Prediction of the Reactivity Hazards for Organic Peroxides Using the QSPR Approach

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ABSTRACT

Organic peroxides can thermally decompose and may lead to runaway reactions. These reactivity hazards have been reported as one of the main causes for fire and explosion in process industries. The risk associated with runaway reactions of organic peroxides can be minimized by employing the inherently safer design (ISD) principles: substitution and moderation of hazardous peroxides in chemical processes. However, the application of ISD concepts requires lengthy evaluations and classification of reactivity hazards of organic peroxides, which are impractical to be done through experimental approach due to the large number of peroxide members and great variations in their reactivity hazards. In this work, the quantitative structure−property relationship (QSPR) was used to predict the detected onset temperature (T0) and heat of decomposition (Qd) of organic peroxides for the estimation of thermal stability and severity of runaway reactions. In addition to the conventional descriptors used in QSPR, we used other properties of the peroxides such as concentration and the number of peroxide functional group as additional descriptors to construct accurate and economic models to predict reactivity hazards. Partial least-squares method (PLS) and multiple linear regression method (MLR) were used to model T0 and Qd. It was found that the regression model derived from the PLS method give better prediction for reactivity hazards of organic peroxides. Sensitivity analyses were also performed to identify important descriptors contributing to the reactivity hazards of organic peroxides. The proposed study describes a new approach to identify the reactivity hazards of organic peroxides that may lead to safe practices in the process industries.