

SC13

Extended Thermal Analysis by Advanced Software Programs: Kinetics, Purity, and Multicomponent Analysis

J.R. Opfermann, E. Kaisersberger
NETZSCH-Gerätebau GmbH, Selb, D

The modern analysis technique is characterized by an enhanced level of automation and enhanced speed of measurement. Both developments result in the fact that a large amount of data is acquired. On the basis of these data now the possibility is opened to make deeper analysis as before. Now a new problem is created: the problem of data mining, consisting in differentiation of various effects and understanding of running processes in the sample.

With 'Advanced Software' NETZSCH-Geratebau offers a library of programs, supporting the work of scientists and engineers in the field of thermal analysis. In this library a series of modern techniques of data analysis are combined.

Thermokinetics

This program contains different methods of multiple-scan analysis, based on thermoanalytical data

(DSC, TGA, Mass spectrometry, Rheometry and Vulcmetry):

- model-free analysis according to Friedman, Ozawa-Flynn-Wall and ASTM E698,
- model-fit with up to 4-step reactions, using 16 different reaction types,
- many possibilities of prediction and optimization.

Two other programs, ChemRheo and Thermal Simulation, allow on the basis of results of Thermokinetics the kinetic analysis of rheometric data and simulations of thermal behavior, respectively. Finally, the connection between the expanded FEM program ANSYS and Thermokinetics is closed by a new module and allows simulation of thermal behavior under more complex conditions.

With this program two problems of purity determination, based on DSC melting scans, are solved: a) the determination of thermal resistance, using the purity as criterion, improves the confidence of estimation in the range of high purity calibration, b) the use of non-approximated formulas improves the accuracy of higher values of impurity and enlarges the range of analysis.

Multicomponent Analysis

On the basis of the well known Partial Least Squares (PLS) techniques this program allows the combination of measurements of various types (DSC, TGA, MS, FTIR) in one analysis. This opens a new situation of data mining and robust solutions of quantitative thermal analysis. The power is demonstrated on the quantitative determination of microwax in paraffin and of determination of individual contents of LDPE, HDPE and PP in mixtures.