METHOD FOR RECONCILING A MODEL OF COMPOSITION

ABSTRACT

Method for determining the composition of a material, including obtaining a reference model of composition (MoC) of the material based on a molecular formula distribution of the material, and reconciling, using at least one computer processor, the reference MoC to match at least one target property of the material, is provided. The reference MoC can be expressed as a combination of molecular lumps with associated reference percent. The reconciliation can be carried out using by constrained optimization of information entropy, and the optimization can be performed on a more coarse-grained basis relative to the reference MoC.

(FIG. 1)

METHOD FOR RECONCILING A MODEL OF COMPOSITION OF A MATERIAL FROM A PETROLEUM STREAM

ABSTRACT

Method for determining the composition of a material, including obtaining a reference model of composition (MoC) of the material based on a molecular formula distribution of the material, and reconciling, using at least one computer processor, the reference MoC to match at least one target property of the material, is provided. The reference MoC can be expressed as a combination of molecular lumps with associated reference percent. The reconciliation can be carried out using by constrained optimization of information entropy, and the optimization can be performed on a more coarse-grained basis relative to the reference MoC.

(FIG. 1)