On-line reaction calorimetry optimisation of safety parameters

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Abstract

Optimisation of the addition profile of semi batch reactions increases the safety of the process as well as the productivity. The development of a tool to perform an on-line optimisation at the lab-scale is a challenging task. It is partially addressed in this paper.

Most of the chemical reactions in the fine chemicals industry are performed in semi-batch mode. One of the key reactant (it will be called B) is added, usually at a constant rate, while the other one (A) is already present in the reactor. The concentration of B in the reactor is a function of two rates: the reaction rate and the addition rate. If the reaction rate is high, it is possible to assume that the concentration of B in the reactor is zero at any time. If the chemical rate is low (in comparison to the addition rate) the concentration of B will continuously increase during the addition, reaching a maximum value with the completion of the addition of a stoechiometric amount of B (this is true for almost all kinetics). In this second case there is a certain accumulation of the reactant B in the reactor. This accumulation is called thermal accumulation because the reactant B is well distributed in the reactor; there is no inhomogeneity like multiple phases, clusters, or unstirred zones. Stopping the feed of B in this case will not stop the chemical reaction precisely because there is some reactant B already at disposal in the reactor.

This is a major concern in the process safety field in case of a cooling breakdown during an exothermal reaction. Such a breakdown can happen for example if the coolant circulation pumps fail but also if it is not possible to stir the reaction mass or if the mass is viscous leading to a situation of heat confinement. Depending on the accumulation and the energy of the reaction this can lead to an important uncontrolled temperature rise. The consequences of such run-away can be dramatic.

The reaction calorimeter CPA 202 from the company ChemiSens is build in such a way that the heat produced by a reaction has to pass through the base of the reactor were it will be quantified. The heat release rate is always known and no baseline has to be drawn a posteriori. With this tool it is possible determine on-line the thermal conversion and to force the system to reach an "ideal accumulation profile" by calculating on-line the thermal accumulation and comparing it to an allowed value.

This paper will focus on the effectiveness of this tool. The accumulation of a reaction will be optimised and the safety assessment of the reaction before and after optimisation will be discussed.