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Molecule-based kinetic Monte Carlo modeling of hydrotreating processes applied to Light Cycle Oil gas oils MAX KOLB, Laboratoire de Chimie, Ecole Normale Supérieure de Lyon, F-69364 Lyon, France, LUIS PEREIRA DE OLIVEIRA, Luis.Pereiradeoliveira@gmail.com, JAN J. VERSTRAETE, IFP Energies nouvelles, BP 3, 69360 Solaize, France — A novel kinetic modeling strategy for refining processes for heavy petroleum fractions is proposed. The approach allows to overcome the notorious lack of molecular details in describing the petroleum fractions. The simulation of the reactions process consists of a two-step procedure. In the first step, a mixture of molecules representing the feedstock of the process is generated via two sucessive molecular reconstruction algorithms. The first algorithm, termed stochastic reconstruction, generates an equimolar set of molecules with the appropriate analytical properties via a Monte Carlo method. The second algorithm, called reconstruction by entropy maximization, adjusts the molar fractions of the generated molecules in order to further improve the properties of the mixture. In the second step, a kinetic Monte Carlo method is used to simulate the effect of the refining reactions on the previously generated set of molecules. The full two-step methodology has been applied to the hydrotreating of LCO gas oils and to the hydrocracking of vacuum residues from different origins (e.g. Athabasca).

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