conducted have been provided in Fig 5 and 6.
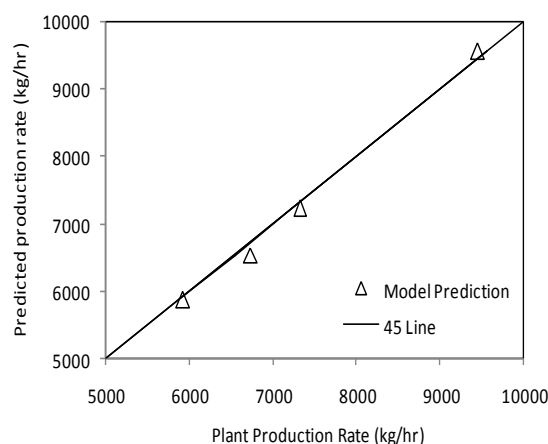

Fig 3: Comparing the experimental data with the values of simulation for HDPE production rate.
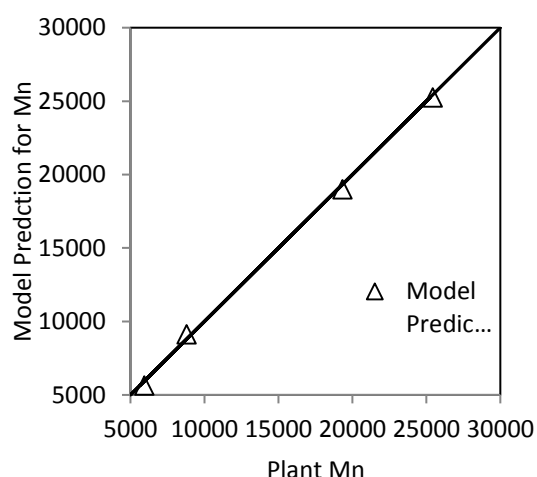

Fig 4. Comparing the experimental data with the values of simulation for M_n of the produced polymer.

In Fig 5, changes in the conversion rate in the reactors and the overall conversion rate of the unit with the changes in the input flow rate have been

shown. As can be seen in the chart, the conversion rate in the reactors has decreased with an increase in the flow rate, which can be due to the fact that with increased flow rate, greater amount of ethylene enters into the reactor and the rate of unreacted ethylene increases. Hence, the conversion rate has been reduced. In Fig 6, the changes in the amount of the produced polymer along with the changes in the rate of the input feed into the unit have been displayed. As is clear from the chart, the amount of the polymer produced has increased with an increase in the input feed into the first reactor, which is an expected phenomenon. So, it should be considered that with an increase in the rate of the input feed into the unit, the amount of the polymer produced increases despite decreasing the conversion percentage. In Fig 7, the effect of changes in the input flow rate on the PDI rate of the produced polymer has been shown. As can be observed in the chart, with increased flow rate of the input feed into the unit, PDI of the polymers produced in the first and second reactors increases, which has a negative impact on the quality of the polymer produced. In polymer processes, it is desirable that movement be made towards the PDI equal to 1, which in this state, all the chains of the produced polymer will have the same length and there will be no dispersion in the chains. However, despite the increase in PDI of the produced polymer, its amount is not to the extent that it is considered to be unacceptable. In Fig 8, it is determined that with increased input feed into the first reactor, the M_n rate of the produced polymer in the first reactor decreases. In other words, the produced polymer will have a shorter chain, but M_n of the produced polymer in the output of the second reactor which is the amount of the final M_n increases and polymer chains with greater length are formed. This can lead to increased strength of the produced polymer.
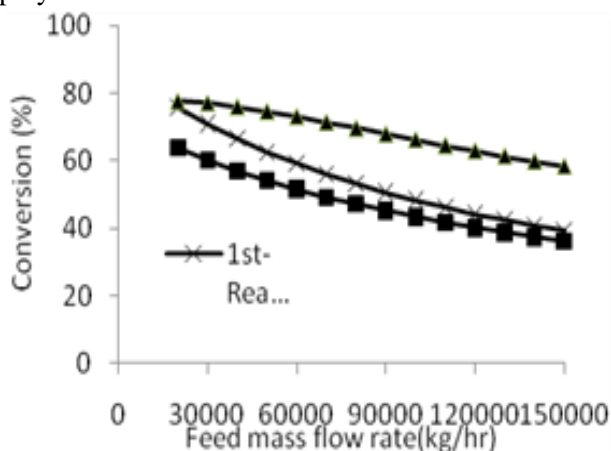

Fig 5. Examining the effect of changes in the input feed into the first reactor on the conversion rate in the reactors.
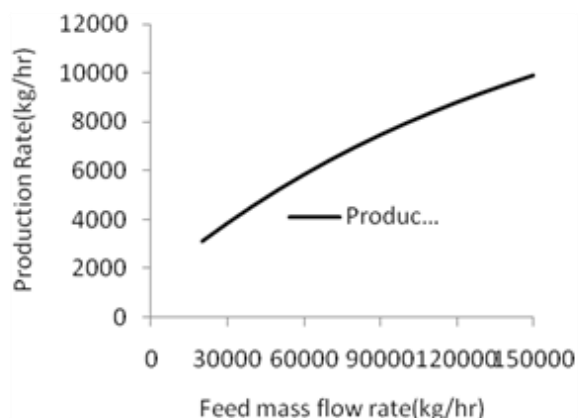

Fig 6. Examining the effect of changes in the input feed into the first reactor on the rate of HDPE produced
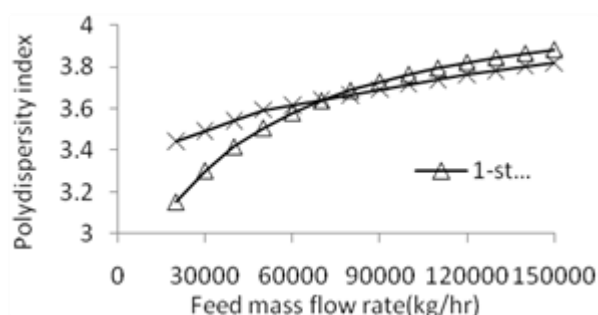

Fig 7. Examining the effect of changes in the input feed into the first reactor on PDI
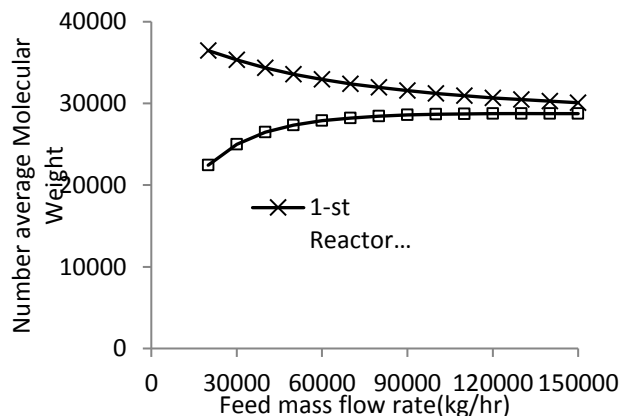

Fig 8. Examining the effect of changes in the input feed into the first reactor on M_n of the produced polymer.

3.2.2 Investigating the impact of the flow rate of the input feed into the second reactor

In this section, the results obtained from the changes in the flow rate of the input feed into the second reactor on the conversion rate, the amount of the produced polymer, PDI and M_n of the polymer have been provided. The results of these investigations have been shown in Fig 9 and 10.

In Fig 9, the effect of changes in the flow rate of the feed in the second reactor on the conversion rate

in the reactors has been displayed. As expected, these changes did not make any impact on the conversion rate in the first reactor. But similar to the previous state, the conversion rate of the second reactor and the overall conversion rate of the reactors have decreased with an increase in the amount of feed, which can be due to increased unreacted ethylene in the output current. In Fig 8.4, the amount of the produced polymer with increased feed of the second reactor has been displayed. As expected, in this state, the rate of polymer production has increased almost linearly with an increase in the amount of feed. Fig 11 shows the changes in PDI of the polymer produced in this state. As expected, changes in the input feed into the second reactor do not have any impact on PDI rate of the produced polymer. But similar to the previous state, they increase the PDI rate of the produced polymer in the second reactor which is the final PDI of the produced polymer. This has a negative impact on the process. Fig 12 shows the changes in M_n of the produced polymer in this state. Similar to the previous states, these changes have not made any impact on the M_n rate of the polymer produced from the first reactor. But they have reduced the amount of the final M_n of the polymer. In other words, they caused to form polymers with shorter chain length.
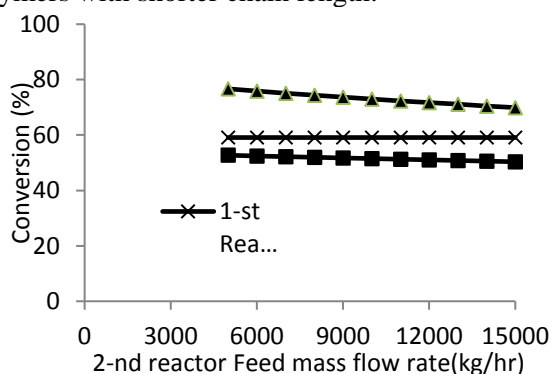

Fig 9. Examining the effect of changes in the input feed into the second reactor on the conversion rate in the reactors.
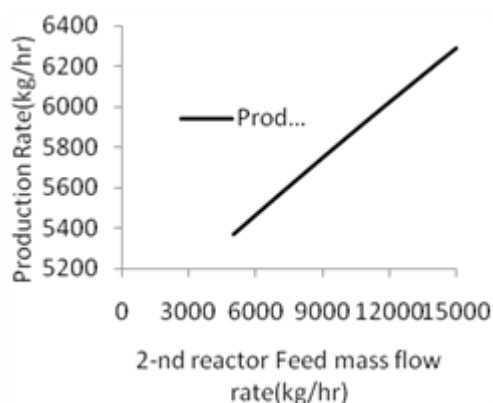

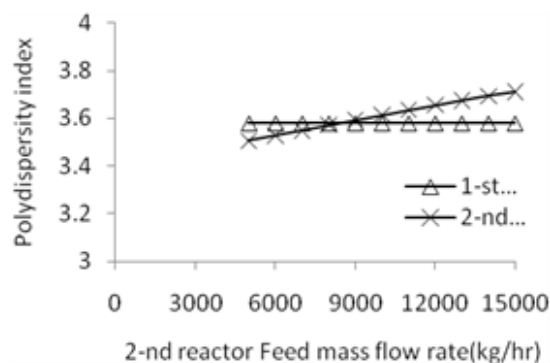**Fig 10.** Examining the effect of changes in the input feed into the second reactor on the rate of HDPE produced.

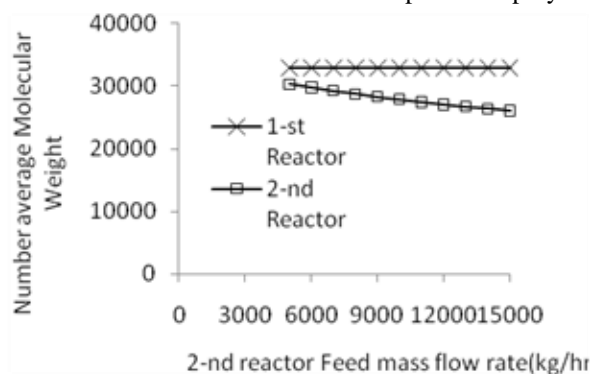**Fig 11:** Examining the effect of changes in the input feed into the second reactor on PDI of the produced polymer.

Fig 12. Examining the effect of changes in the input feed into the second reactor on M_n of the produced polymer.

3.2 Investigating the impact of changes in temperature and pressure of the first reactor

Temperature and pressure are among the most important operating parameters and examining the influence of their changes on the process behavior of the system is of crucial importance. In this section, temperature and pressure of the first reactor were changed in the determined range and its effect on the overall conversion rate of the process, the amount of the produced polymer, M_n and PDI of the produced polymer was analyzed. The obtained results have been presented in Fig 13 and 14. In Fig 13, the impact of simultaneous changes in pressure and temperature on the conversion rate has been displayed. As is clear from the Fig, increased pressure and decreased temperature have positive effects on the overall conversion rate of the reactor and increase it. Therefore, by remaining other operating parameters as constant, working in high pressure and low temperature is recommended to increase the conversion rate. Examining the effects of changes in pressure and temperature on the production rate is exactly similar to the previous state. Since the amount of input feed is constant in this state, the amount of the polymer produced will increase with an increase in the conversion rate. Thus, the process of changes in the amount of polymer production along with the changes in

pressure and temperature shown in Fig 14 is similar to the previous state. By studying the charts in Fig 15 and 16, it becomes clear that increased pressure and decreased temperature reduce the PDI rate of the produced polymer and increase the amount of M_n. Hence, it can be said that overall, an increase in pressure and a reduction in temperature will have positive effects on the system's performance and efficiency.

3.2.2 Investigating the impact of the flow rate of the input feed into the second reactor

In this section, the results obtained from the changes in the flow rate of the input feed into the second reactor on the conversion rate, the amount of the produced polymer, PDI and M_n of the polymer have been provided. The results of these investigations have been shown in Fig 9 and 10.

In Fig 9, the effect of changes in the flow rate of the feed in the second reactor on the conversion rate in the reactors has been displayed. As expected, these changes did not make any impact on the conversion rate in the first reactor. But similar to the previous state, the conversion rate of the second reactor and the overall conversion rate of the reactors have decreased with an increase in the amount of feed, which can be due to increased unreacted ethylene in the output current. In Fig 8.4, the amount of the produced polymer with increased feed of the second reactor has been displayed. As expected, in this state, the rate of polymer production has increased almost linearly with an increase in the amount of feed. Fig 11 shows the changes in PDI of the polymer produced in this state. As expected, changes in the input feed into the second reactor do not have any impact on PDI rate of the produced polymer. But similar to the previous state, they increase the PDI rate of the produced polymer in the second reactor which is the final PDI of the produced polymer. This has a negative impact on the process. Fig 12 shows the changes in M_n of the produced polymer in this state. Similar to the previous states, these changes have not made any impact on the M_n rate of the polymer produced from the first reactor. But they have reduced the amount of the final M_n of the polymer. In other words, they caused to form polymers with shorter chain length.
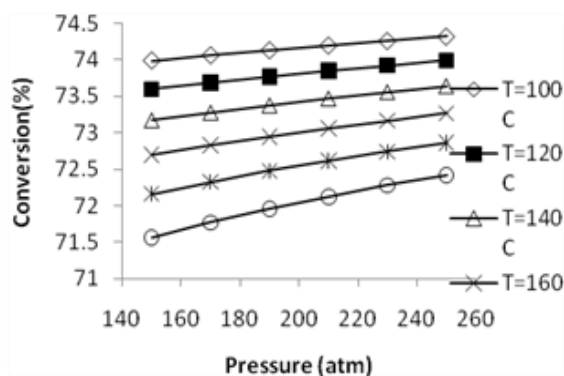

Fig 13. Examining the effect of changes in pressure and temperature of the first reactor on the conversion rate in the reactors.
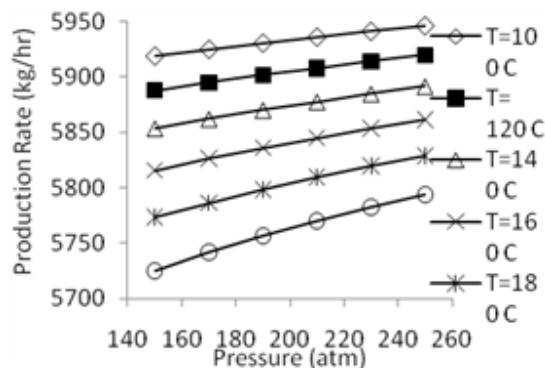

Fig 14. Examining the effect of changes in pressure and temperature of the first reactor on the amount of HDPE produced.
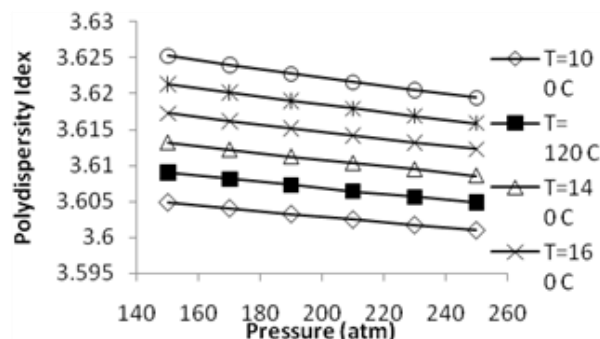

Fig 15. Examining the effect of changes in pressure and temperature of the first reactor on the PDI rate of the produced polymer.
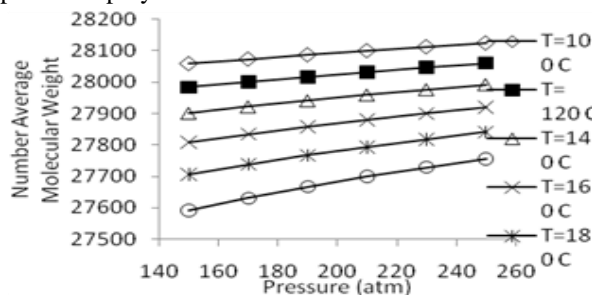

Fig 16. Examining the effect of changes in pressure and temperature of the first reactor on the M_n rate of the produced polymer.

3.3 Investigating the impact of changes in temperature and pressure of the second reactor

The effect of changes in the amount of operating parameters of temperature and pressure in the second reactor on the conversion rate of the reactor, the amount of the polymer produced, PDI and M_n of the produced polymer was also analyzed and the results in this state have been shown in Figs 15.4 and 18.4. Effects of these changes are similar to the state of the first reactor and only in this state, the values of increasing and decreasing the parameters are different compared to the previous state.
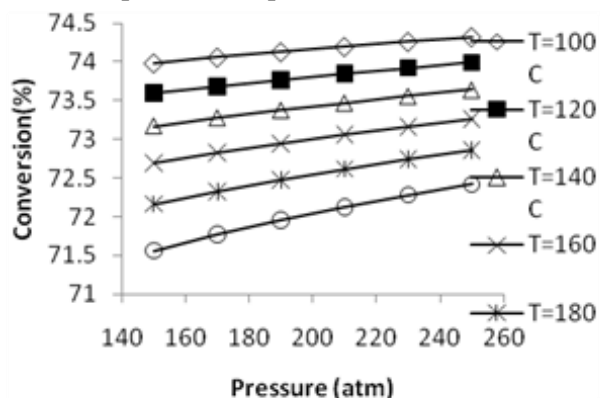

Fig 17. Examining the effect of changes in temperature and pressure of the second reactor on the conversion rate in the reactors.
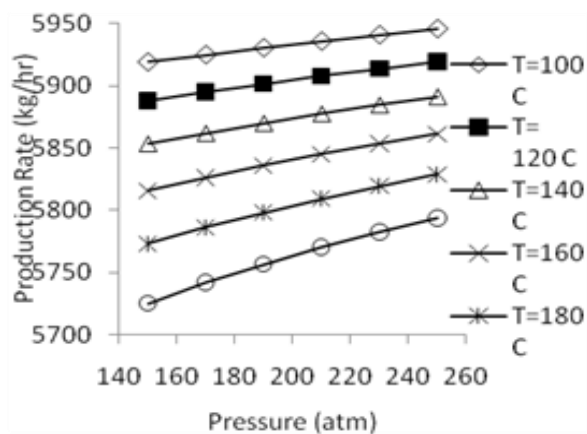

Fig 18. Examining the effect of changes in temperature and pressure of the second reactor on the amount of HDPE produced.
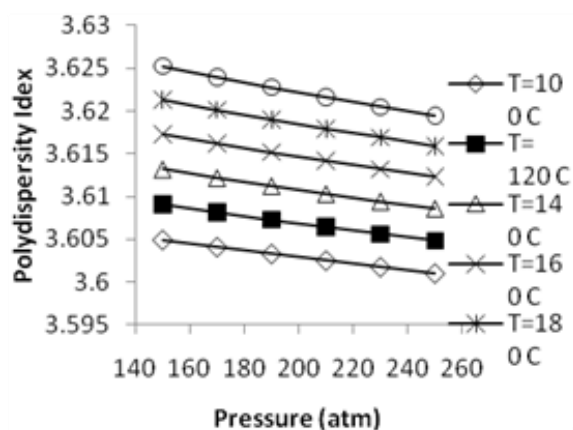

Fig 19. Examining the effect of changes in temperature and pressure of the second reactor on the PDI rate of the produced polymer.

3.4 Investigating the impact of temperature and pressure of separation operation

In the final flash drum, the produced polymer is separated from unreacted ethylene gases and the solvent used which is hexane. Temperature and pressure are among the effective parameters of the separation operation. In this section, the temperature was changed from 100° C to 175° C and the pressure was changed from 2 atm to 16 atm and the impact of these changes on the retrieval rate of ethylene and hexane which are respectively the unreacted gas and solvent used was evaluated.

In Fig 19.4, the effect of simultaneous changes in temperature and pressure on the retrieval rate of ethylene has been displayed. In Fig 20.4, the effect of simultaneous changes in temperature and pressure on the retrieval rate of hexane has been shown.

As is evident in both charts, at a constant temperature, the amount of retrieval is reduced with increased pressure, which is an expected phenomenon because increased pressure enhances
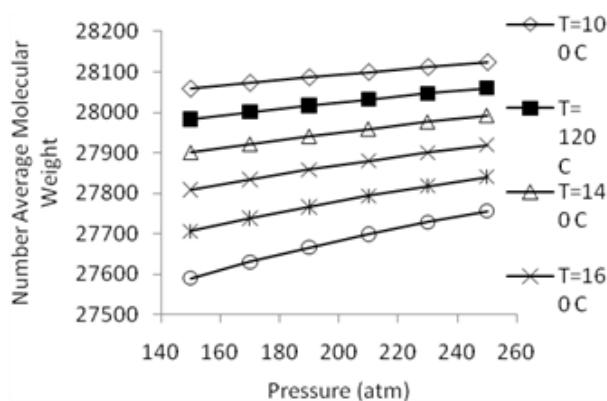

Fig 20. Examining the effect of changes in temperature and pressure of the second reactor on the M_n rate of the produced polymer.

the solubility of the unreacted gas in the polymer, which causes to reduce the rate of retrieval. On the

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other hand, at constant pressure, increased temperature has a positive effect on the rate of retrieval and increases it, which is an expected phenomenon since increased temperature reduces the solubility of gas in liquid. So, separation operation is better to be done at high temperature and low pressure to enhance the retrieval of unreacted gases and the solvent used. This makes the produced polymer more pure.
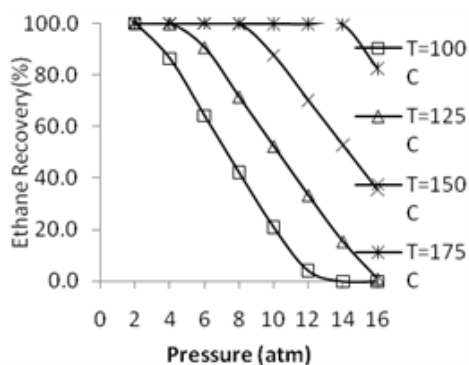

Fig 21. Examining the effect of changes in temperature and pressure of the separation operation on the retrieval rate of ethylene.

- Increasing the input feed into the first reactor reduces the conversion rate but increases the amount of the produced polymer. On the other hand, it increases PDI and M_n of the polymer.
- Increasing the flow rate of the input feed into the second reactor has no effect on the function of the first reactor. On the other hand, it reduces the overall conversion rate and increases the amount of the produced polymer. Besides, it enhances PDI and decreases the rate of M_n.
- Increased pressure and decreased temperature of the reactor increase the conversion rate and the amount of the polymer produced. Additionally, these changes reduce the PDI rate of the produced polymer and increase the rate of M_n.
- Increased pressure and decreased temperature of the second reactor also have the same effects as the changes in the temperature and pressure of the first reactor and the only difference with the changes of the first reactor is in the changed values.
- Separation operation is better to be performed at high temperature and low pressure because this makes the produced polymer more pure.

4. CONCLUSION

The overall results of the project can be expressed as follows:

- By having detailed information of ethylene polymerization process, one can accurately predict the performance of the polymerization system using Aspen Polymer software.
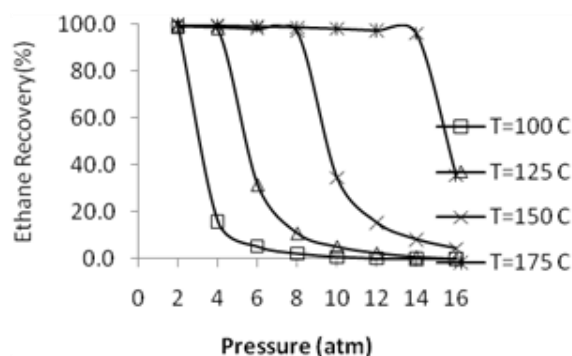

Fig 22. Examining the effect of changes in temperature and pressure of the separation operation on the retrieval rate of hexane.

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