the cases of first-order reversible and nonreversible reactions in the reactor and also to open systems, but the Laplace transform inversions are more complicated. For nonlinear production rate equations, numerical methods must be used, but it is advisable to use normalized Equations (5), (6), and (7) rather than (1), (2), and (4).

## NOTATION

$A$ = coefficients in the series; cross section area of the column, $cm^2$
$c$ = fluid phase concentration, g/cc
$F$ = volumetric fluid phase flow rate, cc/s
$K_p$ = overall stationary phase mass transfer coefficient, cm/s
$L$ = total bed height of the sorbent bed, cm
$q$ = stationary phase concentration, g/cc
$R$ = solute production rate in source, g/s
$s$ = Laplace transformation variable
$S_0$ = sorbent particle specific surface area, $cm^{-1}$
$t$ = time, s
$v$ = interstitial fluid phase velocity in sorbent bed, cm/s
$V$ = volume of source, cc
$x$ = normalized fluid phase concentration, dimensionless
$y$ = normalized stationary phase concentration, dimensionless
$\epsilon$ = void fraction in sorbent bed, dimensionless
$\lambda$ = equilibrium distribution coefficient, dimensionless

**Subscripts and Superscripts**

$*$ denotes an equilibrium concentration
$n$ = index
$\kappa$ = index, exponent
in denotes concentration at sorbent bed inlet
out denotes concentration at sorbent bed outlet
$-$ denotes a Laplace transformed variable

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# On the Maximum Temperature Rise in Gas-Solid Reactions

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The temperature rise within a solid particle during gas-solid reactions, such as the reduction of metal oxides and the regeneration of catalyst pellets by burning off coke deposits, can be quite large. These temperature rises can introduce some difficulties. For instance, in the case of the metal oxide reduction, severe sintering may occur, thus retarding the reaction rate. The temperature rise during catalyst regeneration may cause damage to the catalyst.

Recently, Luss and Amundson (1969) reported the solution to the problem for diffusion-controlled shrinking-core systems. Their solution for a spherical pellet requires numerical integration. It is the purpose of this note to present an analytical solution for the temperature rise, which is exact for an infinite slab and is a good approximation for a spherical pellet. Asymptotic and approximate solutions for the maximum temperature rise that are more convenient to use and give more insight into the problem are also given.

The results of Luss and Amundson show that the maximum temperature rise within the pellet is quite insensitive to the modified Nusselt number, $Nu^* \equiv ha/\lambda_s$, for $Nu^* = 0 \sim 3$. Therefore, for the purpose of estimating the maximum temperature rise, it is reasonable to assume $Nu^* = 0$, that is, the resistance to the heat transfer within the pellet is much smaller compared to that between the solid and the fluid around the pellet. Under this condition the temperature within the pellet is uniform, and the governing equation becomes much simpler.

It was also shown by Luss and Amundson that, for $Sh^* \equiv k_c a/D_e$ greater than 10, the maximum temperature rise occurs a short period after the start of the reaction—when the reaction front is near the external surface. This suggests that, as a first approximation, we can neglect the curvature of the sphere in calculating the maximum temperature rise.

Using the same nomenclature used by Luss and Amundson, the temperature difference $T = T_s - T_g$ between a slab-like pellet and a gas is governed by the following relationship:

$$a\rho_s C_s \frac{dT}{dt} + hT = Q \qquad (1)$$

The position of the reaction front in a slab is given by the following [for example, see Sohn and Szekely, (1972). The relationship may be obtained by differentiating Equation (44) in the reference for $F_p = 1$ and large $\hat{\sigma}^2$, which corresponds to the diffusion-controlled shrinking-core system for a slab]:

$$\frac{dy}{dt} = \frac{n\, D_e C_A}{C_B a^2} \frac{1}{\left\{ y - \left(1 + \frac{1}{Sh^*}\right) \right\}} \tag{2}$$

The rate of heat generation $Q$ is given by

$$Q = -\, C_B\, (-\,\Delta H)_B\, a \frac{dy}{dt} \tag{3}$$

Combining Equations (1) to (3) and rearranging in dimensionless form, we obtain

$$\frac{d\theta}{d\delta} + A \left( \delta + \frac{1}{Sh^*} \right) \theta = A \tag{4}$$

where

$$\delta \equiv 1 - y \tag{5}$$

$$\theta \equiv \frac{h\, a\, T}{(-\,\Delta H)_B D_e n\, C_A} \tag{6}$$

and

$$A \equiv \frac{h}{\rho_s C_s} \left(\frac{A_p}{V_p}\right) \cdot \frac{C_B}{D_e\, n\, C_A} \left(\frac{V_p}{A_p}\right)^2 \tag{7}$$

Equation (4) is identical to the relationship obtained for a spherical pellet by linearizing the corresponding equation for $y$ close to 1, provided that $A$ is defined as in Equation (7). In view of the fact that for a spherical pellet the maximum temperature rise occurs for a small value of $\delta$, one can anticipate that the solution to Equation (4) will be approximately correct for a spherical pellet as well as pellets of other geometries.

The boundary condition for Equation (4) is

$$\theta = 0, \quad \text{at} \quad \delta = 0 \tag{8}$$

The solution is given by

$$\theta = \sqrt{2A}\, e^{-x^2} \{D(x) - D(\alpha)\} \tag{9}$$

where

$$x \equiv \sqrt{\frac{A}{2}} \left( \delta + \frac{1}{Sh^*} \right) \tag{10}$$

$$\alpha \equiv \frac{1}{Sh^*} \sqrt{\frac{A}{2}} \tag{11}$$

and $D(X)$ is given by the so-called "Dawson's integral" defined by

$$e^{-\omega^2} D(\omega) = e^{-\omega^2} \int_0^{\omega} e^{t^2}\, dt \tag{12}$$

The value of this function is tabulated in literature (Abramowitz and Stegun, 1965; Rosser, 1948), and can also be obtained from the following power series expressions (Rosser, 1948):

$$e^{\omega^2} D(\omega) = \sum_{n=1}^{\infty} \frac{(-2)^n}{1 \cdot 3 \cdot 5 \cdots (2n+1)}\, \omega^{2n+1}, \quad \text{for all } \omega \tag{13}$$

$$\cong \frac{1}{2\,\omega} \left\{ 1 + \sum_{m=1}^{\infty} \frac{1 \cdot 3 \cdot 5 \cdots (2m-1)}{(2\omega^2)^m} \right\}, \quad \text{for large } \omega \tag{14}$$

Figure 1 shows the comparison for the maximum temperature rise $\theta_m$ obtained from the closed form solution of Equation (9) and that obtained numerically by Luss and Amundson. The straight line corresponds to the large $\alpha$ asymptote as determined by Equation (20) below. It is seen that there is a good agreement for $A > 10$. For smaller values of $A$, the two solutions differ considerably because under such conditions the maximum temperature rise occurs for a large value of $\delta$—some distance in the interior of the pellet, introducing a greater effect of curvature for a spherical pellet. (See Figure 2.) In this region, however, the temperature rise is small and of no great significance. Therefore, $\theta_m$ obtained from the closed form solution of Equation (9), which is exact for an infinite slab, can be used for a spherical pellet (or for pellets of other geometries) for $A > 10$.

Figure 2 shows the comparison for the location of the reaction front for which the maximum temperature rise occurs. The result shows, not surprisingly, that for $A > 10$, the two solutions agree well. The asymptotic value of $y_m$ as $Sh^* \rightarrow \infty$ for an infinite slab is given by Equation (17) below.

From the solution given by Equation (9), some asymptotic solutions and approximate solutions can be obtained for $\theta_m$ as a function of $A$ and $Sh^*$.

#### ASYMPTOTIC SOLUTION FOR LARGE $SH^*$

As $Sh^*$ becomes large, that is, as $\alpha \rightarrow 0$, Equation (9) reduces to

$$\theta = \sqrt{2A}\, e^{-x^2} D(x) \tag{15}$$

The maximum value of the Dawson's integral occurs at $x = 0.924$ and its value is 0.541. Therefore,

$$\theta_{m,\, Sh^* \rightarrow \infty} = 0.765 \sqrt{A} \tag{16}$$

and $\theta_m$ occurs at

$$\delta_{Sh^* \rightarrow \infty} = \frac{1.31}{\sqrt{A}} \tag{17}$$

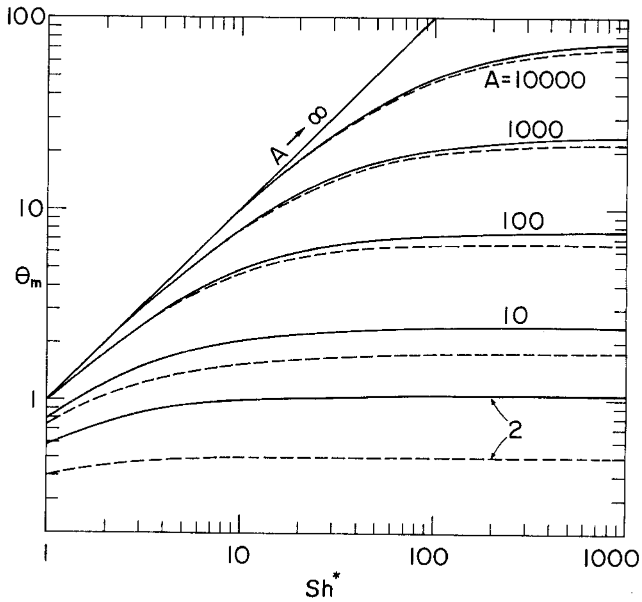


Fig. 1. Comparison between the solutions for an infinite slab and for a spherical pellet. ——— Exact solution for slab-like pellets or approximate solutions for pellets of other geometries; - - - - - Exact solution for spherical pellets.

The asymptotic solution for $\theta_m$ is shown in Figure 3, and is seen to agree satisfactorily with the exact solution for $\alpha \leqq 0.1$.

## APPROXIMATE SOLUTIONS

For small but finite values of $\alpha$, we obtain the following approximate solution from Equations (9) and (13):

$$x_{m,\ \text{small}\ \alpha} = \frac{\alpha + \sqrt{\alpha^2 + 2}}{2} \qquad (18)$$

and

$$\theta_{m,\ \text{small}\ \alpha} = \sqrt{2A}\left\{ \exp - \left(\frac{\alpha + \sqrt{\alpha^2+2}}{2}\right)^2 \right\} \cdot \left\{ D\left(\frac{\alpha + \sqrt{\alpha^2+2}}{2}\right) - D(\alpha) \right\} \qquad (19)$$

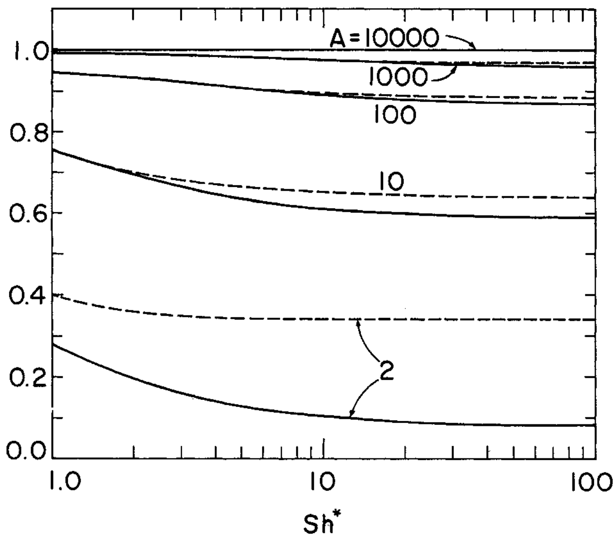


**Fig. 2. Comparison of the location of $y_m$. ——— Exact solution for slab-like pellets or approximate solution for pellets of other geometries; - - - - - Exact solution for spherical pellets.**

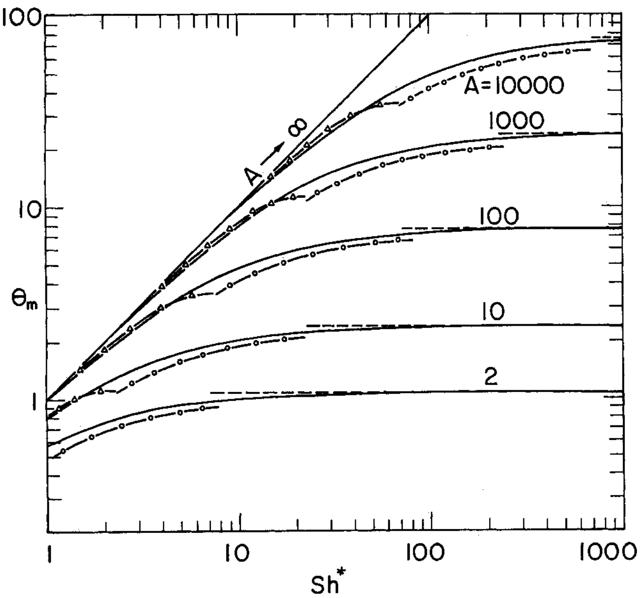


**Fig. 3. Asymptotic and approximate analytic solutions for the maximum temperature rise. ——— Exact solution; - - - - - Asymptotic solution ($\alpha \leqq 0.1$); -o-o- Approximate solution ($0.1 < \alpha < 1$); -Δ-Δ- Approximate solution ($1 \leqq \alpha$).**

This approximate solution is shown in Figure 3 and is seen to agree well with the exact solution for $0.1 < \alpha < 1$.

For large values of $\alpha$, we obtain the following from Equations (9) and (14):

$$\theta_{m,\ \alpha \to \infty} = Sh^* \left(1 - \frac{1}{2\alpha^2}\right) \qquad (20)$$

However, it has been found that the following gives a better approximation:

$$\theta_{m,\ \alpha \to \infty} = Sh^* \left[ \frac{1}{1 + \dfrac{1}{\alpha^2}} \right] \qquad (21)$$

Equation (21) is also shown in Figure 3. A satisfactory agreement exists with the exact solution for $1 \leqq \alpha$.

The results obtained here correspond to systems with $Nu^* = 0$, that is, a uniform pellet temperature at a given instance, which changes with time. They would, however, be valid approximately for systems with $Nu^* = 0 \sim 3$, which would cover most practical conditions. [See Figures 4 and 6 of Luss and Amundson (1969).]

## NOTATION

$a$ = half thickness of an infinite slab, or radius of a long cylinder or a sphere
$A_p$ = external surface area of the pellet
$c_s$ = specific heat of the pellet
$C_A$, $C_B$ = molar concentration of gas and solid, respectively
$D_e$ = effective diffusivity
$h$ = heat transfer coefficient
$(-\Delta H)_B$ = heat of reaction of solid reactant
$k_c$ = mass transfer coefficient
$n$ = number of moles of solid reacted per unit mole of gas
$r_c$ = position of reaction front
$t$ = time
$T$ = temperature difference between the solid and the ambient fluid
$V_p$ = volume of the pellet
$y$ = dimensionless position of reaction front from the center of the pellet ($y = r_c/a$)
$y_m$ = $y$ for which the maximum temperature rise occurs
$\theta_m$ = maximum value of $\theta$
$\lambda_s$ = thermal conductivity of the pellet
$\rho_s$ = density of the pellet

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