Journal of Thermal Analysis, Vol. 8 (1975) 349—350

Short communication

A SOLUTION OF THE EXPONENTIAL INTEGRAL IN THE NON-ISOTHERMAL KINETICS FOR LINEAR HEATING

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(Received October 16, 1974)

A simple and satisfactorily accurate solution of the exponential integral in the non-isothermal kinetic equation for linear heating is proposed:

$$\int_0^T e^{-E/RT} \mathrm{d}T = \frac{RT^2}{E + 2\,RT}\, e^{-E/RT}$$

In the theory and practice of non-isothermal investigations, the solution of the general kinetic equation

$$\int_0^\alpha \frac{\mathrm{d}\alpha}{f(\alpha)} = \frac{A}{q} \int_0^T e^{-E/RT}\, \mathrm{d}T \tag{1}$$

(with symbols used as customary) is of great importance. For the case of hyperbolic heating $\frac{1}{T} = a - qt$, the solution of the right-hand side of Eq. (1) does not give rise to difficulties [1]:

$$F(\alpha) = \frac{AR}{qE} e^{-E/RT} \tag{2}$$

Substantial difficulties arise, however, when Eq. (1) must be solved for the case of linear heating $T = b + qt$. Various approximations for solving the exponential integral have been reported in the literature [2, 3]. Among these, the best approach is yielded by the solution of Coats and Redfern [4, 5]:

$$F(\alpha) = \frac{A}{q}\left(1 - \frac{2\,RT}{E}\right)\frac{RT^2}{E} e^{-E/RT} \tag{3}$$

We propose a new solution of Eq. (1) (without quoting the algoritm of integration), namely

$$F(\alpha) = \frac{A}{q} \cdot \frac{RT^2}{E + 2RT} e^{-E/RT} \tag{4}$$

We shall demonstrate that Eq. (4) is more accurate than Eq. (3). For this purpose, let us differentiate the right-hand side of Eq. (3), yielding, after the necessary mathematical transformations,

$$\frac{dF}{dT} = \frac{A}{q}\left(1 - \frac{6R^2T^2}{E^2}\right) e^{-E/RT} \tag{5}$$

Subjecting Eq. (4) to similar mathematical operations leads to

$$\frac{dF}{dT} = \frac{A}{q}\left\{1 - \frac{2R^2T^2}{(E + 2RT)^2}\right\} e^{-E/RT} \tag{6}$$

In the general case, $\frac{6R^2T^2}{E^2} \ll 1$ and $\frac{2R^2T^2}{(E + RT)^2} \ll 1$, but $\frac{2R^2T^2}{(E + 2RT)^2} < \frac{6R^2T^2}{E^2}$ and consequently the proposed solution of Eq. (1) in the form of Eq. (4) is more accurate.

References

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