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On the effectiveness factor calculation for a reaction – diffusion process in an immobilized biocatalyst pellet

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Abstract

This contribution deals with effectiveness factor (η) and concentration profile of key component estimations when a single independent reaction takes place in a porous catalyst structure where enzymes are immobilized. The procedure is quite general since any kinetic expression can be handled and the case of catalytic activity distribution can also be taken into account. With the knowledge of kinetic parameters and effective diffusivity η and concentration profiles can be estimated through very simple algebraic equations. Thus, the numerical solution of a non linear second order boundary value differential equation, which usually needs some spline scheme, is avoided.

The obtained approximate results are compared with numerical findings for the case of slab geometry where a very simple numerical procedure can be used to solve the resulting differential non linear equation. Approximate results are shown very accurate in the whole range of kinetic parameters, even in those cases where the reaction kinetics shows an apparent negative order of reaction and η values can be above unity. Tables are used to better compare approximate and numerical values. Concentration profile predictions are also very accurate in the region nearby the external surface of the catalyst particle.

These approximate results are used to establish criteria to analyze experimental kinetic data in those cases where diffusional phenomena, that could affect chemical parameter estimations, must be avoided.
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Keywords: Effectiveness factor prediction; Enzyme immobilization; Concentration profiles; Michaelis–Menten kinetic; Kinetic data analysis. Thiele modulus

1. Introduction

Mittal [1] pointed out the main advantages of enzyme immobilization in food processing. Usually, these techniques involve adsorption, covalent attachment, cross linking, entrapment and encapsulation. The support structure needs pore size of appropriate dimensions to ensure uniform enzyme concentration inside the resulting catalyst and a reasonable rate of diffusion of substrates and reaction products. When these conditions are not fully met non uniform enzyme concentration within the catalyst results and/or strong diffusional internal limitations with significant overall reaction decays. According to engineering purposes a number of experimental reactors have been reported [1] to test this kind of biological catalysts.

In recent years, there is an increasing concern to estimate effectiveness factor (η) in bioengineering processes where immobilized enzymes are used as catalysts. Since the kinetic expression is usually non linear in term of concentration, numerical procedures are needed to solve the resulting governing differential equation for the concentration profile inside the pellets. These procedures are not straightforward as shown by Kubicek and Hvalacek [2] and Villadsen and Michelsen [3].

Recently Li et al. [4] presented an approximate procedure to estimate η when chemical kinetics are well represented by the Michaelis–Menten equation. They basically assumed that substrate concentration can be represented by a polynomial up to third degree in the dimensionless position (x) of

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Nomenclature

a	auxiliary parameter defined by Eq. (14)
A	auxiliary variable defined by Eq. (17a)
C	dimensional key component concentration (mol/l)
D	effective diffusivity of key component (cm^2/s)
E	percent deviation $\lvert(\eta_N - \eta_A)/\eta_N\rvert \times 100$
$f(x)$	normalized spatial catalytic activity function (see Eq. (5))
$F(\gamma)$	variable defined by Eq. (21)
$g(x)$	auxiliary variable defined by Eq. (17c)
K_m	Michaelis–Menten dimensional kinetic parameter (mol/l)
L	dimensional characteristic catalyst dimension (cm)
m	geometrical parameter 0, 1, 2
n	reaction order
r	rate of reaction (mol/l s)
r_m	Michaelis–Menten dimensional kinetic parameter (mol/l s)
R	dimensionless rate of reaction, Eq. (2c)
$R'(1)$	first derivative of R with respect to γ evaluate at $\gamma = 1$
x	dimensionless spatial coordinate (x'/L)
x'	dimensional spatial coordinate (cm)
z	auxiliary function of γ and γ_c (Eq. (22))

Greek Letters

α	auxiliary parameter defined by Eq. (12)
β	dimensionless kinetic parameter (C_s/K_m)
γ	dimensionless concentration (C/C_s)
γ^*	value of γ that satisfy $R(\gamma^*) = 0$
$(\gamma_c)_{lim}$	value of γ given by Eq. (26)
ε	auxiliary parameter given by Eq. (24)
η	effectiveness factor
$(\eta_A)_{max}$	maximum value of η when $R'(1) < 0$ (see Eq. (28))
λ	auxiliary variable defined by Eq. (17b)
ρ	auxiliary parameter defined by Eq. (7)
σ	auxiliary parameter given by Eq. (11)
ϕ	Thiele modulus given by Eq. (2d)
ϕ^*	modified Thiele modulus (ϕ/ρ)

Subscripts

A	refers to approximate values
C	refers to value at $x = 0$
e	refers to exact value
L	refers to Li et al. [4] definitions
N	refers to numerical estimated value
s	refers to value at $x = 1$

a spherical particle. The polynomial coefficients are determined once the expression is introduced in the resulting differential equation and terms of like power are equated. They [4] also presented a comparison among approximate and numerical η predictions where is clearly shown that η behavior is not as expected and deviations becomes very large as Thiele modulus increases. A numerical "shooting" procedure is also mentioned but no details are given in the publication. However, it is well known that numerical procedure reported in the literature becomes unstable, unless some spline scheme is put forward (Villadsen and Michelsen [3]). On the other hand, plain shooting procedure can become non convergent when the Thiele modulus is greater than 2, approximately, depending upon the expression used to represent the chemical kinetics.

The aim of this contribution is to clearly show that an early procedure developed by Gottifredi and Gonzo [5] can be safely used to estimate η with great accuracy. The procedure is very simple and straightforward. η can be estimated through a unique algebraic equation and the parameters needed can be calculated analytically or, with very complex kinetic expressions, by direct quadrature.

It is further assumed that the enzyme concentration within the porous catalyst structure is not uniform. Nevertheless, as will be seen, the procedure is completely general instead of being restricted to a given kinetic expression and/or pellet geometry. In order to compare approximate η estimated values, a stable and simple numerical procedure is also shown that, unfortunately, is only applicable to slab geometry. Nevertheless, in this case, it is quite useful to show the accuracy of η approximate predictions and also, to test an approximate algebraic expression to predict concentration profiles inside the pellet. The effect of diffusional phenomena on kinetic data is also discussed.

2. Theory

Let us consider the case of a single independent reaction taking place inside the catalyst porous structure at steady state and where isothermal conditions prevail. With these assumptions the mass continuity equation can be written in dimensionless form as:

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

where x denotes the spatial coordinate, γ the key component concentration, $f(x)$ the normalized catalytic activity distribution function, $R(\gamma)$ the rate of reaction and ϕ the Thiele modulus:

$$x = \frac{x'}{L}; \tag{2a}$$

$$\gamma = \frac{C}{C_s}; \tag{2b}$$

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