Chemical Reactivity Assessments in R&D

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Abstract: The evaluation of reactive chemical hazards at the pilot and manufacturing scale, using laboratory testing, is increasingly used and has been well documented. However, reactive chemical hazard evaluation at the R&D scale presents special challenges. The typical hazard testing program requires a significant amount of sample, often takes time (> 3 days) to complete, and is can be quite costly. On the other hand, the synthesis of new molecules in the R&D environment often produces only a few grams, occurs quickly (<2 days), may only happen once and many synthetic reactions may be carried out before a suitable candidate for scale-up will be found. However, with each new synthesis there is the risk of injury, possibly serious or fatal, caused by unexpected and maybe violent reactivity.

While it may not be possible at the R&D stage of product development to define the critical limits of temperature, pressure, concentration, and safe dosing rates of processes it is possible to identify the potential hazards of the planned synthesis.

This paper describes a staged approach for chemical reactivity hazard evaluation and assessment applicable to an R&D environment. We will describe these initial phases of the R&D hazard evaluation process that rely on only data that can be obtained from the open literature. We will also indicate how the need for additional assessments can be determined from this initial hazard review.