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Prediction of Adiabatic Temperature and Pressure Runaways through Kinetic Analysis of Combined DSC/HFMC and ARC/VSP Data

The prevention and mitigation of thermal runaway remain major challenges in the chemical process industries. Reliable prediction of temperature and pressure evolution following a loss of cooling is essential for process hazard assessment, emergency relief system design, reactor scale-up and the development of inherently safer processes. This work presents an integrated kinetic methodology that combines heat-release and gas-generation analyses to provide a comprehensive description of runaway reaction behaviour.

The approach exploits the complementary capabilities of differential scanning calorimetry (DSC), heat-flow microcalorimetry (HFMC), accelerating rate calorimetry (ARC) and Vent Sizing Package (VSP) experiments performed under temperature-programmed, pseudo-adiabatic or adiabatic conditions. Advanced kinetic analysis of heat-flow and adiabatic calorimetric data is used to derive kinetic models for both intended and decomposition reactions, including complex multi-step and autocatalytic mechanisms. These models enable prediction of reaction rates, conversion profiles, self-heating rates (dT/dt), and heat-release rates (dQ/dt) under arbitrary thermal histories.

In parallel, pressure data obtained from ARC, VSP or related experiments are analysed to quantify gas-generation kinetics. The measured pressure is decomposed into contributions arising from thermal expansion and chemical gas formation, allowing the determination of reaction-induced gas evolution as a function of temperature. The resulting kinetic model predicts the evolution of pressure and its rate of increase (dP/dt).

The combination of heat-release and gas-generation kinetics provides a unified framework for reconstructing and simulating thermal runaway scenarios under adiabatic and pseudo-adiabatic conditions, accounting for the coupled evolution of temperature, heat release and pressure. The methodology enables the determination of key process safety parameters, including the maximum temperature of the synthesis reaction (MTSR), the time to maximum rate under adiabatic conditions (TMR_{ad}) and adiabatic decomposition temperatures (e.g., ADT₂₄). Compared with approaches relying exclusively on adiabatic calorimetry, the proposed methodology enhances the prediction of runaway behaviour while providing the kinetic information required for emergency relief system design, reactor engineering, process scale-up and quantitative risk assessment.