Accepted Manuscript

Review

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PII: S1385-8947(18)31800-X
DOI: https://doi.org/10.1016/j.cej.2018.09.083
Reference: CEJ 19922

To appear in: *Chemical Engineering Journal*

Received Date: 9 May 2018
Revised Date: 17 August 2018
Accepted Date: 10 September 2018

Please cite this article as: Y. Ren, Z. Liao, J. Sun, B. Jiang, J. Wang, Y. Yang, Q. Wu, Molecular Reconstruction: Recent Progress Toward Composition Modeling of Petroleum Fractions, *Chemical Engineering Journal* (2018), doi: https://doi.org/10.1016/j.cej.2018.09.083

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Molecular Reconstruction: Recent Progress Toward Composition Modeling of Petroleum Fractions

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Abstract

Molecular reconstruction is popular in current oil refinery modelling. It aims to understand the refining process from the molecular level, to predict product properties accurately, to optimize the processes, and to increase the value of each molecule. Molecular reconstruction technology determines the detailed molecular composition of petroleum fractions through obtainable bulk properties and chemical details. In this paper, the existing molecular reconstruction models involving models with a set of predefined deterministic molecules, stochastic reconstruction method, structure-oriented lumping method, molecular type-homologous series matrix method, reconstruction by entropy maximization method, stochastic reconstruction-entropy maximization method and state space representation method are reviewed and compared. The credibility of the simulated composition and the drawbacks of molecular reconstruction technique are also discussed.

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