Thermal analysis and intrinsic activation energy estimation to predict hazardous chemical pathways

Aldeeb, A. A., W. J. Rogers, and M. S. Mannan
Mary Kay O'Connor Process Safety Center

Chemical Engineering Department
Texas A&M University
College Station TX 77843-3122
Email: mannan@tamu.edu

ABSTRACT

Evaluation of reactive chemical hazards is critical for the design and operation of safer chemical processes.
Overall system thermodynamic and kinetic parameters can be measured using various thermal analysis techniques, which are primary tools for identifying chemical reactivity hazards. Although thermodynamic parameters are essential for reactivity assessment, identifying hazardous reaction pathways also is important.
Reaction pathway estimation is possible by applying correlations based on thermodynamic-energy relationships.
Intrinsic activation energy is a concept to identify reaction pathways that are more likely because they require less activation energy for initiation. In this research thermal analysis is performed using the RSST and the APTAC calorimeters. Also, intrinsic activation energies are estimated by applying the Polanyi and the Marcus equations to predict hazardous pathways of reactive systems. These predictions will focus the reactivity assessment on systems causing significant and rapid increases in temperature, pressure, or gas evolution.