Understanding the Role of Process Chemistry in Fires and Explosions

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ABSTRACT

Chemical incidents involving fires and explosions cannot be prevented only through command and control regulatory requirements, but prevention requires understanding the fundamental root causes.

When heat generated by an exothermic reaction exceeds the heat removal capability of the system, the exothermic reaction will accelerate and may lead to a thermal runaway reaction, explosion, and fire.

The understanding of the role of process chemistry as a root cause of fires and explosions in the chemical process industry requires knowledge of the maximum quantities of both energy and gas that are generated by the primary and secondary exothermic reactions. Also, the rates of energy and gas production are of utmost importance.

Evaluation of the maximum amounts of energy and gas produced and their rates of generation are usually accomplished by experimental methods. Experimental thermal analyses can provide an overall reactivity evaluation, but they are often unable to explain the reaction mechanisms needed for safe process chemistry.

Moreover, experimental analyses of all reaction pathways are expensive and sometimes impractical.

This paper provides a structured approach for chemical reactivity hazard evaluation using computational methods coupled with experimental techniques. This systematic approach helps to minimize experimental work and identifies the most important parameters in evaluating process fire and explosion hazards and provides a more comprehensive understanding of process chemistry.

A reactive system involved in selected industrial fires and explosions is analyzed to test the validity of this systematic approach. Providing a better understanding of the reactive system chemistry and reducing the experimental work were among the main objectives of this study.