

How to deal with a criticality class 5 – calorimetric studies

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In thermal process safety, in order to know if a reaction is hazardous or not, it is classified in 5 different classes by means of safety data.

A process safety study of a chlorination reaction ($\text{POCl}_3 + \text{PCl}_5 + \text{C} \rightarrow \text{P} + \text{HCl}$) was investigated by calorimetric measurements. At first the thermal process safety parameters, e.g. reaction heat, accumulation, adiabatic temperature increase (ΔT_{ad}) and Maximum Temperature of the Synthesis Reaction (MTSR) were determined by Reaction Calorimetry (RC1). Then the thermal stability of the reaction mass was studied by Calvet Calorimetry (C80) in order to elaborate a cooling failure scenario and define the criticality class.

In this work the reaction was firstly performed in a semi-batch mode with the reactant C dosed in two portions. This process showed an exothermic reaction with a total energy of 116 kJ/kg, which corresponds to an adiabatic temperature increase of 97°C. Thus, in case of cooling failure at the time of maximum accumulation (87%), the temperature will reach 165°C. In addition, the thermal stability of the final reaction mass is problematic. One critical exotherm was observed from 129°C with an energy of more than 1387 kJ/kg. However the initial reaction mass is stable since no exotherm was detected until 300°C. Thus, the process belongs to the criticality class 5. This class means that the scenario of the cooling failure will trigger the decomposition within a short period of time and the boiling point cannot be used as a safety barrier. Normally this class should be avoided and the process should be redesigned.

Nevertheless, based on the considerations above, a safety countermeasure, in this case a quench method was studied in order to avoid the runaway in case of cooling failure. The safety parameters are studied and discussed in this presentation.

This example shows how a more detailed safety study opens possibilities for conducting a criticality class 5 process in a safe way, by taking well adapted safety measures.