Addendum to "A simple kinetic method for the determination of the reaction model from non-isothermal experiments"

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To the Editor,

In 2010, J. Farjas, N. Butchosa, and P. Poura at the University of Girona published an article in the Journal of Thermal Analysis and Calorimetry titled "A simple kinetic method for the determination of the reaction model from non-isothermal experiments" [1]. The article describes an approach to determining reaction order from the shape of the reaction exothermic peak using the time at full-widthat-half-maximum ($\Delta t_{\rm FWHM}$) as the metric. Equation 24 of that publication relates the value of the parameter $\Delta t_{\rm FWHM}$ to reaction order nor for *n*th order reactions, through third-order polynomials in n. Because the purpose of the article is to obtain n from $\Delta t_{\rm FWHM}$ a relationship where $\Delta t_{\rm FWHM}$ is the independent variable would be more useful to users. In correspondence, Dr. Farjas has re-examined the data and offers the following relationship for this purpose.

$$n = -0.39374 + 0.36063\Delta t'_{\text{FWHM}} + 0.08934\Delta t'_{\text{FWHM}}^{2}$$

The difference between the exact and approximate values of *n* in this equation is below 0.04 for 0.11 < n < 3.96 covering the complete practical range for *n*.

 $\Delta t'_{\rm FWHM}$ can be determined from the value of time's half width at half maximum at infinite heating rate, $\Delta t'_{\rm FWHM}/A$, where *A* is the pre-exponential term of the rate constant. Both *A* and $\Delta t'_{\rm FWHM}/A$ can be obtained from the *y*-intercept of the Kissinger and ln($\Delta t_{\rm FWHM}$) versus the reciprocal of peak temperature plots, respectively.

Readers of the original article may well wish to add this relationship to the original article as a useful expansion.

Reference

 Farjas J, Butchosa N, Roura P. A simple kinetic method for the determination of reaction model from non-isothermal experiments. J Therm Anal Calorim. 2010;102:615–25.

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