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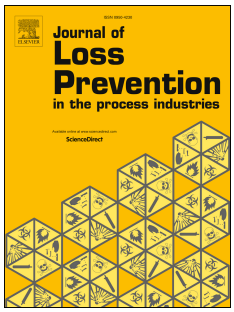

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Predicting the Superheat Limit Temperature of Binary Mixtures Based on the Quantitative Structure Property Relationship

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ABSTRACT:

This study was devoted to develop the quantitative relationship model between the superheat limit temperature of binary mixtures and their molecular structures based on the quantitative structure-property relationship. The integral additive descriptors method was used to calculate the molecular descriptors of binary mixtures. The genetic algorithm combined with the multiple linear regression (GA-MLR) was used to select optimal subset of descriptors which had significant contribution to the superheat limit temperature. Three different external validations, which checked the stability and predictive capability of the obtained models, were employed to build the models. And the applicability domain for the models was also defined. The results showed the presented models were valid and predictive and there was strong linear relationship between the superheat limit temperature of binary mixtures and their molecular structures. This study can provide a new way to predict the superheat limit temperature of binary mixtures.

Keywords: Quantitative structure property relationship; Superheat limit temperature; Binary mixtures.

1. Introduction

The superheat liquid is the liquid when its temperature is higher than its boiling point but it doesn't boil and it is at the metastable state. Thus it is easy to explode or react violently when certain kinds of perturbation happen to the system. The liquid superheat has caused some of the most common and destructive accidents in the process industry, such as the boiling liquid expanding vapor explosion (BLEVE) (Makhviladze & Yakush, 2005; Abbasi T & Abbasi S. A., 2007; A.C. van den berg, 2008; Russell A. O., Juan C. R. & Suzanne A. S., 2011).

There have been many experimental and theoretical methods to determine the superheat limit temperature (SLT). The most common experimental approach is using the droplet explosion technique. Homogeneous nucleation theory, equations of state and Antoine equation are the most commonly used theoretical approaches (Sugales & Trujillo, 1990). There are also equations based on chemical thermodynamics or kinetics to predict the superheat limit temperature of binary-mixed liquids. However, the SLT of some chemicals are not easily gotten from the experimental methods and the equations used in theoretical methods either are complicated to calculate or have less accurate predicted results. Furthermore, the number of new mixtures being used in the process industry increases rapidly each year. Therefore, it is necessary to propose a new, quick and easy applicable way to predict the superheat limit temperature in order to have a clear understanding of the risk of them.

One promising method for predicting the superheat limit temperature is the quantitative structure-property relation (QSPR) approach. The QSPR study has been proved to be an effective way to predict various chemical, physical and biological properties of desired chemicals (Katritaky, Lobanov & Karelson, 1995; Katritaky & Fara, 2005; Patel, Ng & Mannan, 2009; Katritaky, Kuanar, Slavov, Hall, Karelson, & Dobchev, 2010; Pan, Jiang, Ding, Wang & Jiang, 2010; Reyes, Patel & Mannan, 2011; Zhou, Jiang, Pan & Wang, 2015). QSPR is a method which can reveal the relationship between the molecular structures and desired properties at the molecular level. Comparing with other theoretical methods, there are 3 advantages of this approach. Frist, it requires only the knowledge of the chemical structures instead of any other chemical thermodynamics or kinetics, so it can predict the desired properties quickly and efficiently. Second, the molecular descriptors, which are used to calculate solely from molecular structures, have definite physical meaning. Through them, the physicochemical information that has significant contribution to the desired properties could be found and represented easily. Third, the developed QSPR model would even be applicable theoretically for the new chemicals as long as they are in the applicability domain of the model and their molecular structures are already known (Pan, Zhang, Jiang & Ding, 2014).

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