Reactor Dynamic Investigation applied to the Morton case

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Scale-up of chemical processes, particularly those involving fed-batch is well-known to be a problematic area of chemical engineering. It is also costly when something goes wrong in terms of productivity or process safety. Indeed, a specific problem encountered in such installations is the accumulation of non-converted reactants, which may lead to an uncontrolled temperature increase in case of malfunction of process control. Therefore, mastering this aspect is one of the most important and challenging process safety tasks.

Moreover, the demand for faster time-to-market and the increasing product variety requires more versatile production plants capable of producing from small amounts up to several hundreds of tons per year. Nevertheless, a majority of the scale-up methods available nowadays are applied on a case to case as there is no general methodology; it is more a compromise between general rules, know-how and more complex approaches. Therefore, how to design a reactor to be versatile enough and, at the same time, adapted to a particular reaction system remains an open question.

The answer to this question is non-trivial and needs the establishment of an innovative approach considering the following aspects separately: 1) reaction kinetics, 2) reactor dynamics, and 3) risk assessment. Consequently, in order to overcome the case to case approach, two different procedures were developed: the Reactor Dynamic Investigation (RDI) and the Reaction Kinetic Investigation (RKI).

The RDI is a procedure based on temperature ramp measurements and process control theory in order to create an accurate reactor model. While, the RKI is based on calorimetric measurements and a hypothesis of the reaction scheme used to develop a kinetic model of the reaction. The obtained models are then linked and used simultaneously to perform the safety assessment determining if the reactor will be capable to manage the heat released by the considered reaction system.

The reaction system considered in this study is the one taking place in the Morton International inc. accident in New Jersey (1998), involving a synthesis reaction followed by an autocatalytic decomposition of the product. The proposed investigation procedures were then applied considering simultaneously the latter, a 100L reactor dynamics and a scale-down approach in a 0.5L Mettler-Toledo RC1.

In short, compared to conventional scale-up, it was showed that establishing the relationship between reactor dynamics and reaction kinetics simplifies and decreases the development time of several steps. Moreover, using the models contributes significantly to a better understanding of the system. Indeed, the experiments at large-scale can be planned in an optimal way in order to find the best possible operating conditions considering safety and productivity issues.