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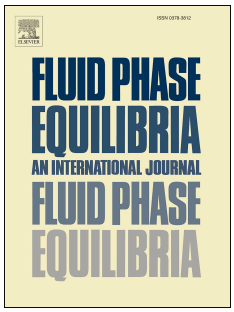

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Distributive structure-properties relationship for flash point of multiple components mixture

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Abstract

Flash point (FP) is an important reference property for characterizing the fire hazards of any combustible material in the field of petro-chemical processes and functional materials designing, whereas, obtaining FP data for flammable liquids is difficult owing to several limitations. Herein, the distributive structure-properties relationship (DSPR) method for simultaneously investigating the relationship between the structure and the FP for multiple-component mixtures (mono/ binary/ternary component) was proposed and was composed of a DSPR model and hybrid norm indexes. Serial of validation metrics prove that this model exhibited good predictive and generalization abilities in prediction of FP for multiple-component mixtures. Thus, this new method and hybrid indexes proposed in this work is effective for the characteristic of the relationship between structure and FP and might have larger applications in chemical process safety.

Keywords: flash point; flammable liquids; mixtures; SPR; norm indexes

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