

Theoretical and Experimental Techniques for the Evaluation of Reactive Chemical Hazards

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ABSTRACT

Evaluation of reactive chemical hazards is critical for the design and operation of safer chemical plant processes.

Much effort is needed for experimental techniques to measure thermal reactivity of chemical systems. Studying all the various reaction pathways experimentally however is very expensive. Therefore, it is essential to employ simplified screening tools to reduce the number of experiments and to identify the most energetic pathways.

A systematic approach will be presented for the evaluation of reactive chemical hazards. This approach is based on a combination of numerical computational methods and experimental thermal analysis techniques.

Numerical computational methods are used to predict reaction stoichiometries, thermodynamics, and kinetics, which will help to exclude thermodynamically infeasible and non-hazardous reaction pathways.

The experimental techniques are used to evaluate the most energetic systems for more accurate thermodynamic and kinetics parameters or to replace inadequate numerical methods. This approach employing theoretical and experimental analyses was used to evaluate the decomposition reaction of di-tert-butyl peroxide (DTBP) in toluene. The results of this analysis was compared to literature data for this system.