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Modified Molecular Matrix Model for Predicting Molecular Composition of Naphtha☆

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Abstract To improve the naphtha composition prediction model based on molecular type homologous series matrix (MTHS), this paper puts forward a novel molecular matrix to characterize the naphtha composition and the normal distribution hypothesis to better describe the molecular composition distribution within each homologous series of the molecular matrix. Through prediction calculation of eight groups of naphtha samples and eight groups of gasoline samples, it is verified that the normal distribution hypothesis is more applicable than gamma distribution hypothesis for the prediction model. According to the prediction results of the samples, the restrain range of normal distribution parameters during model computing process is summarized. With the bulk properties of naphtha samples and the value range of distribution parameters as input conditions, this study utilizes the improved novel molecular matrix to predict the composition of naphtha samples. As the results show, the novel molecular matrix can predict more detailed composition information of naphtha and improve prediction accuracy with less unknown parameters.

Keywords MTHS molecular matrix, distribution assumption, naphtha, molecular composition, prediction model