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EFFECT OF BACK MIXING ON THE PERFORMANCE OF TUBULAR-FLOW REACTORS

[1,2]Selahattin Gültekin and [1]Alimzhan Kalbekov

[1]Kyrgyz-Turkish Manas University, Chemical Engineering Department -Bishkek, Kyrgyzstan
[2]Uskudar University, Bioengineering Department-Istanbul, Turkey

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ABSTRACT

In chemical reaction engineering; *Plug-Flow-Reactor* (PFR) and *Continuous-Stirred-Tank-Reactor* (CSTR) are ideal reactors and are based on extremely simplified assumptions. One can predict the performance of these ideal reactors easily, but this prediction may deviate from reality considerably. In a tubular-flow reactor, *dispersion-model* can be used to predict the performance of real reactors. Degree of dispersion is represented by $Peclet\ \left(Pe = \frac{uL}{D}\right)$ number. In a PFR, $Pe \rightarrow \infty$, and in a CSTR, Pe = 0. In real reactors, degree of backmixing is between those of PFR and CSTR. From mole balance one could get the following equation in terms of conversion of limiting component A, X_A for an nth -order reaction.

$$\frac{D}{uL}\frac{d^2X_A}{dz^2} - \frac{dX_A}{dz} + k\tau C_{Ao}^{n-1}(1 - X_A)^n = 0$$

Where, *z = dimensionless distance along the reactor, D = dispersion coefficient, L = length of reactor, u = linear velocity, k = reaction rate constant,* τ = space time, *n = order of reaction.*

If Pe (uL/D) number = ∞, the above equation reduces to PFR equation. n = 1 and n = 2 were selected with Pe = 0.1, 0.3, 0.5, 1, 3, 5, 10, 100 as parameters. The model equation was solved symbolically by MATLAB. For positive orders, backmixing has an adverse effect on the fractional conversion. In this study, for variety of Pe numbers' effect on backmixing is simulated for 1st and 2nd order reactions. This study has indicated that in a tubular-flow reactor, dispersion has negative effects on performance of tubular-flow reactor. Larger the Pe number, the more conversion is obtained for a *fixed reactor size and dimensions.* These findings are presented in tabular and graphical forms.

***Corresponding author**

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INTRODUCTION

Chemical reactors are heart of the chemical industry. All productions and separation processes are based on the performance of the reactor. There is variety of classifications of reactors such as homogeneous vs heterogeneous, batch vs continuous, ideal vs non-ideal and so on. Ideal reactors such as batch, CSTR and PFR are based on idealized assumptions. That is, in a batch we have 100% mixing, no dead-volumes, in CSTRs again 100% perfect mixing is assumed. In PFR no backmixing but 100% redial mixing is assumed. Temperature, pressure, concentration and density are constant at any cross-section in an ideal PFR. Of course, none of these simplified assumptions reflects the reality. Hence, reactor performance based on idealization may predict far away from the true performance. In order to implement non-ideality in a real reactor design, some models have been developed, such as *dispersion model, combination of reactors model* (*CSTR + PFR*) or *recycle reactor model* given in the literature (Smith, 1981; Schmidt, 1998; Levenspiel, 1999; Walas, 1999;

Carberry, 2001; Davis and Davis, 2003; Fogler, 2011; Froment and Bischoff, 2011). In this study, we have considered dispersion-model with different Peclet (Pe=uL/D) numbers for 1st order and 2nd order reactions. Simulations were carried out with MATLAB package program.

SIMULATION RESULTS AND DISCUSSIONS

A mole balance with axial dispersion model can be obtained for an nth order reaction A → products in terms of conversion.

Table 1. Effect of Pe on conversion for a first-order reaction

Pe	0.1	0.3	0.5	1	3	5	10	100
x	0.342	0.631	0.756	0.883	0.971	0.989	0.997	0.999

The following *second order differential equation* for an n^{th} -order reaction can be obtained

$$\frac{D}{uL}\frac{d^2X_A}{dz^2}-\frac{dX_A}{dz}+k\tau C_{Ao}^{n-1}(1-X_A)^n=0$$

Where, D = Dispersion coefficient
u = Linear velocity
L = Length of reactor
X_A = Fractional conversion
τ = Space time
k = Specific reaction rate
C_{Ao} = Initial concentration of reactant A
y = Distance along the reactor
z = Dimensionless distance (y/L)

By definition $\frac{uL}{D}=\frac{convection}{diffusion}=Pe$ number

Then the above equation can be written as

$$\frac{1}{Pe}\frac{d^2X_A}{dz^2}-\frac{dX_A}{dz}+k\tau C_{Ao}^{n-1}(1-X_A)^n=0$$

Notice when Pe → ∞, equation reduces to an ideal plug flow reactor. When Pe = 0, then one has an ideal CSTR. Therefore, we may chose different Pe numbers as parameters and solve for the conversion for the predefined C_{Ao}, τ, and k for the 1st order. The results were compared with ideal case (i.e. with no backmixing). We have observed from the simulations that when Pe ≠ ∞ , there will be an adverse effect on conversion. In fact, the simulation results are shown in *Table 1* and in "*Fig. 1*" with Pe numbers as parameters confirm the arguments that are put forward. The higher the Pe number, the more conversion. Higher value of Pe number refers to less degree of axial dispersion.

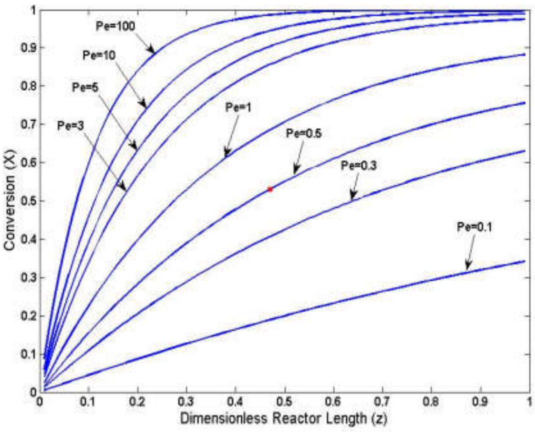

Fig. 1. Effect of Pe on conversion along the reactor for a first-order reaction

The 2nd order reaction was attempted to be solved with two boundary conditions. Unfortunately, analytical solution could not be obtained by MATLAB. Therefore, we search through literature and found information on graphical solutions (Levenspiel, 1959 and Levenspiel, 1961).

We picked up Pe = ¼,; τ = 5 min, k = 2 L/(mol-min), C_{Ao} = 1 mol/L.

- For a second order reaction, we have founded $X_A \approx 0.85$ at z=1 (i.e. at reactor exit)
- For the same conditions for a 1st -order reaction $X_A \approx 0.98$ at z=1
- For a 1st -order reaction in an ideal tubular reactor $X_A \approx 0.99$ at z=1

As can be seen that the higher the order of the reaction, the more pronounced the adverse effect of backmixing. Physical understanding of these cases can be explained through unnecessary reacting packages in the reactor medium due to backmixing.

Conclusions

- None of ideal reactor model performances will predict the reality due to extremely simplified assumptions.
- Backmixing in a tubular reactor will have a definite adverse effect on performance of the reactor.
- The higher the reaction order, the higher the adverse effect of backmixing.

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