Flow calorimetry as a scale-up tool for highly energetic flow processes

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Flow chemistry enables new synthetic routes with highly energetic and hazardous chemicals and their safe and sustainable processing, e.g. in API production [1–3]. Once the process has been developed, it comes to scale-up. This requires reliable thermokinetic data of the flow process, as they may differ from batch processes [4]. In addition, the flow calorimetry test reactor should correspond to a scale-down of a production flow reactor, i.e. the reactor volume or diameter should not be too small.
In this talk, we will show the principle of isoperibolic flow calorimetry using the milli-scale flow calorimeter (17 or 44 ml) [5,6], and how to scale-up these processes in terms of constant heat transfer. As part of an Innosuisse project, a software for evaluating the calorimetry was developed together with the group of D. M. Meier at the IMPE of the ZHAW. It allows to calculate the heat of reaction, reaction enthalpy, adiabatic temperature rise, process half-life as well as the specific heat transfer capacity based on the axial temperature profile, physical data of the reaction mixture and flow reactor properties. In addition to thermodynamic data, kinetic data are also to be extracted from the temperature profile. Using both reaction enthalpy and kinetics allows simulation of the temperature profile in a large-scale tube bundle mixer-heat exchanger with similar heat transfer capacity. This enables scale-up of highly exothermic reactions from 0.5 to about 500 L/h.

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