

Scale-up From RC1 and ARC safety tests using Dynochem.
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ABSTRACT:

The effect of temperature on reaction kinetics, both for desired and undesired reactions is of great importance. Inability to control the heat release from an exothermic reaction can lead to poor yields, low selectivity, especially for stereospecific reactions, and even unsafe operation (excessive gas generation, both from the desired and undesired chemistry, liquid boilup rate) upon scale-up of an API chemical synthesis. Recent advances in laboratory automation and calorimetry have increased both quality and quantity of experimental information; however, translating the information into fundamental understanding of the underlying chemical and physical mechanisms of interest can represent a challenge. To this end, Dynochem was used to fit experimental data (heat flow and gas generation) from several calorimeters (SuperCRC, ARC, RC-1). This data was then used to determine the safe scale-up parameters for a variety of cases: The maximum addition rate of a reagent under cryogenic condition (SuperCRC data); the maximum safe heating rate for a gas-generating rearrangement (RC-1 data); and the required condenser size for an unstable material during distillation (ARC data).