

26e Extension of Structure Oriented Lumping to Vacuum Residua

Stephen B. Jaffe

The method of Structure Oriented Lumping (SOL) for describing the composition, chemical reactions and properties of complex hydrocarbon mixtures has been extended to molecules found in vacuum residua. Residua molecules, in turn, are represented as multi-core molecules comprising linked single-core species found in the lower boiling petroleum fractions. The SOL approach of describing the molecular structure with vectors of structural increments is retained along with the addition of information about the core linkages. The extended vector representation meshes seamlessly with the conventional SOL. Properties of residua may be readily calculated and models of residua conversion processes developed using this formalism.