SAFE SCALE-UP OF CHEMICAL REACTORS USING THE SCALE-DOWN APPROACH

B. Zufferey[1], F. Stoessel[2]
[1]benoit.zufferey@firmenich.com, Firmenich SA, La Plaine, Genève.
[2]francis.stoessel@swissi.ch, Chemical Process Safety, Institute of Chemical and Biological Process Science, Swiss Federal Institute of Technology Lausanne (EPFL)

A successful process development is achieved if the concordance, between laboratory and plant scales, of the three main time constants is respected:

- reaction time constant
- full scale equipment dynamics time constant
- mixing time constant.

In this work, the first two items will be discussed, of course also related to safety aspects. The reaction time constant may be determined at laboratory scale using the data provided by a reaction calorimeter, in our case the RC1® commercialised by Mettler Toledo. Thermal characteristics of the reaction like heat production rate, necessary cooling power, reactant accumulation, etc., are fundamental for safe reactor operation and process design. However, an industrial chemical reactor not only behaves according to the kinetics of the reaction but also to the dynamics of its temperature control system. Scale-up to the large capacity industrial reactor may be limited because the control is performed indirectly via the heat transferred between the fluid circulating in the jacket and the reactant mixture. The transfer area to volume ratio decreases as the size of the reactor increases, leading to serious limitations of the heat transfer capacity of the jacket. Additionally, many problems occur due to the thermal inertia (long time constant) of the jacket wall. Moreover, reaction enthalpies, kinetic parameters and hence product selectivity and global safety are known to be temperature-dependent. Therefore, only the combination of both reactions kinetics and reactor dynamics allows describing and predicting the behaviour of an industrial reactor with respect to productivity, selectivity and safety. Currently, commercialised calorimeters, and among them the RC1®, enable for an ideal control of the temperature even for very exothermic reactions. But they do not allow identifying the effect of the temperature control dynamics of full scale equipment. **In this work, we have developed a «scale-down» methodology allowing to reproduce the exact temperature course of an industrial reactor at laboratory scale, and this, without explicit knowledge of the reaction kinetics.**

By so doing, the new way to use the reaction calorimeter RC1® will allow simulating the thermal behaviour of plant reactors, resulting in a better understanding of full scale production issues, in terms of productivity and quality. Moreover, the assessment of safety scenarios will be more accurate, first because the starting temperature in case of a cooling failure corresponds to that of plant conditions and second because the reaction enthalpy, the heat production rate and the thermal accumulation also more correctly reflect full scale reality. It was thus the goal of this work to develop a tool that helps to eliminate most of costly late development changes and leads to breakthrough improvements in quality, safety and time-to-market.