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Short communication

Approximate expression for the effectiveness factor estimation and a simple numerical method for concentration profile calculation in porous catalyst

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Abstract

The model of steady state diffusion and reaction in a catalyst pellet where a single reaction takes place is analyzed with the scope to predict effectiveness factor through a very simple and practical procedure. Non-linear usual reaction kinetics are used to investigate the agreement among exact or numerical predictions with approximate results. In all cases studied maximum deviations in the whole range of ϕ values are below 4% which turns the procedure attractive and useful. To perform numerical integration of the classical non-linear diffusion and reaction differential equation a new procedure was used that avoid usual instabilities or the introduction of spline collocation methods when concentration profiles are very steep. Concentration resulting profiles are compared with those generated by an early expression proposed by the authors.
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1. Introduction

Recently, Sun et al. [1] presented a new procedure, based on the Adomian decomposition method, to obtain approximate solutions for the non-linear diffusion and reaction differential mass balance equation in catalyst pellets. The dimensionless concentration profile inside the catalyst, as well as the effectiveness factor, can be calculated using this procedure. However, three, and even more (up to six), terms of the Adomian polynomial are necessary to obtain concentration (γ) or effectiveness factor (η) values in agreement with numerical or exact prediction. The number of terms depends upon the complexity of the kinetic expression and on the Thiele modulus value. Nevertheless, as the Thiele modulus (ϕ) increases (i.e., $\phi \geq 2$), η deviations in relation to exact values become larger than 100%.

In this contribution a previous developed perturbation and matching procedure [2] is applied to obtain effectiveness factor predictions through a very simple resulting algebraic expression which produces results in close agreement (maximum deviation 4%) for the whole range of ϕ and for kinetic expressions investigated. In addition a new numerical procedure is used to calculate dimensionless concentration profiles and effectiveness factor which is very straightforward and rapidly convergent.

An approximate expression, developed by Gottifredi et al. [3], to estimate dimensionless concentration profiles inside a catalyst pellet, with the knowledge of η is also tested with predictions obtained through the numerical procedure.

2. Theoretical development

It will be assumed that a single reaction is taking place inside the catalyst pellet of characteristic length L and that isothermal conditions prevail. The continuity equation for the

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Nomenclature

a	dimensionless parameter given by Eq. (11)
A	dimensionless variable defined by Eq. (13)
C	dimensional concentration (kmol/m^3)
D	effective diffusivity of key component (m^2/h)
f	auxiliary function defined by Eq. (18)
g	auxiliary function defined by Eq. (13)
K	dimensionless kinetic parameter used in Eq. (22)
L	catalyst particle characteristic dimension (m)
m	parameter used to define geometrical shape
N	reaction order
r	dimensional rate of reaction (kmol/m^3 h)
R	dimensionless rate of reaction defined by Eq. (2)
x	dimensionless coordinate defined by Eq. (2)
x'	dimensional coordinate (m)

Greek letters

γ	dimensionless concentration (see Eq. (2))
ε	auxiliary parameter defined by Eq. (20)
η	effectiveness factor defined by Eq. (4)
λ	auxiliary parameter defined by Eq. (13)
ρ_1	auxiliary parameter defined by Eq. (9)
σ_1	auxiliary parameter defined by Eq. (7)
ϕ	Thiele modulus defined by Eq. (2)
ϕ^*	modified Thiele modulus given by Eq. (8)

Subscripts

c	denotes property calculated at $x = 0$
s	denotes property calculated at $x = 1$

dimensionless key component concentration can be written as

$$x^{-m}\frac{\mathrm{d}}{\mathrm{d}x}\left(x^m\frac{\mathrm{d}\gamma}{\mathrm{d}x}\right) = \phi^2 R(\gamma) \tag{1}$$

where the following dimensionless variables were defined:

$$\gamma = \frac{C}{C_\mathrm{s}}, \qquad x = \frac{x'}{L}, \qquad \phi = L\sqrt{\frac{r_\mathrm{s}}{DC_\mathrm{s}}},$$

$$R(\gamma) = \frac{r(C)}{r(C_\mathrm{s})} \tag{2}$$

Here C represents the dimensional concentration, D the effective diffusivity, $r(C)$ the dimensional rate of reaction and ϕ the Thiele modulus, respectively. $m = 0, 1, 2$ stands for the geometrical shape of the catalyst particle, while subscript 's' denotes values of the corresponding variables evaluated at the outer surface of the pellet.

Assuming negligible external mass transfer resistance Eq. (1) must be solved with the following boundary conditions:

$$\gamma = 1, \quad x = 1, \qquad \frac{\mathrm{d}\gamma}{\mathrm{d}x} = 0, \quad x = 0 \tag{3}$$

Under realistic situations Eq. (1) does not have an analytical solution since $R(\gamma)$ is usually a non-linear function of γ. Most of the results found in the literature are obtained through the application of numerical methods that can become unstable when $\phi^2 \geq 1$. Fortunately, from a chemical engineering point of view, one is not interested in solving Eq. (1) but rather in estimating the effectiveness factor (η) given by:

$$\eta = (m+1)\int_0^1 [R(\gamma)x^m]\,\mathrm{d}x \tag{4}$$

By integrating Eq. (4) once, with boundary condition given by Eq. (3), it can be easily shown that:

$$\eta = \frac{m+1}{\phi^2}\left(\frac{\mathrm{d}\gamma}{\mathrm{d}x}\right)_{x=1} \tag{5}$$

Both Eqs. (4) and (5), can be used to deduce appropriate expressions to predict η values.

2.1. Approximate effectiveness factor estimation

Gottifredi and Gonzo [2] using the perturbation technique have shown that, for small values of ϕ, η depends on ϕ, up to term of the order ϕ^2 as follows:

$$\eta \approx 1 - \sigma_1\phi^2 + \mathrm{O}(\phi^4) \quad (\phi^2 \ll 1) \tag{6}$$

with

$$\sigma_1 = \frac{R'(1)}{(m+1)(m+3)} \tag{7}$$

where $R'(1)$ denotes first derivative with respect to γ, evaluated at $\gamma = 1$.

For large values of ϕ ($\phi \gg 1$), assuming that $\gamma = 0$ in the center of the pellet, the well-known Petersen [4] and Bischoff [5] approximate expression is valid:

$$\eta \approx \frac{\rho_1}{\phi} = \frac{1}{\phi^*} \quad (\phi^2 \gg 1) \tag{8}$$

where the parameter ρ_1 satisfies the following expression:

$$\rho_1 = (m+1)\left[2\int_0^1 R(\gamma)\,\mathrm{d}\gamma\right]^{1/2} \tag{9}$$

Gottifredi et al. [3], proposed an algebraic equation to match Eqs. (6) and (8):

$$\eta = [\phi^{*2} + \exp(-a\phi^{*2})]^{-1/2} \tag{10}$$

By comparing Eqs. (6) and (8) with Eq. (10), the unknown parameter "a" is found to be:

$$a = 1 - 2\sigma_1\rho_1^2 \tag{11}$$

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