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Modeling of Fixed-Bed Reactor for Hydrogenation of Acetylene in the Olefin Unit's

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Abstract. During this investigation, modeling of fixed-bed reactor for hydrogenation of acetylene was performed on the basis of the pseudo-homogeneous model and adiabatic process. The current mass and energy equations were solved by using a numerical approach. Subsequently, in order to show the advantages of the model, the results were compared with the real values of an industrial reactor. Results show that the temperatures obtained agreed well with the real temperatures of operation. Modeling for both cases of plug and dispersed flows have been presented. Also, the results show that the model predicted less ethylene formation for plug flow in comparison with the dispersed flow. This can be explained by the existence of any phenomena which lead to mixing that occurs in the verse direction. In addition, plug flow converted more acetylene in comparison with the dispersed flow.

Keywords: fixed-bed reactor, hydrogenation, numerical approach, pseudo-homogeneous model, catalytic reaction**.**

1. Introduction

Fixed-bed reactors are including one or more tube filled with catalyst particles and work vertically. Small amount of acetylene is harmful to the catalyst used in polymerization. Therefore, the acetylene in the ethylene stream must be hydrogenated in fixed-bed reactors at Olefin units. Modeling of fixed-bed reactors were carried out using two methods of heterogeneous and pseudo-homogeneous. Modeling of heterogeneous is able to give us satisfied results. However, the difficulty of solving lots of nonlinear equation is the main problem of this method. Therefore, solving equations in pseudo-homogeneous model is easier, but the results are not accurate compared to heterogeneous model. Modeling of fixed-bed reactor is one of the attractive researches for chemical engineers. Various researches are available for modeling of fixed-bed reactors, including: Szukiewicz and coworkers [1], studied the modeling of fixed bed reactor for selective hydrogenation of acetylene. De Smet and coworkers [2], the design of adiabatic fixed-bed reactors for the partial oxidation of methane to synthesis gas. Gobbo and coworkers [3], modeling and optimization of a front-end system for acetylene hydrogenation reactors. Authayanunand coworkers [4], modeling of an industrial fixed-bed reactor based on lumped kinetic models for hydrogenation of pyrolysis gasoline. Mostoufi and coworkers [5], hydrogenation of acetylene kinetic studies and reactor modeling. Current research considered modeling of fixed-bed reactor for hydrogenation of acetylene on the basis of the pseudo-homogeneous model and adiabatic process. Results were compared with hydrogenation reactor of Jam petrochemical company.

2. Numerical Assessment

2.1.Numerical Procedure

For the modeling of fixed-bed reactor, given the pseudo-homogenous reactions to it, the energy and mass equations of the system should be extracted appropriately for fluid and solid phases existing in the system. Given an established Plug flow (plug model), energy and mass equations of the system are as follows [5]-[7]:

$$u\frac{dC_i}{dz}=\rho_c\frac{1-\varepsilon}{\varepsilon}r_i \tag{1}$$

$$\frac{F}{A}C_P\frac{dT}{dz}=\rho_c\frac{(1-\varepsilon)}{\varepsilon}\sum\Delta H_i r_i \tag{2}$$

When the dispersion of the gas phase is considered (dispersed model), mass equation is as follows:

$$\frac{D_i}{u}\frac{d^2C_i}{dz^2}-\frac{dC_i}{dz}+\frac{\rho_c(1-\varepsilon)}{\varepsilon u}r_i=0 \tag{3}$$

Since the thermal dispersion coefficient is very small compared to the mass dispersion coefficient, the energy equation has been constant.

The boundary layer conditions necessary to solve simultaneous equations of mass and energy are as follows:

$$z=0;\ C_{i_0}=-\frac{D_i}{u}\left(\frac{\partial C_i}{\partial z}\right)_{z=0^+}+C_i(0^+,t) \tag{4}$$

$$z=L;\ \frac{\partial C_i}{\partial z}=0 \tag{5}$$

Temperature and concentration profiles of system can be achieved by solving mass and energy equations by utilization of the specified boundary layer conditions. Kinetic equations are as follows [5], [8]:

$$r_{C_2H_2}=\frac{k_1 p_{C_2H_2}p_{H_2}}{\left(1+k_2p_{C_2H_4}\right)\left(1+k_3p_{H_2}\right)} \tag{6}$$

$$r_{C_2H_6}=\frac{k_4 p_{C_2H_4}p_{H_2}}{\left(1+k_5p_{C_2H_4}\right)^{1.25}\left(1+k_6p_{H_2}\right)} \tag{7}$$

Table 1 indicated a list of related parameters to the hydrogenation reactor of Jam petrochemical company. Values are obtained by examination and manufacturer submitted evidences.

Table 1: catalyst properties and boundary layer conditions

No.	Specification
1	Size and Shape: 2-4 mm sphere
2	Density of catalyst: 1400 kg/m^3
3	Pd content (ppm): 300 with support Al_2O_3
4	Volume of particle : Vp=1.414*10^-3 m^3
5	Heat capacity of catalyst: C_S = 1000 j/kg K
6	Thermal conductivity of catalyst: Ks=0. 28211 w/m.k
7	Porosity of bed: ε=40%
8	Heat capacity of gas: Cpg (500 °C & 1bar) = 38.13 j/mol K
9	Density of gas: ρ g (480° C & 1 bar) = 0.65 kg/m^3
10	Bulk density: ρ B=720 kg/m^3
11	Reactor diameter: D = 3.92 m
12	Length of reactor: z = 3.35 m

2.2.Validation of a Numerical Model

The presented pseudo-homogeneous model is solved for simulation of acetylene hydrogenation reactor with desired conditions and utilization of parameters listed in Table 1. Results of simulation compared with actual amounts of industrial hydrogenation reactor and it can be seen in Fig. 1.

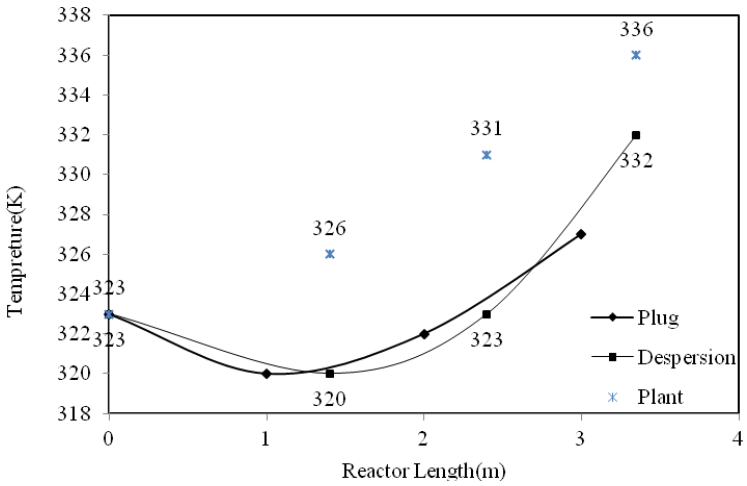

Fig. 1: Comparison of temperature changes derived from the model with industry reactor

As it can be seen, the results are well predicted by the model used in the experiment and temperature results are so close to operation condition results. Therefore, for other parameters, output data are available only. However, results of simulation compared with industrial hydrogenation, also relative errors between the calculated values and industry are shown in Table 2.

Table 2: relative errors between calculated values and industry

10%	Ethylene formation
8%	Ethane (Mol %)
6%	Acetylene (Mol %)
10.6%	Hydrogen (Mol %)

3. Result and Discussion

Important parameters in hydrogenation process are included: bed temperature, acetylene conversion and ethane and ethylene formation.

3.1. Bed Temperature

In order to prevent structural damage to the catalyst, it is important that the bed temperature should not exceed a specified and desirable temperature which is also the maximum permissible temperature of the catalyst. In Fig. 1, the reactor temperature profile obtained from this study was compared with the temperature of industrial acetylene converter units.

3.2. Acetylene Changes

The purpose of the reactor is reduced of acetylene in ethylene production. In Fig. 2, the level of acetylene changes has been shown along the reactor. As can be seen in Fig. 2, only half of acetylene is removed in the first bed and the residue conversion must be done in a second bed. Thus, the length of the reactor is not sufficient to complete the reaction. Also, the amount of acetylene output of the reactor in plug flow is less than the dispersed flow. In other words the conversion of acetylene in plug flow is more than dispersed flow.

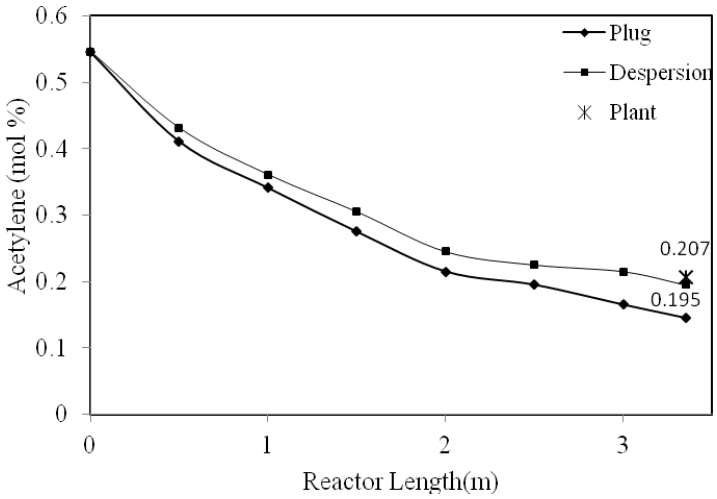

Fig. 2: Concentration variation of Acetylene the length of the reactor

3.3. Ethylene and Ethane Formation

As it can be seen in the Fig. 3 and Fig. 4, plug flow forecasted less ethylene and ethane formation compared to dispersed flow and it is because of existence some phenomena which lead to mixing occurs in the verse direction.

$$X_{C_2H_4} = \frac{F_{C_2H_4} - X_{C_2H_4(in)}}{F_{C_2H_4(in)}} \quad (8)$$

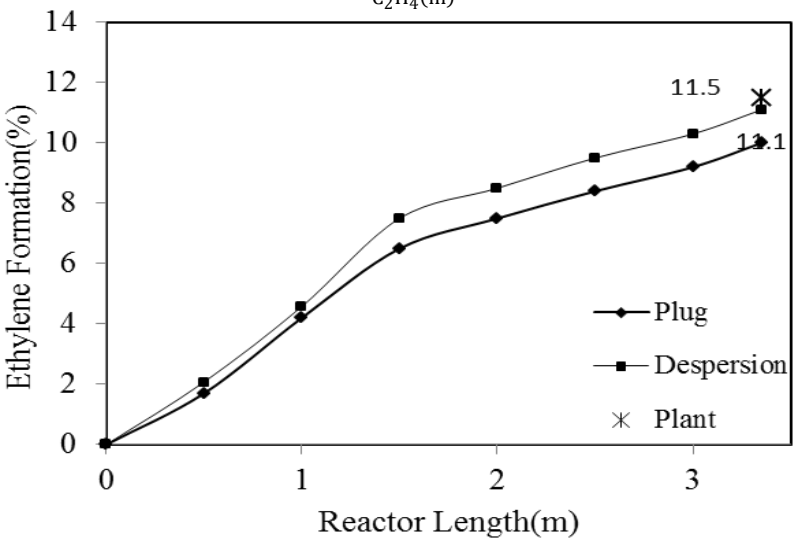

Fig. 3: Ethylene formation vs reactor length

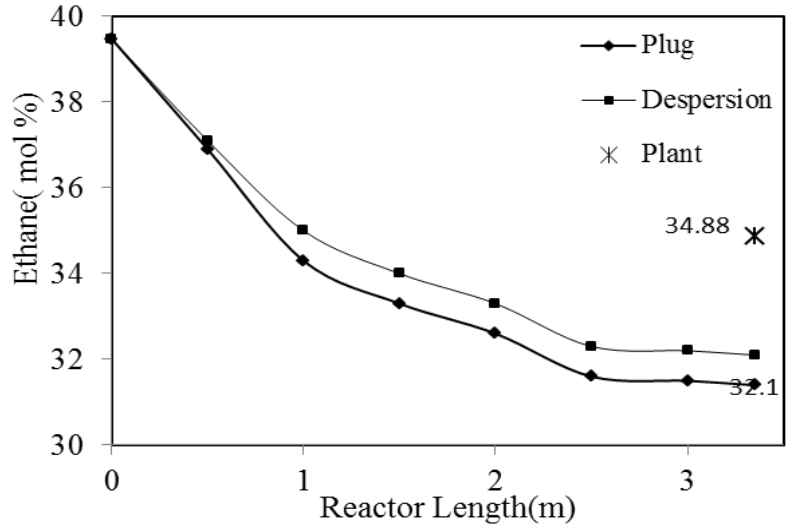

Fig. 4: Ethane formation vs reactor length

4. Conclusion

As it can be seen in this research, the results are well predicted by the model used in the experiment and temperature results are so close to operation condition results. So that the results of both cases of plug and dispersed flows are shown less ethylene and Ethane formation for plug flow in comparison with the dispersed flow, on the other hand, plug flow converted more acetylene in comparison with the dispersed flow.

5. References

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