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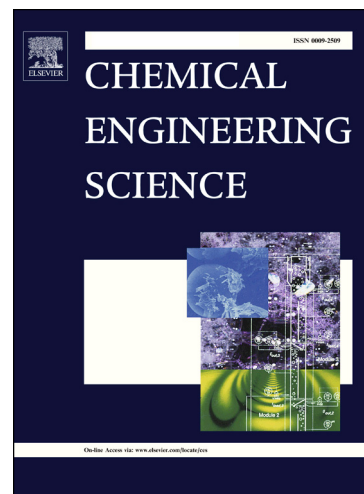
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Molecular characterization of petroleum fractions using state space representation and its application for predicting naphtha pyrolysis product distributions

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Abstract: Molecular model of petroleum fractions plays an important role in the designing, simulation and optimization for petrochemical processes such as pyrolysis process, catalytic reforming, fluid catalytic cracking (FCC) and so on. However, it is very difficult to exactly characterize the composition distributions due to its internal complexity and containing numerous redundant information and measuring errors although many efforts have been made so far. As an improvement of the work in (Mei, *et al*, 2016), a molecular-based representation method within a multi-dimensional state space is developed in this paper. In this method, each pure component in the petroleum mixtures is defined as a state variable and any petroleum fractions can be geometrically represented as a point in a multi-dimensional linear state space, in which a conception of basis fractions is further introduced by defining a group of linear independent vectors so that any petroleum fractions within the specified range (e.g. naphtha) can be obtained through a linear combination by such basis fractions. The redundant information and

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