PREDICTION OF THERMAL AGING OF MATERIALS BY MODIFIED KINETIC ANALYSIS BASED ON LIMITED AMOUNT OF EXPERIMENTAL POINTS

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The investigation of materials aging process at ambient temperatures is experimentally very difficult due to its very low rates and small changes of physicochemical properties. Commonly applied methods of thermal-aging determination are therefore based on measuring material properties at several elevated temperatures followed by plotting log of time-to end-of-life at each temperature against the reciprocal of absolute temperature and, finally, calculating best-fit straight line by regression analysis. In this study we propose a modified method for the kinetic analysis of experimental data. In proposed modification both, n-th order and autocatalytic kinetic models are applied, what results in much better fit of experimental data. The method used to compare different models takes into account not only the quality of regression fit, but also the number of data points and number of parameters in specific models based on the Akaike information criterion (AIC) [1]. Such procedure allows concluding which model is more likely to be correct. The proposed method delimits also the borders of the prediction band based on the bootstrap method [2-3] (e.g. confidence interval 95%) showing scatter of the data and allows considering uncertainty of the best-fit curve being very important for thermal aging predictions. Advantages of new method will be illustrated by results of investigations of thermal aging process of some polymers, biopharmaceutical products and energetic materials. The proposed method was validated among others (fig.1) by comparing results of the predictions with subsequent measurements performed at various temperatures after longer period (c.a. 9 months) of storage time.

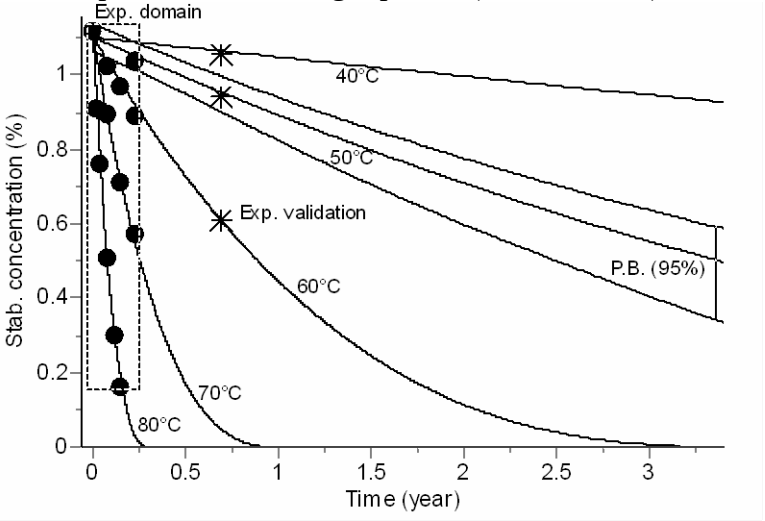

Fig.1 Prediction of change of stabilizer concentration in double base propellant based on the data collected in experimental domain depicted on the plot. Prediction curves at 40, 50 and 60°C were verified by the experimental points marked by asterisks. The prediction band PB is shown for the simulations of the process course at 50°C.

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