Quantitative Structure Property Relationship Studies for Predicting Dust Explosibility Characteristics (Kst, Pmax) of Organic Chemical Dusts

Olga J. Reyes, Suhani J. Patel, and M. Sam Mannan

Mary Kay O'Connor Process Safety Center, Artie McFerrin Department of Chemical Engineering, Texas A&M University System, College Station, Texas 77843-312

ABSTRACT

In the chemical process industry, hazardous chemical dusts have recently been the cause of many severe incidents leading to fatalities and injuries. It is important to characterize the hazards posed by dust materials. Thus, in this work the quantitative structure property relationship (QSPR) technique has been used to predict the explosibility characteristics (i.e., KSt, Pmax) of chemical dusts. The data set consisted of 31 chemical dusts, further divided into training and test sets. The mathematical models were developed using Material Studio 5.0 software and the genetic function approximation (GFA) algorithm. The final predictive models for the maximum overpressure (Pmax) and dust deflagration index (KSt) are cubic equations with 5 parameters and high correlation coefficients (R2 for the models are 0.96 and 0.91, respectively). The correlations also took into account the effect of the dust particle size by using the median value as a parameter in the developed models. This is essential because dust explosion behavior is principally governed by particle size. Such prediction models for hazardous dust properties serve as an indication for design and protective measures against dust explosions as well as they can be applied for hazard classification and screening of dust materials.