FORMULATION AND NUMERIC CALCULATION OF NON-ISOTHERMAL EFFECTIVENESS FACTOR FOR FINITE CYLINDRICAL CATALYSTS WITH BI-DIMENSIONAL DIFFUSION

BIBIAN HOYOS† , JUAN GUILLERMO CADAVID‡ and HERMES RANGEL‡

† *Escuela de Procesos y Energía. Universidad Nacional de Colombia, A. A. 1027. Medellín, Colombia.*
bahoyos@perseus.unalmed.edu.co

‡ *Facultad de Ingeniería. Universidad Nacional de Colombia, Transv 38 Diag 40. Bogotá D. C, Colombia.*
jcadavid@ing.unal.edu.co

Abstract–– **A model for calculating the effectiveness factor and the concentration and temperature profiles for finite cylindrical either hollow or solid catalyst particles is presented. The model accounts for dispersion in both radial and axial directions and non-isothermal behavior. The resulting differential partial equations system is discretized by a centered finite difference method and a program written for the Excel™ electronic sheet solves the highly nonlinear algebraic system. The numerical technique can be extended for any kinetic expression; for illustration, some results for n -th order reactions rate expressions are shown.**

Keywords–– **Effectiveness factor, Finite cylindrical catalysts, Bi-dimensional dispersion, Non-isothermal model.**

I. INTRODUCTION

In heterogeneous catalytic studies it is important to establish the mechanism that is limiting the overall rate of transformation within the catalytic particle, that is, to know whether the diffusive effects are controlling the process rate, or whether the chemical reaction at the particles surface controls.

To have an idea of the relative importance of diffusion and chemical reaction phenomenon, an effectiveness factor for catalytic particles is defined, for a steady state flow condition, as

$$\eta = \frac{\text{Actual amount of substance reacting in the whole particle}}{\text{Amount that would react if the whole particle were at the external surface temperature and concentration}} \quad (1)$$

which can also be expressed in terms of molar velocity through the external surface particle by

$$\eta = \frac{\left(\begin{array}{c}\text{Molar velocity of component}\\ \text{i through the external}\\ \text{surface particle}\end{array}\right) \times \left(\begin{array}{c}\text{External surface}\\ \text{area of catalytic}\end{array}\right)}{\left(\begin{array}{c}\text{Formation rate of component}\\ \text{i at the external surface}\\ \text{temperature and concentration}\end{array}\right) \times \left(\begin{array}{c}\text{volume of}\\ \text{catalytic particle}\end{array}\right)} \quad (2)$$

As stated by Eqn. 2, a value of unit for the effectiveness factor (for isothermal conditions) indicates that there are not diffusive barriers to the overall rate of transformation and the activation energy of the chemical reaction at the surface of the particle is the rate determinant step. An effectiveness factor less than unit shows that the diffusive effects are important in the control of global velocity of transformation: the smaller the effectiveness factor is, the larger importance of the physical processes of mass transfer are.

The case of an effectiveness factor greater than unit can also appear, which indicates that heat transfer effects are important, and even though in appearance this would be an ideal situation, in practice this is not recommendable due to catalytic deactivation originated by high temperatures within the particle.

There are a great number of published articles where the parameters of major influence in the effectiveness factor are studied. Among those parameters, the particle geometry is perhaps of major concern. In particular, the studies for cylindrical pores (Carberry, 1961), for spherical particles (Smith, 1956; Carberry, 1976), for flat slabs (Morbidelli *et al.*, 1982a) for cylindrical pellets (Morbidelli *et al.*, 1982b), and more recently, the investigation of Wang *et al.*, (1994) for rectangular reticulated particles are remarkable. Doraiswamy and Sharma (1984) showed a good summary of the geometric influence in the effectiveness factor and in the concentration profiles inside the particle.

The influence of the kinetic expression for the chemical reaction in the effectiveness factor is also an aspect widely studied: there are studies for first and second order rate expressions (Wakao *et al.*, 1978; Lee, 1979; Lin *et al.*, 1986), for reactions type Langmuir-Hinsehelwood (Krasuk and Smith, 1965; Morbidelli *et al.*, 1982a,b), for negative order rate expressions (Morbidelli and Varma, 1983) and even for multiple reactions (Wohlfahrt, 1982). Doraiswamy and Sharma (1984) , Satterfield and Sherwood (1963) and Satterfield (1991) also showed the analytic equations of effectiveness factor for a great number of reactions with highly complexes kinetic expressions.

Almost all works in literature consider in their mathematical models the diffusion phenomenon in