Advanced tools for prediction of thermal ageing, safety analysis and migration from food packaging

B. Roduit [1] and V. Dudler [2]

[1] Advanced Kinetics and Technology Solutions (AKTS AG) TECHNO-Pôle, CH-3960 Siders - http://www.akts.com
[2] Swiss Federal Office of Public Health (OFSP), Division of Food Science, CH-3003 Bern - http://www.admin.ch/bag

An advanced study on the thermal behaviour was carried out by hyphenated techniques using a biopolymer as a model reaction. In order to apply correctly the EGA signals for the description of the kinetics of the decomposition reactions, the interaction between thermoanalytical and mass spectrometric curves in TA-MS system must be known. If the time lag between the thermoanalytical curve (e.g. DTG) and EGA signal (e.g. MS) is negligible, then the spectroscopic signal can be used not only for the qualitative analysis of the gaseous products but also for the kinetic description of the process [1]. The study focused on the prediction of the thermal stability of aged and reference samples both in extended temperature ranges and under temperature conditions at which ordinary investigation would be very difficult. These difficulties are prevalent at low temperatures (requiring very long investigation scanning times), as well when under specific temperature fluctuations [2]. Complex temperature profiles were considered such as isothermal, non-isothermal, stepwise, modulated, shock, adiabatic conditions [3] and additionally temperature profiles reflecting real atmospheric temperature changes (yearly temperature profiles of different climates with daily minimal and maximal fluctuations). Employing Finite Element Methods (FEM), the technique was extended to predict the amount of a substance (decomposition products, additives, contaminant or residual monomer) that can migrate from a plastic packaging material into the wrapped food. The technique allowed the simulation of complex packaging (different geometries and multilayer films). Calculation of the diffusive process was based on Fick's law. It considered the Arrhenius equation and the last version of the Piringer model with refined Ap constant for the approximation of the diffusion coefficients [4, 5]. Diffusion and concentration distribution inside all package layers can be computed for both the migrant and the food components.

During the lecture, on-line calculations using AKTS-TA- and SML-software will illustrate the determination of the kinetics and application of FEM for the prediction of the migration. The decomposition of the biopolymer will be used as a case study.

REFERENCES

1. B. Roduit, M. Maciejewski and A. Baiker, Influence of experimental conditions on the kinetic parameters of gas-solid reactions - parametric sensitivity of thermal analysis, Thermochim. Acta 282/283, 101-119, 1996.
2. B. Roduit, Computational aspects of kinetic analysis. Part E: The ICTAC Kinetics Project - Numerical techniques and kinetics of solid state processes, Thermochim. Acta 355, 171-180, 2000.
3. F. Stoessel, J. Steinbach, A. Eberz: Plant and process safety, exothermic and pressure inducing chemical reactions, In: Ullmann's encyclopedia of industrial chemistry. Weise E (Eds), VCH, Weinheim (1995):343-354.
4. O. Piringer, Food Additives and Contaminants, 11 (1994) 221.
5. Materials and articles in contact with foodstuffs – Plastics: Estimation of migration by generally recognized diffusion models in support of EU Directive 90/128/EEC (Migration modelling), CEN/TC194/SC1/WG4 N106, version 1, August 2001.