

Note

AN ATTEMPT FOR A NEW CLASSIFICATION OF THE METHODS USED TO EVALUATE NON-ISOTHERMAL KINETIC PARAMETERS

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The most common, well-known and -used classification of the methods applied to evaluate non-isothermal kinetic parameters was given by Flynn–Wall [1] and Šesták–Šatava–Wendlandt [2]. The classification is based on a mathematical criterion using mainly differentiation or integration to get the necessary equations from which the values of the kinetic parameters can be obtained.

In this note a new classification of the non-isothermal kinetics methods based of the extent of the (α, t, T) interval is suggested. According to our classification the following groups of methods should be distinguished.

(1) Methods which use the integration over all the values of (α, t, T)

Notation \rightarrow

Examples. The methods worked by van Krevelen et al. [3], Reich–Levis [4], Coats–Redfern [5], Ozawa [6], Urbanovici–Segal [7].

Advantages. (a) The methods are rather insensitive to experimental errors; (b) the kinetic equations are easy to linearize.

Disadvantages. The methods are insensitive to the eventual changes of the kinetic parameters.

(2) Methods which use integration over small values of (α, t, T)

Notation \leftarrow

Examples. The methods worked by Urbanovici–Segal [8].

Advantages. (a) The methods are sensitive to the changes of the kinetic parameters; (b) the temperature integral can be easily solved.

Disadvantages. (a) The methods are sensitive to experimental errors mainly for very small intervals of (α, t, T) values; (b) complicated working formulae.

*(3) Methods which use point values of the experimental data (α , t, T)**Notation* —●—

Examples. The methods worked by van Krevelen et al. [3] Freeman–Carroll [9], Kissinger [10], Turner–Schnitzer [11], Achar–Brindley–Sharp [12], Piloyan [13], Alakhverdov–Steopin [14].

Advantages. The methods are sensitive to the eventual changes of the kinetic parameters.

Disadvantages. The methods are sensitive to the experimental errors (mainly to the errors of the reaction rate evaluation).

Concerning the correspondence between our classification and that reported in the literature [1,2], it is easy to see that the groups of methods \rightarrow and \leftarrow correspond to the integral methods while the group $\rightarrow\bullet\leftarrow$ corresponds to the differential, and difference-differential ones.

REFERENCES

- 1 J.H. Flynn and L.A. Wall, J. Res. Natl. Bur. Stand., Sect. A, 70 (1960) 487.
- 2 J. Šesták, V. Šatava and W.W. Wendlandt, Thermochim. Acta, 7 (1973) 333.
- 3 D.W. van Krevelen, C. van Heerden and F.J. Huntjens, Fuel, 30 (1951) 253.
- 4 L. Reich and D.E. Levis, Makromol. Chem., 66 (1963) 102.
- 5 A.W. Coats and J.P. Redfern, Nature (London), 201 (1964) 68.
- 6 T. Ozawa, Bull. Chem. Soc. Jpn., 38 (1965) 1881.
- 7 E. Urbanovici and E. Segal, Thermochim. Acta, 80 (1984) 379.
- 8 E. Urbanovici and E. Segal, Thermochim. Acta, 80 (1984) 389; in press.
- 9 E.S. Freeman and B. Carroll, J. Phys. Chem., 62 (1958) 394.
- 10 H.E. Kissinger, Anal. Chem., 29 (1957) 1702.
- 11 R.C. Turner and M. Schnitzer, Soil. Sci., 13 (1963) 225.
- 12 B.N. Achar, G.W. Brindley and J.H. Sharp, Proc. Int. Clay Conf., Jerusalem, 1966, Vol. 1, p. 67.
- 13 F.O. Piloyan, I.O. Ryabchikov and O.S. Novikova, Nature (London), 212 (1966) 1229.
- 14 G.P. Alakhverdov and B.D. Steopin, Zh. Fiz. Khim., 43 (1969) 2268.