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Evaluating Thermal Explosion Hazard of Self-Reactive Substances by Using Kinetics-Based Simulation Approach

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ABSTRACT

Analysis of possible development of runaway at production, storage and use of a chemical product, and subsequent choice of measures that can prevent an accident or mitigate its consequences is one of the main tasks of reaction hazards assessment. A kinetic model evaluated from calorimetric data gives the reliable basis for implementing the analysis by means of numerical simulation. The purpose of this paper is to discuss some features of the approach as applied to such typical problem as determination of critical conditions of thermal explosion for solid and liquid reactive chemicals.

The hierarchical approach is proposed which comprises the use of some simplified theories for preliminary survey with the following numerical simulation for getting more detailed data.

The mathematical models of thermal explosion in solid and liquid reacting systems are presented followed by a basic sketch of the numerical methods chosen for solving the problems.

The practical usefulness of the simulation approach for analyzing explosion development is illustrated with several examples.

The discussed models and methods were embodied in the ThermEx and ConvEx program packages developed by CISP. All the presented results have been obtained by means of this software

Keywords: reaction hazard; thermal explosion; numerical simulation