

## **Assessing the Potential Hazards of Reactive Chemicals**

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### **ABSTRACT**

Strategies for safe and economic process require accurate information about chemicals and chemical reactions, but sufficient information is often not available from traditional sources. The Mary Kay O'Connor Process Safety Center (MKOPSC) at Texas A&M University employs calorimetric measurements and classical and quantum chemistry models to determine properties of chemicals and analyze chemical systems. Molecular simulation and computational methods are now practical engineering tools for predicting thermophysical properties, estimating reaction rates, and for understanding the molecular-level causes of macroscopic behavior measured in the laboratory.

There are important process safety applications of molecular simulation models to supplement experimental measurements, such as the analysis of unstable reaction systems that have caused thermal runaway reactions.

In response to these needs, the Center is developing a systematic method to determine the reactivity and potential hazard of any chemical using a combination of known information, calculations using quantum chemistry and classical models, screen testing, and if necessary, more detailed experimental measurements.