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The Effect of Shape on the Effectiveness of Biporous Pellets[1]

Catalyst pellets with biporous structures are frequently used in industrial operations. When porous catalyst particles are pelletized, the resulting pellet has large macropores, with the small micropores branching out from them. Signal work has been done by Mingle and Smith (*4*) and Carberry (*1*) in evaluating the effectiveness of biporous catalyst pellets. Recently, Ors and Dogu (*5*) defined a new parameter, α, characterizing the ratio of the diffusion times of the micropores to that of the macropores. Jayaraman *et al.* (*2*) studied the general *n*th-order reaction occurring biporous pellets. Recently, Jayaraman (*3*) analyzed the zero-order reaction occurring in a biporous pellet. The aim of the present study is to analyze the effect of the shape on the effectiveness of a biporous pellet. Rester and Aris (*6*) and Rester *et al.* (*7*) have done trend setting work on this for monoporous pellets. They have defined a normalized Thiele modulus based on the volume to external surface area. The effectiveness factor vs this modified modulus is seen to merge for all values with a maximum spread of 16%. An analysis made to see the usefulness of defining such a modulus for the micropore and macropore regions is reported in this communication.

Assuming that a first-order reaction occurs in the micropores of the pellet the mass balance equations can be written in dimensionless form as

—Micropores:

$$\frac{1}{X^n}\frac{d}{dX}\left(X^n\frac{dC_{\mathrm{mi}}}{dX}\right) = \phi_n^2 C_{\mathrm{mi}} \qquad (1)$$

with the boundary conditions

$$\frac{dC_{\mathrm{mi}}}{dX} = 0 \quad \text{at } X = 0 \qquad (2)$$

$$C_{\mathrm{mi}} = C_{\mathrm{ma}} \quad \text{at } X = 1. \qquad (3)$$

—Macropores:

$$\frac{1}{Y^n}\frac{d}{dY}\left(Y^n\frac{dC_{\mathrm{ma}}}{dY}\right) = \alpha_n\left(\frac{dC_{\mathrm{mi}}}{dX}\right)\bigg|_{X=1} \qquad (4)$$

with the boundary conditions

$$\frac{dC_{\mathrm{ma}}}{dY} = 0 \quad \text{at } Y = 0 \qquad (5)$$

$$C_{\mathrm{ma}} = 1 \quad \text{at } Y = 1. \qquad (6)$$

C_{mi} and C_{ma} are the dimensionless reactant concentrations in the micropores and macropores, respectively. X and Y are the corresponding dimensionless length variables; $n = 0$, 1, and 2 for slab, cylinder, and sphere, respectively. ϕ_n is the micropore Thiele modulus defined as

$$\phi_n = L_{\mathrm{mi}}(k/D_{\mathrm{mi}})^{1/2} \qquad (7)$$

and

$$\alpha_n = (n+1)\frac{L_{\mathrm{ma}}^2}{L_{\mathrm{mi}}^2}\frac{D_{\mathrm{mi}}}{D_{\mathrm{ma}}}(1-\varepsilon) \qquad (8)$$

(the other variables are defined in the nomenclature).

As was defined in the case of monoporous pellets by Rester and Aris (*6*), we can define a normalized Thiele modulus for micropores

$$\Lambda_{\mathrm{mi}} = \frac{V_{\mathrm{mi}}}{S_{\mathrm{mi}}}\sqrt{\frac{k}{D_{\mathrm{mi}}}} \qquad (9)$$

or

$$\Lambda_{\mathrm{mi}} = \frac{L_{\mathrm{mi}}}{(n+1)}\sqrt{\frac{k}{D_{\mathrm{mi}}}}. \qquad (10)$$

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The micropore equations can now be integrated with the boundary conditions and the term $\alpha(dC_{\mathrm{mi}}/dX)$ can be written as

$$\alpha_n \left(\frac{dC_{\mathrm{mi}}}{dX}\right)\bigg|_{X=1} = (n+1)^2\Lambda_{\mathrm{ma}}^2 C_{\mathrm{ma}}, \quad (11)$$

where Λ_{ma} is the normalized macropore Thiele modulus defined as

$$\Lambda_{\mathrm{ma}} = \frac{V_{\mathrm{ma}}}{S_{\mathrm{ma}}}\sqrt{\frac{k}{D_{\mathrm{ma}}}\,\eta_{\mathrm{mi}}}, \quad (12)$$

where

$$\eta_{\mathrm{mi}} = \frac{\tanh(\Lambda_{\mathrm{mi}})}{\Lambda_{\mathrm{mi}}} \quad \text{(flat plate)} \quad (13)$$

$$= \frac{2I_1(2\Lambda_{\mathrm{mi}})}{2\Lambda_{\mathrm{mi}}I_0(\Lambda_{\mathrm{mi}})} \quad \text{(cylinder)} \quad (14)$$

$$= \frac{3}{3\Lambda_{\mathrm{mi}}}\left(\frac{1}{\tanh(3\Lambda_{\mathrm{mi}})} - \frac{1}{3\Lambda_{\mathrm{mi}}}\right). \quad \text{(sphere)} \quad (15)$$

Integrating the macropore equation with the boundary conditions and using the usual definition the effectiveness factor can be obtained as

$$\eta_{\mathrm{overall}} = \eta_{\mathrm{mi}}\eta_{\mathrm{ma}}, \quad (16)$$

where

$$\eta_{\mathrm{ma}} = \frac{\tanh(\Lambda_{\mathrm{ma}})}{\Lambda_{\mathrm{ma}}} \quad \text{(flat plate)} \quad (17)$$

$$= \frac{2I_1(2\Lambda_{\mathrm{ma}})}{2\Lambda_{\mathrm{ma}}I_0(\Lambda_{\mathrm{ma}})} \quad \text{(cylinder)} \quad (18)$$

$$= \frac{3}{3\Lambda_{\mathrm{ma}}}\left(\frac{1}{\tanh(3\Lambda_{\mathrm{ma}})} - \frac{1}{3\Lambda_{\mathrm{ma}}}\right). \quad \text{(sphere)} \quad (19)$$

As the overall effectiveness factor is the product of the effectiveness of the micropore and macropore regions, it is logical to expect the deviations in the $\eta - \phi$ curves for the three geometries to be higher than those for the corresponding monodispersed case. The results of the computations indicate that the maximum deviation is found to be around 36%. This deviation is found for both the moduli lying between 1.3 and 1.7. The other significant results are

Error is <20% if
ϕ_{mi} or ma ≤ 1 or ≥ 2 and
ϕ_{mi} or ma ≥ 10 or ≤ 0.4.
Both ϕ_{mi} and $\phi_{\mathrm{ma}} \geq 5$ or ≤ 0.1.
Error is <5% if
Both ϕ_{mi} and $\phi_{\mathrm{ma}} \geq 15$ or ≤ 0.3.

From the above analysis it can be concluded the shape normalization of the Thiele modulus brings together the curves with tolerable accuracy if either the macropore or the micropore Thiele modulus is less than 0.1; or both the micropore and macropore modulii are more than 5; or when either of them is not in the range of 1 and 2, while the value of the other is ≥ 10 or ≤ 0.4.

NOMENCLATURE

C_{ma}	Dimensionless macropore concentration
C_{mi}	Dimensionless micropore concentration
D_{ma}	Macropore diffusion coefficient
D_{mi}	Micropore diffusion coefficient
k	Rate constant
L_{ma}	Macropore length or radius
L_{mi}	Micropore length or radius
X	Dimensionless micropore length variable
Y	Dimensionless micropore length variable
α_n	Parameter defined by Eq. (8)
ε	Macropore porosity
η_{ma}	Macropore effectiveness factor
η_{mi}	Micropore effectiveness
ϕ_{ma}	Macropore Thiele modulus
ϕ_{mi}	Micropore Thiele modulus
Λ_{ma}	Modified macropore Thiele modulus
Λ_{mi}	Modified micropore Thiele modulus

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