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# Molecular reconstruction model based on structure oriented lumping and group contribution methods*

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**Abstract** Molecular management is a promising technology to face challenges in the refining industry, such as more stringent requirements for product oil and heavier crude oil, and to maximize the value of every molecule in petroleum fractions. To achieve molecular management in refining processes, a novel model that is based on structure oriented lumping (SOL) and group contribution (GC) methods was proposed in this study. SOL method was applied to describe a petroleum fraction with structural increments, and GC method aimed to estimate molecular properties. The latter was achieved by associating rules between SOL structural increments and GC structures. A three-step reconstruction algorithm was developed to build a representative set of molecules from partial analytical data. First, structural distribution parameters were optimized with several properties. Then, a molecular library was created by using the optimized parameters. In the final step, maximum information entropy (MIE) method was applied to obtain a molecular fraction. Two industrial samples were used to validate the method, and the simulation results of the feedstock properties agreed well with the experimental data.

**Keywords** molecular reconstruction, structure oriented lumping, group contribution, Monte Carlo, maximum information entropy

## 1 INTRODUCTION

The refining industry today has to comply with higher product-quality specifications, more stringent environmental regulations and heavier crude oil. To address these issues, a promising technology that is termed molecular management, which targets the right molecules to be in the right place, at the right time and at the right price, has been of increasing interest. To achieve molecular management, the feedstock composition should be known with great detail. However, no analytical technique is yet sufficiently effective to detect and quantify the thousands of different compounds in the heavy petroleum fraction. Consequently, it is necessary to reconstruct a mixture from partial analytical data. Several approaches have been described in the literature to represent the petroleum fraction.

Quann and Jaffe [1, 2] proposed a method that is termed structure oriented lumping (SOL) in which they attempted to use a group of structure vectors to describe complex hydrocarbon molecules. Because a structure vector represents a class of molecules with the same functional groups but with different structures, the number of complex hydrocarbons has been reduced from millions to thousands, and the model complexity has been reduced. Jaffe [3] extended this method to heavy petroleum residues and more specifically to a representation of multicore species. This method has been used widely in the oil industry and has received great feedback. However, it is still a challenge to estimate the properties of molecules that are described by structure vectors.

Zhang [4] used a matrix of pseudo compounds that are classified by chemical family and carbon number to characterize the petroleum fraction. There are several other approaches using variations of matrix representations with homologous series [5, 6]. This method can keep much valid information of the feedstock. However, long and complex analyses are needed to obtain this matrix, and it is difficult to apply the method to heavy petroleum residues.

Neurock *et al*.[7] proposed a method that is termed stochastic reconstruction (SR), which characterizes the petroleum fraction by a set of distributions of molecular structural attributes. Monte Carlo (MC) sampling is used

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