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Note

ON THE USE OF THE FUNDAMENTAL EQUATIONS OF NON-ISOTHERMAL KINETICS

E. URBANOVICI and E. SEGAL

Chair of Physical Chemistry and Electrochemical Technology, Faculty of Chemical Engineering, Polytechnical Institute of Bucharest, Bulevardul Republicii 13, Bucharest (Romania)

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The fundamental classical equation of non-isothermal kinetics is [1,2]

$$\frac{d\alpha}{dT} = \frac{A}{\beta} f(\alpha) e^{-E/RT} \tag{1}$$

In this rate equation $A \approx$ const, $E \approx$ const and $f(\alpha)$ keeps, in principle, the same form throughout the whole reaction. Through variable separation and integration, eqn. (1) becomes

$$\int_0^\alpha \frac{d\alpha}{f(\alpha)} = \frac{A}{\beta} \int_0^T e^{-E/RT} dT \tag{2}$$

By introducing the usual notation

$$\int_0^\alpha \frac{d\alpha}{f(\alpha)} = F(\alpha)$$

and

$$\int_0^T e^{-E/RT} dT = I(T)$$

where $F(\alpha)$ and $I(T)$ are the conversion integral and temperature integral, respectively, eqn. (2) takes the shorter form

$$F(\alpha) = \frac{A}{\beta} I(T) \tag{3}$$

These differential and integral kinetic equations can be used to solve the following problems.

Evaluation of E *and* A *as well as calculation of* $f(\alpha)$ *from known values of* α, T *and* $d\alpha/dT$

To determine the non-isothermal kinetic parameters, eqn. (1) is easy to use (from a mathematical standpoint); when using the integral equation (2) one has to take into account that the conversion integral, $F(\alpha)$, and the tempera-

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ture integral, $I(T)$, can be solved only approximately (except some usual cases for $f(\alpha)$ and some non-linear heating programmes for $I(T)$). Thus, one has to take care to use rather simple approximations.

Evaluation of α *from known* E, A, $f(\alpha)$ *and* T

In this case one has to solve eqn. (2) with respect to numerical values needed for the calculation of the temperature integral.

Evaluation of T *from known* E, A, $f(\alpha)$ *and* α

Equation (3) has to be solved with respect to T. The difficulty consists in the presence of T as an integration limit.

Evaluation of α *and* T *from known* E, A, $f(\alpha)$ *and* $d\alpha/d\mathrm{T}$

In this case one has to solve the system of eqns. (1) and (2) with α and T as unknowns.

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