Experimental study of hydrogenation reaction safety

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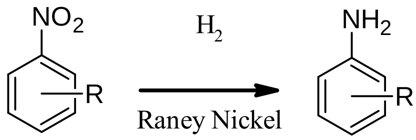
One of the most useful and widely applicable method to reduce chemical substances is without doubt the catalytic hydrogenation which finds diverse applications in industrial chemical processes. Hydrogenations of aromatic nitro compounds are known to be exothermic and are potentially hazardous processes. Indeed, a typical enthalpy for a nitro group reduction is around 560 kJ/mol [1].

In this study, the thermal safety of a nitro-compound hydrogenation process was investigated by calorimetric measurements. At first the thermal process safety parameters, e.g. reaction heat, adiabatic temperature increase (ΔT_{ad}) and Maximum Temperature of the Synthesis Reaction (MTSR) were determined by Reaction Calorimetry (CPA). Then the thermal stability of the reaction mass was studied by Calvet Calorimetry (C80) in order to define the criticality class of the actual process and elaborate failure scenarios.



The hydrogenation reaction was performed at 40°C under hydrogen pressure and the agitation was increased in order to activate the reaction. This process showed an exothermic reaction with an energy of 440 kJ/kg, which corresponds to an adiabatic temperature rise of 230°C. As a consequence, in case of cooling failure with 100% accumulation, the temperature will reach 270°C. In addition, the thermal stability of the initial and final reaction mass was analysed. The initial reaction mixture presents a high decomposition potential. From around 200°C an exothermic decomposition peak is detected with an energy of more than 540 kJ/kg corresponding to an adiabatic temperature rise of more than 280°C. As for the final reaction mixture, its thermal stability is unproblematic since no significant exotherm was observed up to 300°C. Consequently, this process belongs to a criticality class 5. It is therefore essential to define efficient emergency measures in order to ensure the safety of such a process.

An appropriate protection strategy was defined by studying the effect of process parameters such as hydrogen flow and agitation on the failure scenario. This study is a good example showing how to establish safety recommendations for hydrogenation processes based on failure scenarios.

[1] “Thermal Safety of Chemical Processes”, Risk Assessment and Process Design, Francis Stoessel, Wiley-VCH, 2011