

Composition Based Modeling

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Composition Based Modeling represents a significant improvement in the approach to building kinetic models of petroleum systems. The activity is divided into three areas:

The Model of Composition (High Detail Hydrocarbon Analysis)
Describing the chemistry of petroleum mixtures (Structure Oriented Lumping)
Model Delivery Technology

The composition of petroleum is itself viewed as a model. Numerous analytical methods, collectively known as High Detail Hydrocarbon Analysis (HDHA), are employed to represent petroleum as a consistent set of 5000 molecular species. Physical, chemical and performance properties of petroleum are calculated using composition based correlations and are used to "property balance" the HDHA analyses.

Structure Oriented Lumping (SOL) has been developed to describe the reactions of hydrocarbon mixtures. Using SOL individual hydrocarbon molecules are represented as vectors of incremental structural features. These vectors provide a convenient framework to construct rule-based reaction networks of arbitrary size and complexity. Models using SOL typically follow the conversion of molecular species through as many as 100,000 elementary reaction steps.

Composition Based Models have been built for all major petroleum conversion processes including reforming, fluid catalytic cracking, hydrocracking, catalytic hydro-desulfurization and lubricant manufacture. They are presented to the user through a uniform architecture on a PC platform and are in use worldwide to optimize refinery operation.