Sherwood Number for a Swarm of Adsorbing Spheroidal Particles at any Peclet Number

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In previous publications, the authors have developed theoretical models of mass transfer from a slowly moving dilute solution to a swarm of spheroidal adsorbers using the particle-in-cell approach. In the high Peclet number region (Coutelieris et al., 1993), analytical expressions have been provided for the solute concentration, the local and overall Sherwood number, and the adsorption efficiency. In the moderate Pe region ($10 \leq Pe < 1{,}000$) where solute diffusion in the direction of flow becomes non-negligible, a novel boundary condition on the outer surface of the cell has been proposed (Coutelieris et al., 1995), which ensures flux continuity across the surface even in cases where the diffusion layer crosses or lies entirely outside the outer cell boundary (except for the point of impact). Typical concentration profiles, Sherwood number values, and adsorption efficiency values have been calculated numerically as functions of the solid fraction of the swarm, the Peclet number, and the aspect ratio of prolate and oblate spheroids.

From the engineering viewpoint, the overall Sherwood number is the most significant quantity for applications that involve mass transfer to solid surfaces (catalysis, fluidization, filtration, and so on). However, although accurate Sh values for $Pe \gtrsim 10$ can be extracted either from tabulated data or analytical expressions, the region $0 < Pe < 10$ remains, practically, unexplored. The goal of this article is to propose a simple, working expression for the overall Sherwood number Sh_o for prolate and oblate spheroidal adsorbers that can be used for engineering applications over a wide range of Pe values including the limiting cases $Pe = 0$ (diffusion control) and $Pe \to \infty$ (convection control).

For *isolated* spheroids, Clift et al. (1978) proposed an expression for Sh_o which can be cast in the following form

$$Sh_o = \frac{Sh_o^*(a_3)}{2} + \left[\left(\frac{Sh_o^*(a_3)}{2}\right)^3 + K^3 Pe\right]^{1/3} \tag{1}$$

where K is a geometrical factor given in Clift et al. (1978) and $Sh_o^*(a_3)$ is the overall Sherwood number as $Pe \to 0$. For prolate spheroids

$$Sh_o^*(a_3) = 2\sqrt{a_3^2-1}\left[\ln\left(a_3+\sqrt{a_3^2-1}\right)\right]^{-1} \times\left[1+\frac{a_3^2}{\sqrt{a_3^2-1}}\sin^{-1}\left(\frac{\sqrt{a_3^2-1}}{a_3}\right)\right]^{-1} \tag{2a}$$

and for oblate ones

$$\overline{Sh_o^*}(a_3) = 2\sqrt{1-a_3^2}\,[\cos^{-1}(a_3)]^{-1} \times\left[1+\frac{a_3^2}{2\sqrt{1-a_3^2}}\ln\frac{1+\sqrt{1-a_3^2}}{1-\sqrt{1-a_3^2}}\right]^{-1} \tag{2b}$$

where a_3 is the long semiaxis of the prolate spheroid or the short semiaxis of the oblate spheroid.

Equation 1 is exact for $Pe = 0$ but deviates considerably from the numerical results of Masliyah and Epstein (1972) for $Pe \neq 0$ (Figure 1).

A substantially more accurate expression for the overall Sherwood number for isolated spheroids can be obtained with the simple addition of the Sh_o value for $Pe = 0$ and the analytical expression for Sh_o in the high Pe region obtained by Coutelieris et al. (1993), in analogy with the original suggestion of Levich (1962) for isolated spheres. The direct additivity of the diffuse and convective terms can also be derived on the basis of the Langmuir model (see Churchill, 1983). In the case of isolated spheroids this combination gives

$$Sh_o = Sh_o^*(a_3) + 0.997 g_o(a_3) Pe^{1/3} \tag{3}$$

In Eq. 3 $g_o(a_3) \equiv g(a_3, \gamma \to 0)$, where $g(a_3, \gamma)$ is a function of the aspect ratio of the spheroid and of the solid fraction of the swarm γ defined in Coutelieris et al. (1993). Tabulated values of this function for several γ and a_3 values are given in the same publication. [It should be noted here that some analytical expressions in that work can be simplified further using the exact relation $c^2(\tau_\alpha^2 - 1) = 1$]. Equation 3

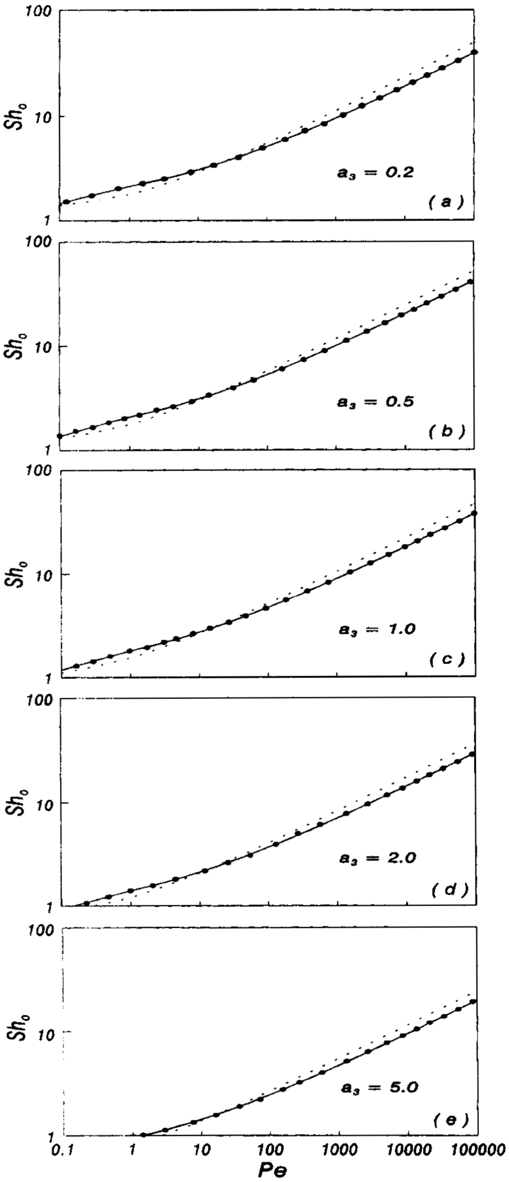


Figure 1. Overall Sherwood number vs. Peclet number for isolated (a, b) oblate spheroids; (c) sphere; (d, e) prolate spheroids.

Comparison between the two approximating formulae (dashed lines: Eq. 1; solid lines: Eq. 3) and numerical solution (marked points).

predicts the exact value at $Pe = 0$, provides accurate Sh_o estimates for $Pe > 1{,}000$ (where only the second term on the righthand side survives), and provides satisfactory estimates of the Sh_o value in the region $0 < Pe < 1{,}000$ (Figure 1) as compared to the numerical values of Masliyah and Epstein (1972), which were reproduced for the sake of this work by the authors. Figure 1 shows that Eq. 1 overestimates the actual Sh_o value for $Pe > \sim 25$ and any aspect ratio examined here ($1/5 \leq a_3 \leq 5$; both prolate and oblate geometries) including the case of spherical adsorber ($a_3 = 1$). On the other hand, Eq. 1 underestimates the actual Sh_o value for $0 < Pe < \sim 10$ and all aspect ratio values examined.

A similar approach is adopted in the present work for the case of mass transfer to a *swarm* of spherical particles modeled as convective mass transfer within a spheroid-in-cell. The approximation reads now

$$Sh_o = Sh'_o(a_3, \gamma) + 0.997 g(a_3, \gamma) Pe^{1/3} \tag{4}$$

where $Sh'_o(a_3, \gamma)$ is the overall Sherwood number at the limit $Pe \to 0$. For prolate spheroids

$$Sh'_o = 2c\left(1 + \frac{a_3^2}{c}\sin^{-1}\frac{c}{a_3}\right)^{-1}\left[\ln\frac{b_1(c + a_3)}{c + b_3}\right]^{-1} \tag{5a}$$

and for oblate ones

$$\overline{Sh}'_o = 2\bar{c}\left(1 + \frac{a_3^2}{2\bar{c}}\ln\frac{1+\bar{c}}{1-\bar{c}}\right)^{-1}[\tan^{-1}(b_3/\bar{c}) - \tan^{-1}(a_3/\bar{c})]^{-1} \tag{5b}$$

where c and $\bar{c}$ are the semifocal lengths of the prolate and oblate spheroids, respectively. Note that the lengths c, $\bar{c}$, b_1 and b_3 can be determined from the quantities a_3 and γ, and, consequently, Sh'_o and $\overline{Sh}'_o$ are functions of a_3 and γ, alone. Alternatively, Eq. 5a can be expressed as

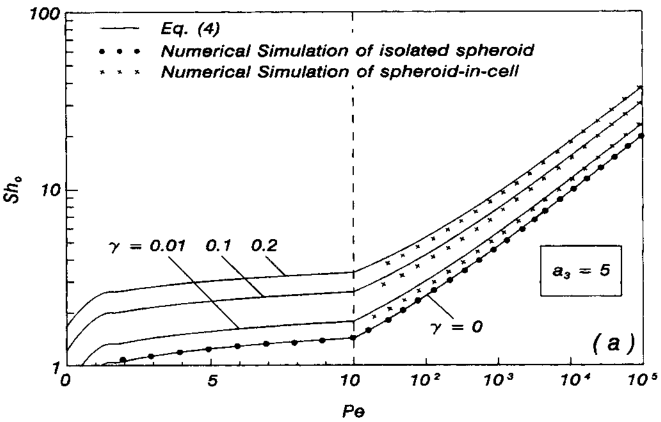
$$Sh'_o = 2\sqrt{\tau_\alpha^2 - 1}\left[\tau_\alpha^2 - 1 + \tau_\alpha^2\sqrt{\tau_\alpha^2 - 1}\sin^{-1}(\tau_\alpha^{-1})\right]^{-1} \times \left[\ln\sqrt{\frac{(\tau_\alpha + 1)(\tau_\beta - 1)}{(\tau_\alpha - 1)(\tau_\beta + 1)}}\right]^{-1} \tag{5c}$$

where τ_α $(= a_3/c)$ and $\tau_\beta (= b_3/c)$ are the values of the (modified) prolate spheroidal coordinate τ at the inner and outer spheroidal surfaces (Dassios et al., 1995). Similarly, Eq. 5b can be expressed as

$$\overline{Sh}'_o = 2\sqrt{\lambda_\alpha^2 + 1}\left[\lambda_\alpha^2 + 1 + \lambda_\alpha^2\sqrt{\lambda_\alpha^2 + 1}\ln\left(\frac{1 + \sqrt{\lambda_\alpha^2 + 1}}{\lambda_\alpha}\right)\right]^{-1} \times \left(\tan^{-1}\lambda_\beta - \tan^{-1}\lambda_\alpha\right) \tag{5d}$$

where $\lambda_\alpha (= a_3/\bar{c})$ and $\lambda_\beta (= b_3/\bar{c})$ are the values of the (modified) oblate spheroidal coordinate λ at the inner and outer spheroidal surfaces. The parameter pairs $(\tau_\alpha, \tau_\beta)$, or $(\lambda_\alpha, \lambda_\beta)$, can be used instead of (a_3, γ).

Figure 2 compares the predictions of Eq. 4 with the numerical predictions of the spheroid-in-cell model, which was developed by Coutelieris et al. (1995) and incorporated the aforementioned boundary condition of flux continuity across the outer cell surface. It was shown in that work that for $Pe \geq 10^3$ the numerical results virtually coincide with the predictions of the analytical solution for high Pe values (Coutelieris et al., 1993). For $Pe = 0$, Eq. 4 obviously yields the exact value, which is a function of the aspect ratio and the solid fraction of the swarm. Note the very good agreement between the predictions of the formula suggested here (Eq. 4) and the numerical results for $Pe \geq 10$ for several values of the solid fraction of the swarm and for relatively high aspect ra-



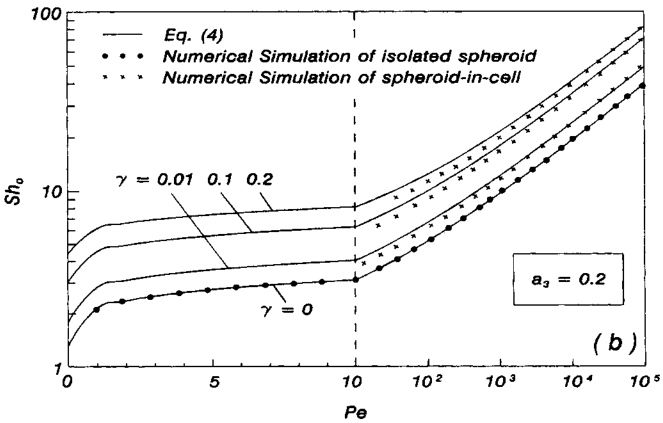


Figure 2. Overall Sherwood number vs. Peclet number in a swarm of adsorbing (a) prolate and (b) oblate spheroids.

Comparison of the predictions of the formula proposed in this work (solid curves) to numerical results.

fraction of the swarm and for relatively high aspect ratio values. The mean relative error over the difficult region $10 < Pe < 10^3$ for all the geometries of Figure 2 is less than 4%.

In conclusion, a simple expression is proposed in this work which can provide reliable estimates of the overall Sherwood number during mass transfer to adsorbing spheroidal particles over the entire range of Pe values. In the limiting case of $\gamma \to 0$ (isolated spheroid), this expression is accurate over the entire Pe value range $[0, \infty)$ within the tolerance accepted in engineering calculations. For mass transfer to a swarm of spheroids, the proposed expression is exact for $Pe = 0$, highly accurate for $Pe \geq 1{,}000$, and sufficiently accurate (better than 4% for $0.2 < a_3 < 5$ and $0 < \gamma \leq 0.2$) for engineering applications in the region $10 < Pe < 1{,}000$. It can also serve for engineering estimates of Sh_o in the region $0 < Pe < 10$, which cannot be investigated within the framework of particle-in-cell approaches as shown recently by Coutelieris et al., (1995) because of the fact that the diffusion layer lies entirely outside the cell envelope and the assumptions that underlie the particle-in-cell concept are strongly violated.

Acknowledgment

This work was supported financially by the Institute of Chemical Engineering and High Temperature Chemical Processes.

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Manuscript received June 17, 1996, and revision received Oct. 10, 1996.