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Short Communication

A SIMPLE BUT VERY CLOSE APPROXIMATION TO THE SERIN–ELLICKSON EQUATION

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The Serin–Ellickson equation,

$$\alpha = 1 - \frac{6}{\pi^2}\sum_{n=1}^{\infty}\left(\frac{1}{n^2}\right)\exp\left(-\frac{n^2\pi^2 Dt}{a^2}\right),$$

where D is the diffusion coefficient and a the radius of a spherical body, can be approximated with high accuracy in a wide range of α values by

$$\alpha = \frac{3x^2}{\pi^2} + \frac{6x}{\pi\sqrt{\pi}},$$

where $x^2 = \frac{D\pi^2 t}{a^2}$.

One of the commonly used expressions in the study of chemical kinetics and diffusion in a spherical body is the Serin–Ellickson equation:

$$\alpha = 1 - \frac{6}{\pi^2}\sum_{n=1}^{\infty}\left(\frac{1}{n^2}\right)e^{-\frac{n^2 D\pi^2 t}{a^2}} \tag{1}$$

where D is the diffusion coefficient, a the radius of the sphere and t the time. D or D/a^2 can be determined by fitting the experiemental $\alpha(t)$ reaction rate curves to Eq. (1). Due to the complex form of this equation, the determination of the D values is time-consuming and involves the use either of standard precalculated tables or graphs or of computerised programmes [1–3].

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In this communication, the authors propose the simplest so far known, but very close approximation of the above equation, overcoming all the routine and laborious calculations normally involved in fitting the experimental data to the Serin–Ellickson equation.

Let us write:

$$x^2 = \frac{D\pi^2 t}{a^2} \tag{2}$$

Equation (1) can be written as:

$$\alpha = 1 - \frac{6}{\pi^2} \sum_{n=1}^{\infty} \left(\frac{1}{n^2}\right) e^{-n^2 x^2} \tag{3}$$

The first differential of Eq. (3), considering x^2 as the variable, is:

$$\frac{d\alpha}{d(x^2)} = \frac{6}{\pi^2} \sum_{n=1}^{\infty} e^{-n^2 x^2} \tag{4}$$

The series in Eq. (4) can be expressed in another way:

$$\sum_{n=1}^{\infty} e^{-n^2 x^2} = -\frac{1}{2} + \frac{\sqrt{\pi}}{x}\left[\frac{1}{2} + \sum_{n=1}^{\infty} e^{-\frac{n^2\pi^2}{x^2}}\right] \tag{5}$$

When $x^2 < 1.4$, the sum of the series on the right-hand side of Eq. (5) becomes very small, and for practical purposes it can be neglected with respect to 1/2.

On the other hand, if $x^2 \cong 1.4$, Eq. (3) gives $\alpha \cong 0.9$. This result implies that for $x^2 < 1.4$ the nearly full range of α usually investigated has been taken into account.

Equation (4) can now be written as:

$$\frac{d\alpha}{d(x^2)} \cong \frac{6}{\pi^2}\left[-\frac{1}{2} + \frac{\sqrt{\pi}}{2x}\right] \tag{6}$$

By integration of Eq. (6) we obtain the following approximation of the Serin–Ellickson equation:

$$\alpha \cong -\frac{3x^2}{\pi^2} + \frac{6x}{\pi\sqrt{\pi}} \tag{7}$$

The difference Δ in the values of α given by the Serin–Ellickson equation (3) and Eq. (7) is less than 10^{-3} for $\alpha \cong 0.9$. It rapidly decreases with decreasing α, as shown in Table 1.

Table 1 Values of Δ for different ranges of α

α	< 0.9	< 0.84	< 0.78	< 0.7
Δ	$< 10^{-3}$	$< 10^{-4}$	$< 10^{-5}$	$< 10^{-7}$

By solving Eq. (7), we obtain:

$$x = \sqrt{\pi}\left[1 - \left(1 - \frac{\pi}{3}\alpha\right)^{\frac{1}{2}}\right] \tag{8}$$

Equation (8) enables the calculation of x from the experimental values of α. From a plot of x^2 against t via Eq. (2) we can obtain $D\pi^2/a^2$ directly, and the value of the diffusion coefficient D if the radius a of the sphere is known.

At this point it may be emphasized that, even if the diffusion coefficient D is a function of t, Eq. (8) allows determination of the experimental curve $D(t)$, which is otherwise very difficult using the original Serin–Ellickson equation directly.

References

1 Comprehensive Chemical Kinetics, Elsevier, Amsterdam, 1969, Vol. 2.

2 Conduction of Heat in Solids, Oxford University Press, 1947.

3 J. Crank, The Mathematics of Diffusion, Oxford University Press, 1956.