An Approximate Analytical Solution for the Diffusion and Reaction Problem in a Catalyst Particle in the Presence of Coke Formation

Miguel A. Morales Cabrera, Tomas Viveros Garcia and Jesus A. Ochoa Tapia
Area de Ingeniería Química, Universidad Autónoma Metropolitana-Iztapalapa
Av. San Rafael Atlixco 186, Col. Vicentina, México, D.F., C.P. 09340, México.
Tel.: (01-55) 58044648/49/50, Fax: (01-55) 58044900, email: jaot@xanum.uam.mx

Introduction

Catalyst deactivation by coke deposition is frequently found in hydrocarbon conversion processes. The quantitative study of the activity-time relation is important to find the optimum design and operation of the reactors for such processes [1,2,3].
The first step in treating the problem is the analysis of the behavior at the single catalyst particle level. The earliest attempt to solve this problem was developed for an isothermal pellet where the irreversible reaction, $A \rightarrow B$ occurs [3]. In that work the effect of deposition on the rate of the main reaction was described by a linear relationship. Recently, a semi-analytical solution for the same problem with linear and exponential deactivation functions was obtained [4].
In this paper, we present an approximate analytical solution for the isothermal diffusion-reaction problem in a catalytic pellet where the irreversible reaction, $A \rightarrow B$, and coke formation occur. The dimensionless form conservation equations for coke and the main reaction key component, in a spherical pellet, are given by

$$\frac{\partial U_C}{\partial \tau} = R_{C0}\left(U_A, U_B\right)\phi_C\left(U_C\right), \qquad \frac{1}{\xi^n}\frac{\partial}{\partial \xi}\left(\xi^n \frac{\partial U_A}{\partial \xi}\right) = h^2 R_{A0}\left(U_A, U_B\right)\phi_A\left(U_C\right) \qquad (1,2)$$

These are subjected to the following initial and boundary conditions:

$$\tau = 0 \qquad 0 \le \xi \le 1 \qquad U_C = 0 \qquad (3)$$

$$\xi = 1 \quad \tau \ge 0, \quad U_A = 1 \quad U_B = U_{BS}; \quad \text{and} \quad \xi = 0 \quad \tau \ge 0 \quad \frac{\partial U_A}{\partial \xi} = \frac{\partial U_B}{\partial \xi} = 0 \qquad (4,5)$$

The method to obtain the analytical solution is based on the linearization of the kinetic terms of the reactant transport equations by expansion in Taylor series [5]. The analytical expressions for the concentration profiles of the reactants are obtained by direct application of the Laplace transform method. This procedure leads to analytical expressions for the effectiveness factor, of the main reaction, in terms of the Thiele modulus (h) and the time (τ).

Results and Discussion

The approximate effectiveness factors predictions are compared with the exact results obtained by numerical integration of the reactant transport equations [3]. Two types of deactivation processes by coke were considered: series and parallel deactivation.

Figure 1 shows the case where series deactivation is considered. For this case, the approximate effectiveness factors predictions are in very good agreement with the exact predictions for moderate Thiele modulus values. The approximate predictions can be considered good, in the whole range of Thiele modulus-time domain, because the maximum deviation from the exact values is less than 20%.

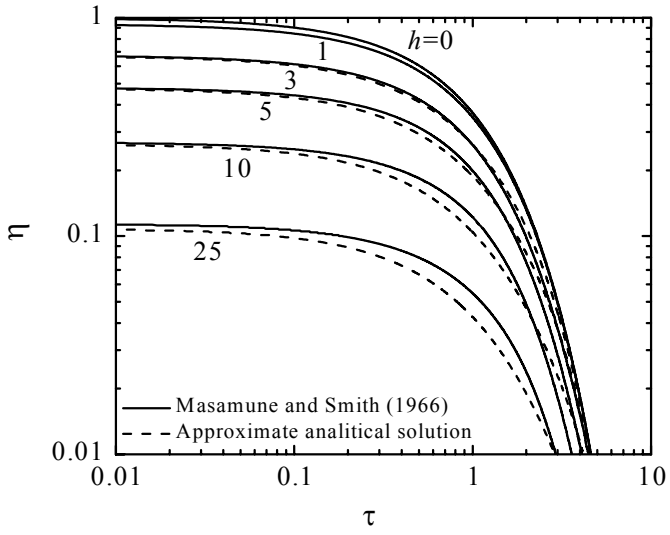

Figure 1. Evolution of the effectiveness factor with time (τ) for series deactivation as function of the Thiele modulus.

The figure shows that, for series deactivation, the extent of deactivation increases with diffusion resistance (larger Thiele modulus, *h*). Therefore, the results can be used to predict the effect of coke deposition on the activity of the catalyst particle at any time for isothermal conditions and first order kinetics.
Finally, the approximate analytical method can be used to solve diffusion reaction problems with higher order kinetics and considering coke deposition described by nonlinear relationships.

References

1. G.F. Froment, K.B. Bischoff. Chemical Reactor Analysis and Design, Wiley, New York. 1979.
2. R. Hughes. Deactivation of Catalysts, Ch. 1, 2 and 6, Academic Press, London. 1984
3. S. Masamune, J.M. Smith. *AICHE J*., 12 (1966) 384.
4. J.C. Gottifredi, G.F. Froment. *Chem. Eng. Sci*., 52 (1997) 1883.
5. J.O. Marroquín de la Rosa, T. Viveros García, J.A. Ochoa Tapia. (1998). *Ind. Eng. Chem. Res*., 37 (1998) 3780.