

## Molecule-based modeling of heavy hydrocarbon structure and reaction

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The considerable interest in molecule-based models of heavy hydrocarbon structure and reaction is motivated by the need to predict both upstream and downstream properties of these materials. This is because the molecular composition is an optimal starting point for the prediction of mixture properties. The potential advantages of molecule-based modeling are thus clear. Less readily apparent, however, is that the development and operation of molecular models comes with a large requirement for model construction and solution time as well as analytical and reactivity information.

The challenge of building molecule-based models is due to the staggering complexity of the complex reaction mixtures. There will often be thousands of potential molecular and intermediate (e.g., ions or radicals) species. The sheer size of the thus-implied modeling problem engenders a conflict between the need for molecular detail and the formulation and solution of the model. Clearly, the use of the computer to not only solve but also formulate the model would be helpful in that it would allow the modeler to focus on the basic chemistry, physics and approximations of the model.

Our recent work has led to the development of such an automated capability to model development. Monte Carlo simulation of feedstock structure casts the modeling problem in molecular terms. Reactivity information is then organized in terms of quantitative linear free energy relationships. The model equations are then built and coded on the computer. Solution of this chemical reaction network, in the context of the chemical reactor, provides a prediction of the molecular composition, which is then organized into any desired commercially relevant outputs.

This approach is illustrated through the development of molecule-based models for petroleum resid structure and reaction. Key results and the underlying bases of analytical, physical-organic and computational chemistry will be discussed.