Accumulation in fed-batch reactor with multiple reaction scheme

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Avoiding incidents related to chemical production is a significant concern in fine chemical industries. On the one hand, chemical risks may be due to reactivity and toxicity of the involved chemicals. On the other hand, controlling chemical reactions (especially exothermic ones) and associated hazards are present as soon as a production is initiated. Through an investigation of the incidents the chemical industry has witnessed, one can mention a large range of issues such as lack of knowledge, wrong consideration of the heat transfer evolution or less efficient mixing through the increase of scale and incorrect estimation of the processing time. A successful scale-up is, therefore, the way that solves these issues correctly and allows to define optimal operating conditions that ensure an inherently safe and efficient process.

A particular problem encountered in the scale-up of fed-batch operations is the thermal potential generated by the accumulation of unconverted reactants but also by the production of hazardous materials. Besides quality issues, such accumulation may lead to an uncontrolled temperature increase in case of process control malfunction and trigger secondary reactions. Therefore, mastering this aspect is one of the most challenging tasks in the development of safe and viable fed-batch processes.

The key factor of success of such a scale-up is the understanding of the physical phenomena governing the chemical processes to bring the different dynamics into real adequacy namely:

a) The chemical reaction dynamics described by the reaction kinetics,
b) The reactor dynamics described by the heat transfer with the cooling system, its control and inertia [1],
c) The mixing dynamics described by the mass transfer provoked by the stirrer motions.

A robust control of these dynamics may lead to an economic and thermally safe process. For that, a novel approach focusing on a combination of dynamic models, safety issues and calorimetric experiments has been developed to answer the two following key questions:

1. How to design a reactor or use an existing one to be versatile enough and, at the same time, adapted to a particular reaction system?
2. How to find the optimal operating conditions to be inherently safe, focusing on an efficient control of thermal potential while remaining economically viable?

The proposed method was investigated for the Morton incident reaction system (New Jersey 1998), composed by a synthesis reaction (SN1) followed by an autocatalytic decomposition of the product [2].

[1] C. Guinand, M. Dabros, T. Meyer, F. Stoessel. *Reactor dynamics investigation based on calorimetric data*. Can. J. Chem. Eng. 95 (2017) 231-240 DOI: 10.1002/cjce.22700

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