THERMAL ANALYSIS AND CALORIMETRY FOR PROCESS SAFETY APPLICATIONS

Gaëlle LEBOURLEUX, Rémi ANDRE, Maxime BOURDON

KEP Technologies EMEA, 12 rue de Verdun, 69300 CALUIRE-ET-CUIRE

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Process safety is more and more implemented in order to first of all, ensure the safety of collaborators and peoples living around the plant. The second objective in to preserve the manufacturing tools and avoid extra cost to repair or rebuilt. The third is to keep a good reputation. Most of industrial accident are covered by media which give a strong visibility to the company. This may affect its image to population, customers and investors.

Additionally, local and continental regulations define the scope of Process Safety and reactive substances management. In Europe, the 2012/18/EU "Seveso III" Directive obliges the operators of establishments where dangerous substances are present in significant quantities to provide the competent authorities with risks analysis, and possible major-accident scenarios. It includes the classification of any substance involved or likely to be present on the site into categories such as "explosives" or "self-reactive substances". Any new substance used or produced on the plant thus requires thermal stability testing to check whether it has to be listed in a dangerous substance category.

Thermal analysis and calorimetry are part of most process safety strategy. A typical testing flow will be the following:

- First, a quick screening using Differential Scanning Calorimetry (DSC). This step mainly aimed at determining the thermal stability of all compounds that may be involved in the reaction: reactants, intermediates, final product. The information will be the temperature at which the decomposition starts and the energy released.
- Following the screening phase, deeper analysis can be made on a selected number of compounds using Rapid Screening Calorimetry (RSC). The thermal stability will be tested on a higher mass of sample and a measure of pressure can be added. This parameter will be useful to evaluate the pressure rise under normal and runaway conditions and give some indications on the quantity of evolved gases. It will help to size a reactor.
- To continue in the reactor sizing, an essential step, is the reaction understanding in standard conditions and more particularly the thermodynamic using Reaction Calorimetry. Heat of reaction parameter will help to evaluate the temperature rise due the reaction. The quantity of gases release and pressure generated during the reaction are also key parameters.
- Once the reaction in normal conditions is characterized, it is time to determine what would be the worst-case scenario and test the main reactants, intermediate and product in runaway conditions using Adiabatic Calorimetry. It will lead to the determination of the largest temperature rise achievable during decomposition.