ADVANCED SIMULATION OF THE COOK-OFF EXPERIMENTS

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Simulation of cook-off i.e. the thermally induced firing of energetic materials is a complicated task that requires the consideration of two issues: (i) the correct description of the kinetics of the process i.e. the temperature dependence of the reaction rate on the temperature and (ii) the precise link between kinetics and thermal behavior of the investigated materials. Both these tasks are strongly related because, without correct heat balance considerations, even the most exact evaluation only of the kinetics based on the experiments carried out in mg scale is of little value for the prediction of the real behaviour of materials in kg or Mg scale. On the other hand, the precise knowledge of the thermal properties of the energetic materials when applied with the data based on too simplified kinetic description of the decomposition (as e.g. still commonly used simple models such as ”zeroth-” or “first” order reaction) will not lead to the correct prediction of the time to ignition of the cook-off experiments as well.

In our former work [1] we have proposed the method of the application of the advanced kinetic description of the decomposition of the energetic material combined with the exact heat balance carried out by Finite Element Analysis. Present study extends the simulation by introducing into consideration an analysis of influence of additional parameters such as thermal conductivity of the materials, their geometry, and different temperature profiles of the surrounding environment.

The thermal decomposition of six propellants: two small calibre types P 3616 Ws (5.56 mm, single base); P 3620 Ws (5.56 mm, EI®) and four medium calibre types FM 3170/21 (23 mm, single base); FM 3031s (25 mm, EI®); VM 0696/102s (30 mm, EI++) and VM 0700/101s (30 mm, EI++) was investigated by Differential Scanning Calorimetry (DSC). The slow cook-off experiments were carried out in cylindrical reactor with the diameter of 47 mm with a heating rate of 3.3°C/h according to STANAG 4382. The results of DSC experiments carried out with at least 3 heating rates in the range of 0.25-4°C/min were elaborated by Thermokinetics software [2]. Obtained kinetic parameters were applied for the simulation of the ignition temperature of the propellants during the slow cook-off and for the determination of the time to maximum rate under adiabatic conditions. The Thermal Safety software [2] enabled also the simulation of the thermal ignition of the propellant conditioned previously for 12h at 80°C and exposed later isothermally for 8h to temperatures between 120-180°C, the determination of the influence of the geometry of the investigated sample and thermal properties of combustible munitions cartridges on the ignition temperature. Additionally, the simulation of the time to ignition in the thermal environment created by the fire at conditions included in EN Standard concerning the fire resistance EN1991-1-2 (2002) was performed.

During the lecture, on-line calculations using AKTS-Thermokinetics- and Thermal-Safety Software will illustrate the determination of the kinetics and simulation of the propellants behavior.

[1] B. Roduit, C. Borgeat, B. Berger, P.Folly, J.N.Aebischer, H.Andres, Ul.Schädeli, J. Therm. Anal. Cal., 85 (2006) 195-202
[2] Advanced Kinetics and Technology Solutions: http://www.akts.com (AKTS-Thermokinetics- and Thermal Safety software).