

ESDU SPD-M8-1

Coarse-grained simulation of asphaltene-hydrocarbon containing systems – Sept. 08 update

Unamended
Issue 1 Oct 2008



Imperial College
London

**Sub-Project D: Thermodynamics
and molecular modelling**

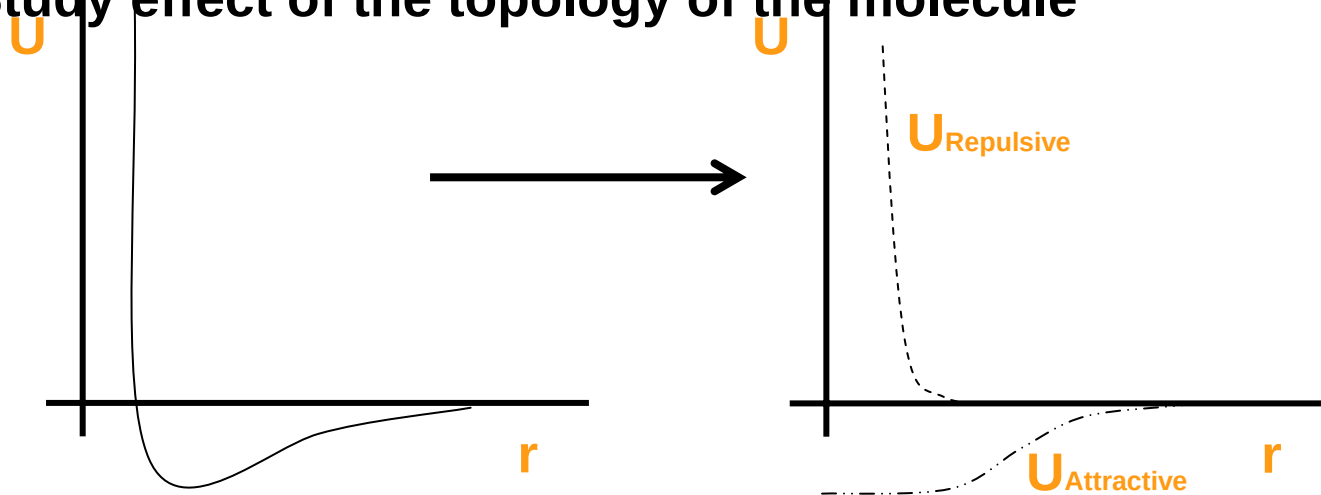
**Coarse-Grained Simulation of
Asphaltene-Hydrocarbon containing
Systems**

Julio Jover

**Amparo Galindo, Andrew Haslam, George Jackson, Erich
Müller and Stephen Richardson**

Objective

- Study the phase behaviour of asphaltene containing systems.
 - Perform a coarse grained simulation by averaging the atomistic details.
 - Decoupling of the interaction in repulsive and attractive terms.
 - Study effect of the topology of the molecule

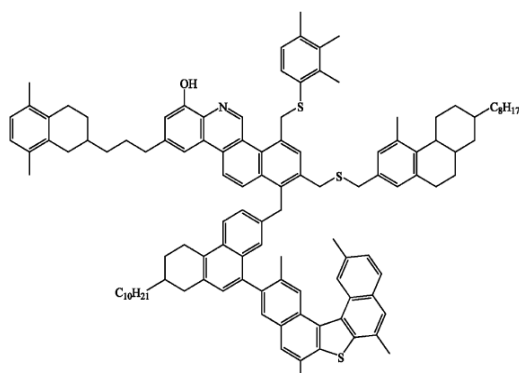


Why Molecular Simulations

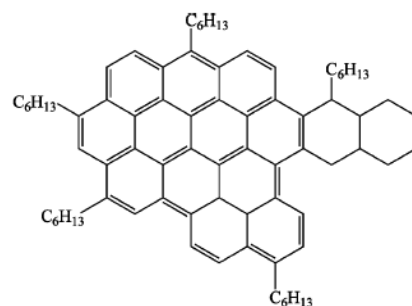
- **Molecular simulations?**
 - **Test the Model**
 - Assymmetry
 - Topology
 - Interaction
- **Molecular Dynamics?**
 - Thermodynamics
 - Structure
 - Diffusion
 - Aggregation / Nucleation

Asphaletene Models:

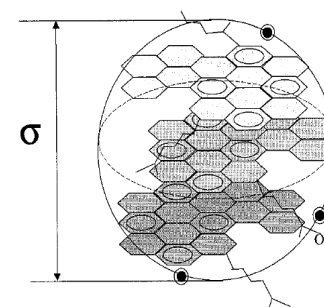
• Theoretical Models:



Archipelago



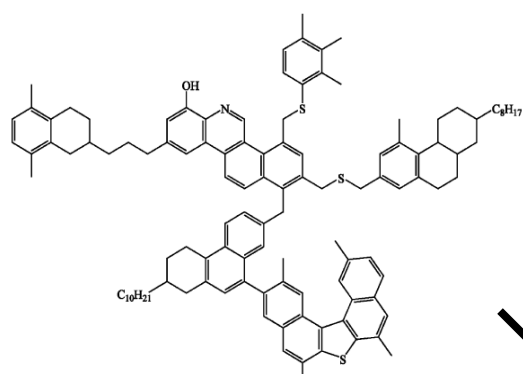
Continental



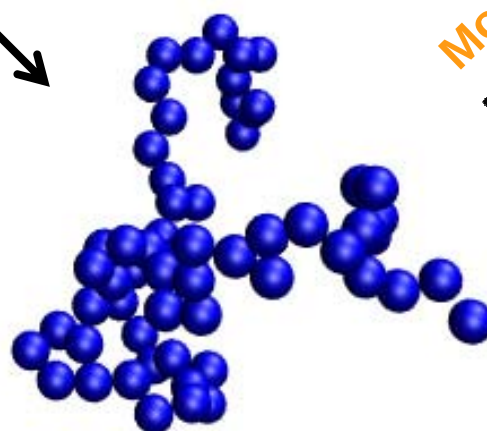
Pre-aggregated
particle

Asphalene Models:

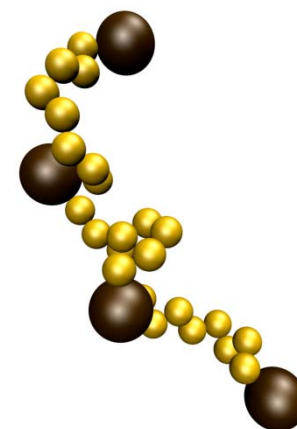
• Refining the Asphaltene Model



Coarse Grained
Molecule 1



Coarse Grained
Molecule 2



More Detail