A Systematic Approach to Reactive Chemicals Analysis

M. Sam Mannan

Mary Kay O'Connor Process Safety Center
Chemical Engineering Department
Texas A&M University System
College Station, Texas 77843-3122, USA
(979) 862-3985, mannan@tamu.edu

Reactive chemicals are chemicals that can, under certain conditions, release very large and potentially dangerous amounts of energy. Reactive chemicals can lead to reactions that differ from the routine mainly in the rate at which they progress. A chemical reaction can be considered routine if the reaction rate is relatively slow or can be easily controlled. It is this question of rate of reaction and ability to control that marks certain chemicals as warranting special precautions and the label "reactive chemical."

The primary difficulty in identifying reactive chemicals stems from the variety of conditions under which certain chemicals can undergo an uncontrollable hazardous reaction. Some chemicals are simply unstable and can vigorously polymerize, decompose or condense, or become self-reactive. Other chemicals can react violently when exposed to common environmental chemicals or conditions. A major difficulty, which arises when one considers the problem as a whole, is that it is often not appreciated that the reactive chemical hazards is seldom a unique characteristic of the chemical or the process itself but highly dependent on the process conditions and mode of operation. For example, a simple property such as flash point can be used to determine the fire or explosion hazard of a substance. In contrast, the identification of a reactive hazard requires the detailed evaluation of both the properties of the substances used and the operating conditions. The dilemma is that many so-called "benign" reactions can become highly reactive or undergo a runaway reaction under slightly different conditions or the introduction of minute impurities.

This paper provides a background of the reactive chemicals problem including a summary of chemical incidents that can be attributed to reactive chemical events. Based on the extent of the problem, a systematic approach to reactive chemicals analysis is suggested. The approach is a tiered framework where one can start with simple screening tools based on thermophysical property and thermodynamic analysis, use of quantum mechanics and transitional state theory, and finally the use of experimental measurements.