DSC baseline interpolations: Importance for kinetic evaluations

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Many powerful tools and methodologies exist nowadays for easy and precise execution of the kinetic analysis and determination of the corresponding kinetic parameters. Accordingly, the decision point regarding the reaction/transformation kinetics has shifted towards acquisition of high quality kinetic data and their correct preparation. With respect to the latter, correct identification and consequent subtraction of the thermokinetic background (baseline, zeroline) belongs to the most important procedures. The tangential area-proportional baseline is the most universal baseline not only because of its correction possibilities but most importantly because it represents true, physically substantiated evolution of the heat capacity in the given system. However, the tangential area-proportional baseline is often not included in the standard operating and evaluation software packages of TA instruments, and its programming requires an iterative approach. Therefore, various, more easily accessible approximations and substitutions are often being utilized, which are based on the interpolation algorithms employing only the pre- and post-peak data. Obviously, usage of these approximations leads to certain distortion of the kinetic data and corresponding introduction of systematic errors into the results of the kinetic analysis.

In the present contribution the errors associated with application of the three most common interpolations — linear, cubic spline and Bezier — will be analyzed and quantified for several typical cases of the thermokinetic background course. In the first batch of theoretically simulated data we will approach the simplest case of a single process with JMA asymmetry exhibiting various differences between the heat capacities of products and reactants. The second batch of theoretically simulated data will then demonstrate the degree of errors arising from usage of inaccurate interpolations in case of different asymmetries of the kinetic peak.

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