Reasonable application of isoconversional methods

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Isoconversional methods are widely applied in thermoanalytical kinetics. They are based on the concept of single-step approximation residing in the substitution of a set of kinetic equations by the single-step rate equation. The main advantage of this approach is that it enables description and modelling of the kinetics of the process without a deeper insight into its mechanism [1,2]. The isoconversional methods can be divided into three groups, i.e. the differential, incremental and integral ones [2] where the latter group is mostly used for the treatment of kinetic data. The Arrhenius equation is mostly applied as the temperature function [3]. It has been demonstrated that also non-Arrhenian functions can be applied and that the Arrhenius and non-Arrhenian temperature functions are equivalent in the temperature range of measurement and describe the experimental data on the same qualitative level. The kinetic parameters from various temperature functions can be then recalculated so that the problems with evaluating the temperature integral can be removed [4]. When extrapolating the conclusions outside the temperature region of measurements, the stability estimates most corresponding with experience are achieved for the non-Arrhenian temperature functions; the Arrhenius function tends to overestimate the material stability [5].

A great flaw of isoconversional methods was recognized only recently. In case of variable activation energy, the integral isoconversional methods are mathematically incorrect and the predicted dependence of conversion vs. time shows nonsensical course [6] (see the figure below). Hence, the integral isoconversional methods should be avoided; the incremental methods could be used instead as demonstrated in [7].

LITERATURE

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