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A Simplified Representation for Nonisothermal Effectiveness Factors

c_s	Surface concentration
y	Dimensionless concentration
x	Dimensionless radial coordinate
R	Radius of the pellet
k	Rate constant
D	Effective diffusivity in the pellet
ϕ	Thiele modulus, $R(k/D)^{1/2}$
β	$+D(-\Delta H)c_s/KT_s$
K	Effective conductivity of the pellet
(ΔH)	Heat of reaction
T_s	Surface temperature
γ	E/R_gT_s
E	Activation energy
R_g	Gas constant
η	Effectiveness factor
η_{iso}	Effectiveness factor if the pellet is isothermal and at temperature T_s
α	$\beta\gamma$

The heat and mass balance equations for a first order irreversible reaction occurring in a nonisothermal spherical pellet can be reduced to the following equation (*1*):

$$\frac{d^2y}{dx^2} + \frac{2}{x}\frac{dy}{dx} = \phi^2 y \exp\left[\gamma\beta\frac{(1-y)}{1+\beta(1-y)}\right], \tag{1}$$

with

$$\frac{dy}{dx} = 0 \qquad \text{at } x = 0, \tag{2}$$

$$y = 1 \qquad \text{at } x = 1. \tag{3}$$

This equation was solved numerically by Weisz and Hicks (*1*) and the results were presented graphically as effectiveness factor, η, vs Thiele modulus, ϕ, with β and γ as parameters. Such graphs cannot be directly utilized for the purpose of reactor design. Reactor design involves numerical solution of coupled nonlinear mass and energy balance equations. The numerical solution requires evaluation of the rate of reaction at every mesh point which in turn involves the evaluation of effectiveness factor. Since the surface temperature and concentration vary from point to point in the reactor, to compute the effectiveness factor, it becomes necessary to solve Eq. (1) numerically, at every mesh point with parameters ϕ, β and γ evaluated at the corresponding surface conditions. An alternative approach would be to obtain a relationship expressing effectiveness factor in terms of parameters of the system, which can be directly substituted in mass and heat balance equations. This approach was first followed by Carberry (*2*) and more recently by Jouven and Aris (*3*) who have considered exothermic first order reaction. Liu (*4*) obtained an empirical expression for the case of a first order endothermic reaction. In the present note a simplified expression which has certain advantages over the results of the previous workers is reported for the case of an exothermic first order irreversible reaction.

Carberry (*2*) solved the heat and mass balance equations for a reaction occurring in a spherical pellet and showed that for a first order reaction, for $\alpha \leqslant 6$ and $\phi > 7.5$, the effectiveness factor can be estimated by the following equation:

$$\eta = \frac{3\exp(\alpha/5)}{\phi}. \tag{4}$$

However, from the results of Weisz and Hicks (*1*), it can be shown that the value of the effectiveness factor can differ by as much as 20%, for the same value of ϕ and $\beta\gamma$, but different values of β and γ. This points out a need for obtaining an expression where β and γ appear independently.

Jouven and Aris (*3*) suggested a procedure to evaluate effectiveness factor, valid over a wide range of parameters, i.e., β from zero to 1.4, γ up to 40, subject to the

condition $\beta\ \gamma < 14$. This region is subdivided into four subregions and the procedure for each subregion is specified. The procedure involves evaluation of certain series using 200 constants which appear as coefficients of the terms in the series. The results illustrated by the authors show excellent agreement. The only drawback is the relative complexity of the method requiring appreciable computer memory and time. It is stated by the authors that the use of the method makes the calculation of η 55 times faster than the numerical solution of the nonlinear boundary value problem specified by Eqs. (1) to (3).

In the present work an empirical equation has been fitted. It has been shown in the literature (*5*), that for a number of reactions of industrial importance $\beta\ \gamma < 6$. Hence attention was focused on this region only. Considering the discrepancy $(\eta - \eta_{iso})$ as the deviation to be correlated with system parameters, it was plotted against η_{iso}. The resulting curves showed that an expression of the type

$$\eta - \eta_{iso} = a(e^{\eta_{iso}} - 1) \qquad (5)$$

holds in the range $\phi > 2$. The constant a was then related to the system parameters using numerical solutions reported by Weisz and Hicks. The resulting equation is as follows:

$$\eta = (e^{1.172\beta(\gamma-8)^{1/2}} - 1)(e^{\eta_{iso}} - 1) + \eta_{iso}, \qquad (6)$$

where

$$\eta_{iso} = \frac{3}{\phi}\left(\frac{1}{\tanh \phi} - \frac{1}{\phi}\right). \qquad (7)$$

The equation is valid for $\phi > 2$ and $\gamma > 8$.

A large number of values obtained by using Eq. (6) and those using Carberry's equation were compared with those obtained by Weisz and Hicks (*1*), in the range $\phi > 7.5$ where Carberry's equation is applicable. Some representative values are illustrated in Table 1. The average absolute deviation with the present correlation was 3.8% the maximum deviation being 10.6%. The corresponding deviations for Carberry's equation are 12.2 and 27.6%. In addition to the above region, i.e., $\phi > 7.5$, Eq. (6) is also valid in the range $2 < \phi < 7.5$. In this range the average absolute deviation was found to be 7.2% and maximum deviation was 20%.

TABLE 1

			Effectiveness factor		
ϕ	β	γ	(Weisz and Hicks solution)	(Carberry's equation)	(Author's equation)
8	0.6	10	0.980	1.245	0.980
15	0.6	10	0.530	0.664	0.530
30	0.6	10	0.260	0.332	0.270
75	0.6	10	0.105	0.133	0.108
8	0.4	10	0.730	0.834	0.693
15	0.4	10	0.395	0.445	0.379
30	0.4	10	0.200	0.223	0.192
75	0.4	10	0.081	0.089	0.081
8	0.3	20	1.15	1.245	1.250
15	0.3	20	0.740	0.664	0.675
30	0.3	20	0.335	0.332	0.338
75	0.3	20	0.135	0.133	0.135
10	0.1	20	0.395	0.361	0.425
20	0.1	20	0.207	0.184	0.219
30	0.1	20	0.142	0.122	0.147
50	0.1	20	0.088	0.073	0.089
75	0.1	20	0.066	0.049	0.059
8	0.1	30	0.620	0.682	0.612
10	0.1	30	0.500	0.547	0.497
15	0.1	30	0.340	0.364	0.337
75	0.1	30	0.075	0.073	0.073

The nature of effectiveness factor vs Thiele modulus plots for non-first order pseudohomogeneous and Langmuir–Hinshelwood models is expected to be the same as that for first order reaction. In view of this an expression of the same type as Eq. (5) can be expected to hold for other rate expressions also. Hutchings and Carberry (*6*) have obtained numerical solution for mass and energy balance equations subject to external heat and mass flux boundary conditions for a reaction obeying Langmuir–Hinshelwood kinetics. For the present analysis, the results for the case of Nusselt and Sherwood numbers approaching infinity were utilized to plot $(\eta - \eta_{iso})$ vs $(e^{\eta_{iso}} - 1)$. A linear plot was obtained for $\phi > 2$, confirming the validity of the above statement. Correlating the constant a of Eq. (5)

with the large number of system parameters required numerical values of η for a wide range of parameter values. Since these were not available, the correlation could not be attempted.

The equation obtained in the present work correlates the values more accurately than Carberry's equation. It separates the effect of parameters β and γ and is also applicable over a wider range. At the same time it involves much less numerical computation compared to those involved in Jouven and Aris' (*3*) procedure. Hence for the engineering design of the systems which lie in the range of this equation, the use of Eq. (6) will result in considerable saving of computer time without sacrificing accuracy.

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