

Accepted Manuscript

Modified Molecular Matrix Model for Predicting Molecular Composition of Naphtha

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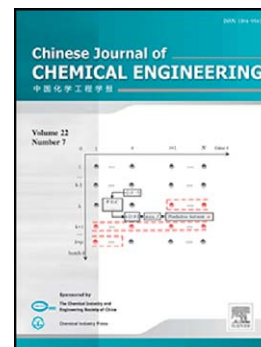
PII: S1004-9541(16)30957-0  
DOI: doi:[10.1016/j.cjche.2017.01.008](https://doi.org/10.1016/j.cjche.2017.01.008)  
Reference: CJCHE 747

To appear in:

Received date: 22 September 2016  
Revised date: 22 December 2016  
Accepted date: 2 January 2017

Please cite this article as: Kun Wang, Shiyu Li, Modified Molecular Matrix Model for Predicting Molecular Composition of Naphtha, (2017), doi:[10.1016/j.cjche.2017.01.008](https://doi.org/10.1016/j.cjche.2017.01.008)

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**Energy, resources and environmental technology**

**Modified Molecular Matrix Model for Predicting Molecular Composition of Naphtha<sup>☆</sup>**

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<sup>☆</sup> Supported by the National Natural Science Foundation of China (U1462206).

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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

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