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TECHNICAL NOTES

Diffusion around oblate ellipsoids—a study on the influence of particle shape on the rate of particle consumption in fluid–particle processes

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INTRODUCTION

IN CHEMICAL engineering it is often required to consider operations in which there are physico-chemical interactions between solid particles and a surrounding fluid. For the discussion which follows relevant examples of these operations are the evaporation or dissolution of solid particles, the combustion of solids and gas phase reactions catalysed by solids. In the quantitative treatment of these operations it is common practice to assume the particles to be spherical and yet this may be far from true (e.g. if the particles come out of a grinding operation). As far as diffusion and reaction rates are concerned it is important to know the error involved in that approximation. Also, if the particles are consumed in the process (e.g. evaporation) it may be important to know how the particle evolves in shape as it is consumed.

The treatment of irregular shapes and most regular shapes could only be done by computer and even then for only a few cases. A shape which lends itself to analytical treatment in problems of diffusion is the ellipsoid. Therefore it was decided to take the oblate ellipsoid as a 'model' of a non-spherical particle and to study the problems of diffusion around it. The results from this study help assess the error involved in approximating real particles by spheres. Only the limiting processes of pure diffusion control and pure kinetic control are considered. In the treatment of diffusion no allowance is made for any convective terms.

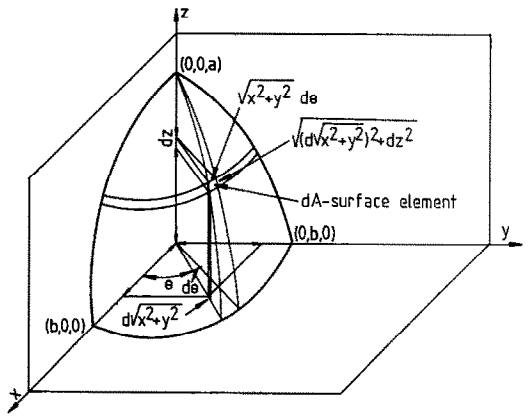

FIG. 1. Geometrical relationship between rectangular and spheroidal coordinates.

DIFFUSION AROUND AN ELLIPSOID

An oblate ellipsoid is generated by rotating an ellipse about its major axis, Fig. 1; the relationship between the rectangular and the spheroidal coordinates is [1]

$$x = e\,sh u \sin\omega \cos\theta \tag{1a}$$

$$y = e\,sh u \sin\omega \sin\theta \tag{1b}$$

$$z = e\,ch u \cos\theta \tag{1c}$$

with $0 \leqslant u < \infty$, $0 \leqslant \omega \leqslant \pi$, $0 \leqslant \theta \leqslant 2\pi$ and e the distance of the focus of the ellipse to the origin.

Consider a particle in a stagnant fluid medium with solute concentration C_∞ far away from the particle, and let the concentration of solute (i.e. diffusing species) be C^* in the fluid adjacent to the particle.

The solute concentration profile has to satisfy the equation of continuity which for steady state and in the absence of reaction in the fluid phase reads div grad $C = 0$ or

$$\frac{\mathrm{d}}{\mathrm{d}u}\left(sh u \frac{\mathrm{d}C}{\mathrm{d}u}\right) = 0 \tag{2}$$

along coordinate u.

The boundary conditions are

$$C = C^*, \quad u = u_s \text{ (i.e. on the particle surface)} \tag{3a}$$

$$C \to C_\infty, \quad u \to \infty \tag{3b}$$

the solution to this problem is

$$C - C_\infty = (C^* - C_\infty)\frac{\ln|\tan(u/2)|}{\ln|\tanh(u/2)|} \tag{4}$$

and the local diffusional flux at any point on the particle surface ($u = u_s$) may be obtained from (4) and Fick's law of diffusion as

$$N_{us} = \frac{D_g(C^* - C_\infty)}{e\sqrt{sh^2 u_s + \sin^2\omega}\,[-\ln|\tanh(u_s/2)|]sh u_s}. \tag{5}$$

This flux may be multiplied by the elemental area of the ellipsoid surface

$$\mathrm{d}A = e^2 sh u_s \sin\omega \sqrt{sh^2 u_s + \sin^2\omega}\,\mathrm{d}\omega\,\mathrm{d}\theta \tag{6}$$

to give, after integration, the total rate of diffusion of solute from the particle

$$R_{el} = \frac{4\pi e D_g}{\ln|\tanh(u_s/2)|}(C^* - C_\infty). \tag{7}$$

It is interesting to compare this rate of diffusion with that for diffusion from the equivalent sphere (i.e. the sphere with the same volume as the ellipsoid)

$$R_0 = 2\pi D_g d(C^* - C_\infty). \tag{8}$$

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NOMENCLATURE

a, a_i	semi-major axis of an oblate ellipsoid. Subscript i refers to initial conditions [m]
A	surface area [m^2]
A_{el}	surface area of ellipsoid [m^2]
A_0	surface area of equivalent sphere (i.e. sphere with same volume as ellipsoid) [m^2]
b, b_i	semi-minor axis of an oblate ellipsoid. Subscript i refers to initial conditions [m]
C	oxygen concentration [mol m^{-3}]
C^*	oxygen concentration at the particle surface [mol m^{-3}]
C_∞	oxygen concentration away from the particle [mol m^{-3}]
d	diameter of the equivalent sphere [m]
D_g	gas phase diffusion coefficient [$m^2\ s^{-1}$]
e	focal distance of ellipsoid [m]
k_c	rate constant for surface reaction [m s^{-1}]
M	molecular weight of solute [kg mol^{-1}]
N_u	diffusional molar flux along coordinate u [mol $m^{-2}\ s^{-1}$]
R_{el}	carbon combustion rate for the ellipsoid [mol s^{-1}]
R_0	carbon combustion rate for the equivalent sphere [mol s^{-1}]
s_u	length of arc along coordinate u for pure diffusion [m]
t	time [s]
u	spheroidal coordinate [m]
x, y, z	rectangular coordinates.

Greek symbols

ρ	mass of solute per unit volume of solid [kg m^{-3}]
ω, θ	spheroidal coordinates.

The relationship between d and the ellipsoid (as defined by e and u_s) is purely geometrical. The ratio R_0/R_{el} may be written as

$$R_0/R_{el} = (sh^2 u_s chu_s)^{1/3}[-\ln|\tanh(u_s/2)|] \quad (9)$$

and the dependence of this ratio on eccentricity (b/a) is shown in Fig. 2. It is apparent from this figure that diffusion from an ellipsoid is faster than diffusion from the equivalent sphere, but the error in taking the ellipsoid for a sphere is less than 20% for $b/a > 0.2$.

Also shown in Fig. 2 is the ratio between the area of the sphere A_0, and that of the ellipsoid with the same volume as the sphere, A_{el}. The difference between the values of R_0/R_{el} and A_0/A_{el} shows that with increasing eccentricity, the increase in surface area of the particle is more pronounced than the corresponding increase in the rate of diffusion.

Workers like Pecanha and Gibbs [2] account for the effect of particle shape on combustion rates of coal particles by means of a shape factor (or sphericity). The above analysis shows that those authors are overestimating combustion rates for non-spherical particles when diffusion control dominates.

Equation (5) gives the instantaneous local flux of solute under steady-state conditions. If the particle is consumed by reaction with the diffusing gas, this equation may be used to predict the evolution in shape of the particle by means of a pseudo-steady-state analysis.

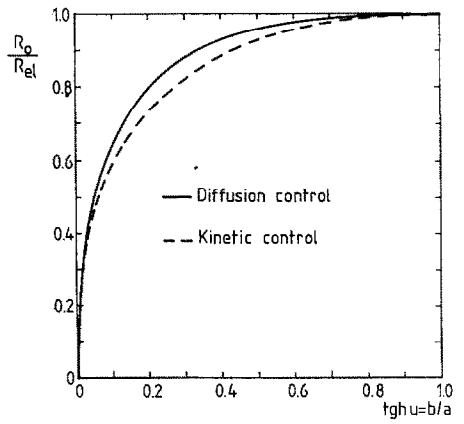

FIG. 2. Dependence of the ratio (R_0/R_{el}) upon particle eccentricity for the extreme conditions of diffusion control and kinetic control (the dashed line also gives the ratio between surface areas of sphere and ellipsoid with the same volume).

This is a somewhat lengthy mathematical exercise which leads to the important conclusion that while shrinking in a process controlled by diffusion, an ellipsoid of revolution with initial eccentricity b/a and focal length e evolves as a succession of ellipsoids of constant eccentricity, b/a, and decreasing focal length. (The authors offer to supply the proof to any interested reader.)

This information, together with equation (9), leads to the conclusion that the ratio between rates of consumption of an ellipsoid and an equivalent sphere is constant throughout the process, when under pure diffusion control.

As a result, in the event of integral analysis of rate data for a burning particle for example [3, 4], the assumption of spherical shape results in an error which may be calculated from Fig. 2 as a function of the initial eccentricity.

PARTICLE CONSUMPTION UNDER PURE KINETIC CONTROL

In processes such as carbon combustion, the particles are consumed by reaction with a gaseous species. The rate of combustion is then determined by the combined influence of reactant diffusion to, and chemical reaction at the particle surface. For high enough temperatures, the rate of particle consumption is 'diffusion controlled' on account of Arrhenius' law. The analysis presented above is applicable then. At lower temperatures carbon particles burn in 'kinetic control' and it is interesting to consider this situation for the sake of comparison.

In the absence of diffusion limitation (i.e. for a slow enough reaction rate) the concentration of gaseous reactant at the particle surface, C^*, is uniform and equal to the concentration far from the particle, C_∞. The local rate of solid reactant consumption per unit external area is then the same at any point on the particle surface, $N_{us} = k_c C_\infty$, where k_c is the kinetic constant (assuming first-order kinetics).

The overall rate of consumption of gaseous reactant over the ellipsoid is then

$$R_{el} = nA_{el}k_c C_\infty \quad (10)$$

where n is the number of moles of gas which react with one mole of solid. This is to be compared with the rate of consumption over the equivalent sphere

$$R_0 = n\pi d^2 k_c C_\infty. \quad (11)$$

The ratio $R_0/R_{el} = \pi d^2/A_{el} (= A_0/A_{el})$ and the dependence of this ratio on ellipsoid eccentricity is shown in Fig. 2. It may be seen that the error in approximating the particle by a sphere is larger in kinetically controlled reactions.

The 'velocity of shrinkage' for points on the particle surface is easily obtained as

$$\frac{ds_u}{dt} = \frac{M}{\rho} N_{us} = \frac{M}{\rho} k_c C_\infty. \quad (12)$$

Where ds_u is the element of length perpendicular to the particle surface and this is constant over the surface of the particle. As a result, the ratio b/a between minor and major axes of the ellipse decreases in the process of reaction and so the burning particle deviates increasingly from a sphere as the reaction proceeds. Indeed, in any period of time, b_i and a_i are reduced by the same amount, say s, and for $b_i < a_i$ it is obvious that $(b_i/a_i) > (b_i - s)/(a_i - s)$.

The evolution of particle shape may be easily obtained from the original ellipsoid by 'peeling off' layers of constant thickness.

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Average Nusselt number on the downward-facing heated plate

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INTRODUCTION

IN A RECENT paper Schulenberg [1] determined analytically the stagnation point heat transfer coefficient for natural convection on the horizontal downward-facing heated plate. In his Fig. 9 he plotted 12 points based upon experimental data for the ratio of average to stagnation point Nusselt number. Hatfield and Edwards [2] had correlated average Nusselt number on the basis of a virtual extension, x_0, of the boundary layer, as shown in Fig. 1, to allow for the finite thickness of the boundary layer as it flowed around the corner of the plate, or outwards onto a horizontal adiabatic extension of length L_a. In this note we apply the virtual displacement concept to find a closed-form correlation based upon Schulenberg's analysis and compare it to the previous correlation [2].

ANALYTICAL BASIS

Given a local Nusselt number Nu_x that varies with local Ra_x, where x is measured from the virtual edge, the average Nu_L based upon total length L is

$$Nu_L = \frac{\bar{h}L}{k} = \frac{L}{k}\frac{2}{L}\int_{x_0}^{x_0+L/2}\left(\frac{k}{x}Nu_x\right)dx. \quad (1)$$

In keeping with the approximate boundary-layer theory of Singh *et al.* [3] and the stagnation point solution of Schulenberg [1], a one-fifth power relationship is assumed

$$Nu_x = C'(Pr)\, Ra_x^{1/5}. \quad (2)$$

The result of Schulenberg for the stagnation point can be expressed as a Nusselt number based upon total length L

$$Nu_0 = \frac{h_0 L}{k} = 2^{2/5} C(Pr)\, Ra_L^{1/5} \quad (3)$$

where for the infinite isothermal strip Schulenberg gives

$$C(Pr) = \frac{0.571 Pr^{1/5}}{(1+1.156Pr^{3/5})^{1/3}}. \quad (4)$$

Coefficient $C'(Pr)$ in equation (2) is related to $C(Pr)$ in equation (3) by equating h_0 to the local heat transfer coefficient at $x_0 + L/2$. Equation (2) may then be substituted into equation (1) and the integration carried out. The result is

$$\frac{\bar{h}}{h_0} = \frac{Nu_L}{Nu_0} = \frac{5}{3}(1+\zeta)^{2/5}[(1+\zeta)^{3/5} - \zeta^{3/5}] \quad (5)$$

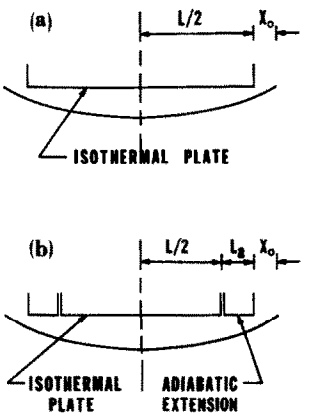

FIG. 1. Schematic of the boundary layer on a heated horizontal plate facing down. (a) Bare edges; (b) adiabatic extensions.