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A Simple Closed-Form Expression for the Geometric Correction Factor for the Weisz Diffusivity Cell

One of the most convenient methods for measuring effective diffusivities in single spherical pellets of catalyst, or other porous materials, was developed by Weisz (*1*), and subsequently analysed theoretically by Meyer and co-workers (*2*). A pellet is forced into an undersized elastic tube which effectively provides a seal over the equatorial zone of the porous sphere whilst leaving its two polar caps exposed; this is illustrated in Fig. 1. In practical situations the geometry may be made to approach closely the ideal form illustrated by placing plastic cable ties around the elastic tube at the points AA indicated in Fig. 1. This ensures a sharp, well-defined particle-tubing contact angle. An effective diffusivity within the pellet is found by exposing the polar caps to flowing gas streams of differing composition and measuring, usually by chromatographic means, the flux of species diffusing through the pellet from one stream to the other. This must be carried out under conditions where the pressure imbalance across the pellet is sufficiently small for the diffusive fluxes to dominate their convective counterparts.

If the pellets being tested are of cylindrical form with a diameter d and a length-to-diameter ratio of unity then the steady-state diffusive flux through the pellet is given by

$$F = D_e \frac{\pi d^2}{4}\left[\frac{C_1 - C_2}{d}\right], \qquad (1)$$

where F is the flux of diffusing species, D_e the effective diffusion coefficient and C_1 and C_2 are the concentrations of diffusing species at the respective pellet ends. The case of the spherical pellet is much more difficult to analyse, but Weisz's approach was to say that the diffusive flux passing through the sphere of diameter d was given by an equation of the same form as Eq. (1), but modified by the inclusion of an empirical geometric correction factor α which accounted for the nonplanar geometry of the porous matrix. By testing spherical pellets, machining them into cylindrical form, and then retesting them. Weisz was able to evaluate this correction factor. For his particular experiments, spheres of nominal diameter 4.2 mm were forced into tubing with an internal diameter of 3.225 mm giving a particle-tubing contact angle γ (see Fig. 1) of a fraction over 50°. Tests on 14 pellets of two types of material gave values of α ranging from 0.61 to 0.90 with an average of 0.78.

Meyer and co-workers (*2*) analysed this same steady-state diffusion problem theoretically and by equating the exact expression for the diffusive flux through the pellet with the empirical equation of Weisz (*1*), referred to above, were able to define α rigorously.

Thus,

$$F = D_e \frac{\pi d^2}{2} \int_0^\gamma \left(\frac{\partial c}{\partial r}\right)\bigg|_{r=d/2} \sin\theta \, d\theta$$

$$= D_e \frac{\pi d}{4}(C_1 - C_2) \cdot \frac{1}{\alpha} \qquad (2)$$

and hence

$$\alpha = \frac{(C_1 - C_2)}{2d} \cdot \frac{1}{\displaystyle\int_0^\gamma \frac{\partial c}{\partial r}\bigg|_{r=d/2} \sin\theta \, d\theta}. \qquad (3)$$

In these equations the term

$$\frac{\partial c}{\partial r}\bigg|_{r=d/2}$$

is the partial derivative of concentration of

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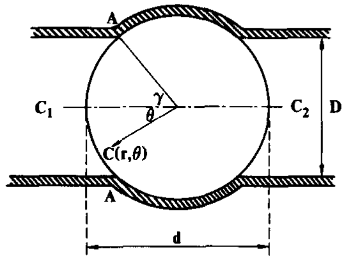

FIG. 1. The geometry of the Weisz diffusion cell.

the diffusing species with respect to the sphere radius at the sphere outer surface and θ is the spherical coordinate as indicated in Fig. 1. Meyer *et al.* (*2*) calculated α as a function of the particle-tubing contact angle γ and presented the results in the form of a graph approximately 4×5 cm in size. In our recent collaborative work with Mills and Duduković on diffusion in porous catalysts (*3*), we needed accurate values of α but found that restrictions placed upon Meyer *et al.* by their employers meant that the detailed calculations, and in particular the numerical results, on which Fig. 2 of the article of Meyer *et al.* was based could not be made generally available (*4*). We felt unable to take data from the small Fig. 2 in Ref. (*2*) with sufficient accuracy for our purposes and therefore decided that the steady-state problem needed to be resolved. This was carried out by Mills and Duduković (*5*), and in Table 1 their data are given for α as a function of the particle-tubing contact angle γ. Also provided for comparison are data taken from Fig. 2 of Meyer *et al.* (*2*) using a Hewlett–Packard 9874 A digitiser. It will be seen that whilst the trends in the two sets of information are essentially identical the work of Meyer *et al.* gives consistently lower values of α than do the computations of Mills and Duduković.

In experimental work we have found it convenient to express the relationship between α and γ in a closed form so that the geometric correction factor can be found for any chosen combination of particle and tubing diameters. A least-squares nonlinear polynomial regression on Mills and Duduković's data has yielded the following specific expression for α; this has been found to be entirely adequate in all our work.

TABLE 1

Data for the Geometric Correction Factor α as a Function of the Particle-Tubing Contact Angle γ

Particle-tubing contact angle γ (degrees)	Geometric correction factor α		
	Mills and Duduković (*5*)	Meyer *et al.* (*2*)	Calculated from Eq. (4)
10	5.441	5.058	5.438
15	3.612	3.372	3.613
20	2.709	2.554	2.707
25	2.160	2.049	2.159
30	1.787	1.678	1.787
35	1.513	1.425	1.514
40	1.300	1.228	1.302
45	1.129	1.066	1.130
50	0.986	0.932	0.986
55	0.863	0.821	0.863
60	0.756	0.730	0.754
65	0.658	0.616	0.656
70	0.568	0.541	0.568
75	0.483	0.470	0.485

Note. The data of Meyer *et al.* are taken from Fig. 2 of Ref. (*2*) and those of Mills and Duduković from Ref. (*5*).

$$\alpha = \frac{24.1016}{\gamma^2} + \frac{49.9549}{\gamma} + 0.249812 - 0.0047407\gamma - 1.40917 \times 10^{-5}\gamma^2, \quad (4)$$

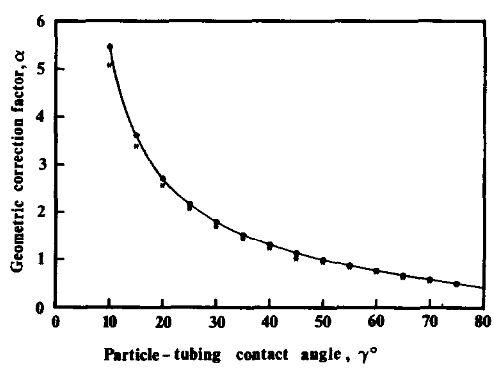

FIG. 2. The geometric correction factor α as a function of particle-tubing contact angle γ. (*) Data of Meyer *et al.* (*2*). (O) Data of Mills and Duduković (*5*). Solid line represents the polynomial approximation given in Eq. (4).

where γ is expressed in degrees.

Values for α found from Eq. (4) are given in Table 1 for comparison purposes and all of the data from this table are presented in Fig. 2. The agreement is seen to be excellent: Eq. (4) gives values for α which, for the tabulated γ range, agree with the respective values given by Mills and Duduković (5) to within much less than 0.5%. Over normal particle-tubing contact angles which lie between 45 and 60° the results of Meyer *et al.* (2) all lie within 6% of the polynomial approximation.

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