Experimental and Computational Methods for Process Safety Research

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ABSTRACT

Since its inception in 1995, the Mary Kay O’Connor Process Safety Center (MKOPSC) has researched the chemical behavior of industrial chemical reactions and processes. Reactions are selected for investigation based on their industrial importance and on major incidents involving injuries or large losses. The thermal behavior of a reaction system is analyzed to identify and assess potential hazards for likely scenarios in which process variables are exceeded or reaction components encounter incompatible materials or contaminants. Experimental information is supplemented with computational methods to estimate measured properties and to guide subsequent tests to the most important system and conditions.

Computational approaches include classical methods, such as the Benson group contribution method, semi-empirical methods, and quantum methods to determine properties at the molecular level. An important purpose of the computational methods is to provide values under conditions when the substances are unstable and cannot be measured accurately or safely, such as the heat of formation of hydroxylamine. Another important need is to supplement experimental data to determine reaction mechanisms for reactive hazard assessment. From these computations and experimental investigations, correlations are developed to extend at lower cost and expertise the detailed results to other systems. QSPR, for example, has been used effectively to relate macroscopic behavior to molecular properties without detailed molecular computations. These approaches and methods will be discussed in relation to the primary objective of reliable process safety information for identifying hazards of reacting systems and the design of safer and more economical industrial processes.