Study on the Prediction of Upper Explosion Limited of Hydrocarbons

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ABSTRACT

The quantitative relationships between the Upper Explosion Limited (UEL) and the molecular structures of hydrocarbon compounds were investigated based on the quantitative structure-property relationship (QSPR). The molecular descriptors of 323 hydrocarbon compounds were calculated by the CODESSA program, and these descriptors were pre-selected by Heuristic Method (HM) and Best Multilinear Regression Method (B-MLR). As a result, the four-descriptor linear models were developed by these two methods to describe the relationship between the molecular structures and UEL. The models were tested by internal and external validations. The results show that, for both models, the predicted UEL values agree well with the experimental ones, and the predicted errors are within the range of the experimental error of UEL measurements and the predicted results are satisfactory.

Key words: Explosion Limits; Quantitative Structure-property Relationship (QSPR); Linear Prediction; Heuristic Method (HM); Best Multilinear Regression Method (B-MLR)