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Up-scaling of DSC data of self-heating materials

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ABSTRACT

The study of thermal properties of various energetic materials was based on the thermoanalytical experiments (Differential Scanning Calorimetry DSC) carried out with few heating rates. Obtained DSC signals, after optimization of the base-line were used for the calculation of the kinetic parameters (KP) KP of the decomposition process applying advanced kinetic software of AKTS [1-3]. The determination of the kinetic parameters was based on the differential iso-conversional method of Friedman [4]. The correctness of the estimation of KP was checked by the comparison of the experimental and predicted courses of the decomposition [1-6].

The slow cook-off (Up-scaling of DSC data to 1 kilogram and more) experiments of the self-reactive materials were carried out with the rate 3.3 °C/h. For the simulation of the experimental results the heat balance based on the Finite Element Analysis (FEA) was applied together with the advanced kinetic description of the reaction. The comparison of the experimental and simulated data indicates that applied procedure resulted in a very good prediction of the temperature of the ignition. Application of commonly used simplified assumptions concerning the mechanism of the decomposition (such as first- or *n-th* order mechanisms) led to significantly worse prediction of the cook-off temperatures.

During the lecture, on-line calculations using AKTS-Thermokinetics and AKTS-Thermal Safety Software will illustrate the determination of the kinetics and present the FEA applications for the prediction of cook-off experiments.

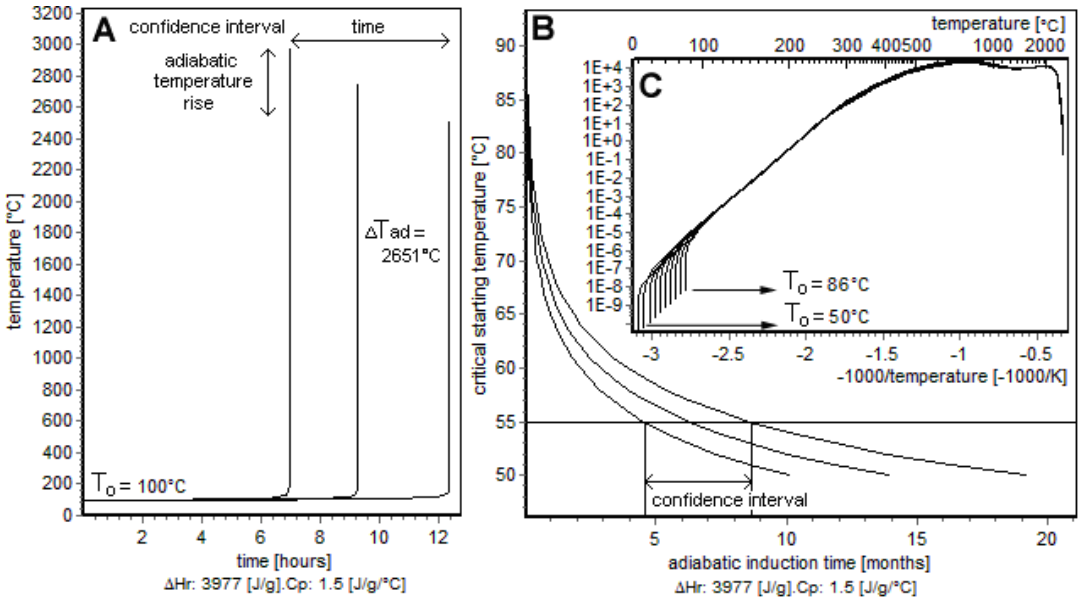

Fig. 1 (A) Adiabatic runaway curves for a boost propellant (isochoric conditions) showing the confidence interval for the prediction (T_{begin}=100°C and $\Delta T_{ad}=\Delta H_r/c_p$=2651±233°C). The confidence interval was determined for 95% probability.
(B) Starting temperature and corresponding adiabatic induction time TMR_{ad} relationship of the boost propellant under isochoric conditions. The choice of the starting temperatures strongly influences the adiabatic induction time (confidence interval: 95% probability). (C) Heat rate curves versus temperature for the boost propellant under isochoric conditions.

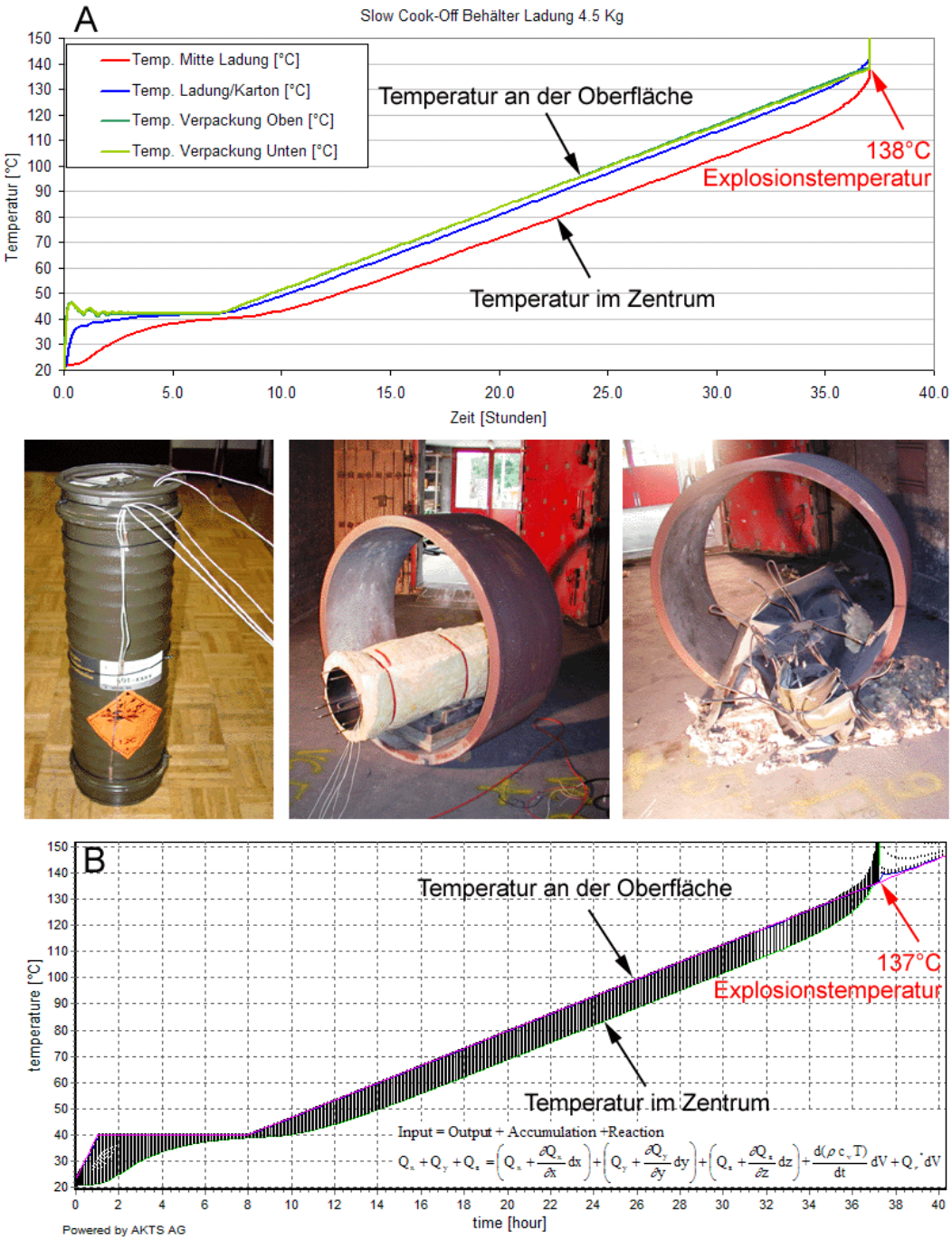

Fig. 2 Slow cook-off experiments of a nitrocellulose based substance (A) and simulation (B). As presented in the figure, the predicted temperature of explosion was 137°C. It is in good agreement with the slow cook-off experiments (138°C).

1. Advanced Kinetics and Technology Solutions: http://www.akts.com (AKTS-Thermokinetics software and AKTS-Thermal Safety software).
2. B. Roduit, Ch. Borgeat, B. Berger, P. Folly, B. Alonso, J.N. Aebischer and F. Stoessel,. J. Therm. Anal. Cal., ICTAC special issue, 80 (2005) 229–236.
3. B. Roduit, Ch. Borgeat, B. Berger, P. Folly, B. Alonso, J.N. Aebischer,. J. Therm. Anal. Cal., ICTAC special issue, 80 (2005) 91–102.
4. H.L. Friedman,. J. Polym. Sci. Part C 6: (1965) 183–195.
5. Stoessel F, Steinbach J, Eberz A: 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.
6. P. Reuse, H. Fierz, Characterisation of pressure and temperature rise of run-away reactions using temperature-programmed measurements, CHISA 2004 Proceedings [510].