

ESDU SPD-M4-3

Coarse grained simulation of asphaltene-hydrocarbon containing systems



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Sub-Project D: Thermodynamics and molecular modelling

Coarse Grained Simulation of Asphaltene-Hydrocarbon containing systems

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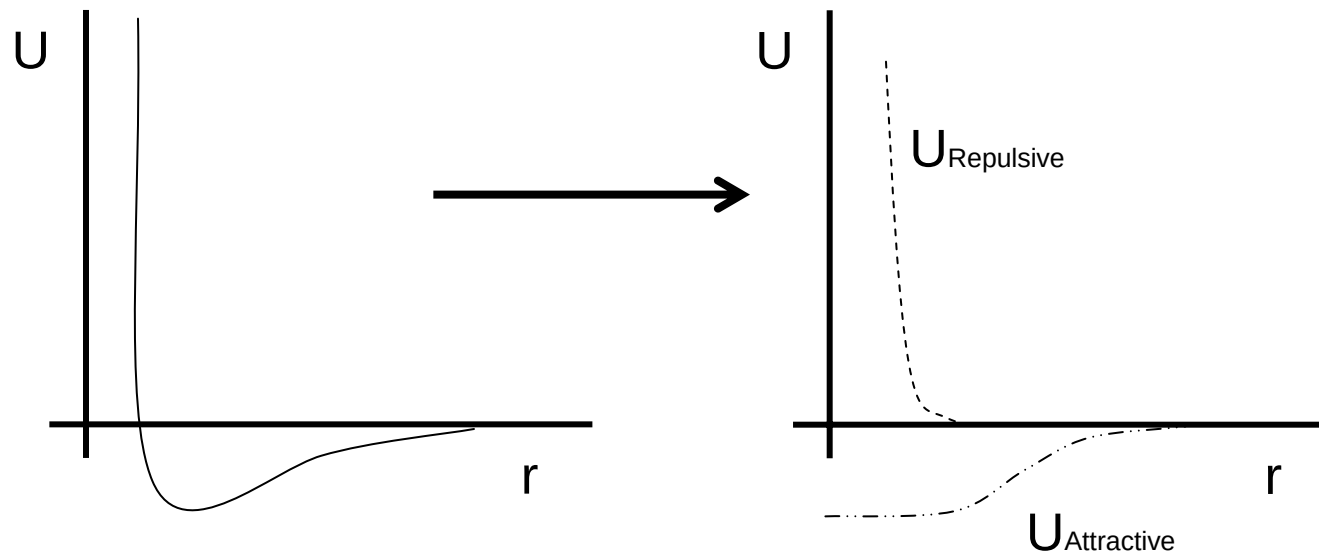
Erich Müller and Stephen Richardson

Outline

- **Objectives**
- **Models**
- **Technique**
- **Validation**
- **Work in progress**
- **Future work**

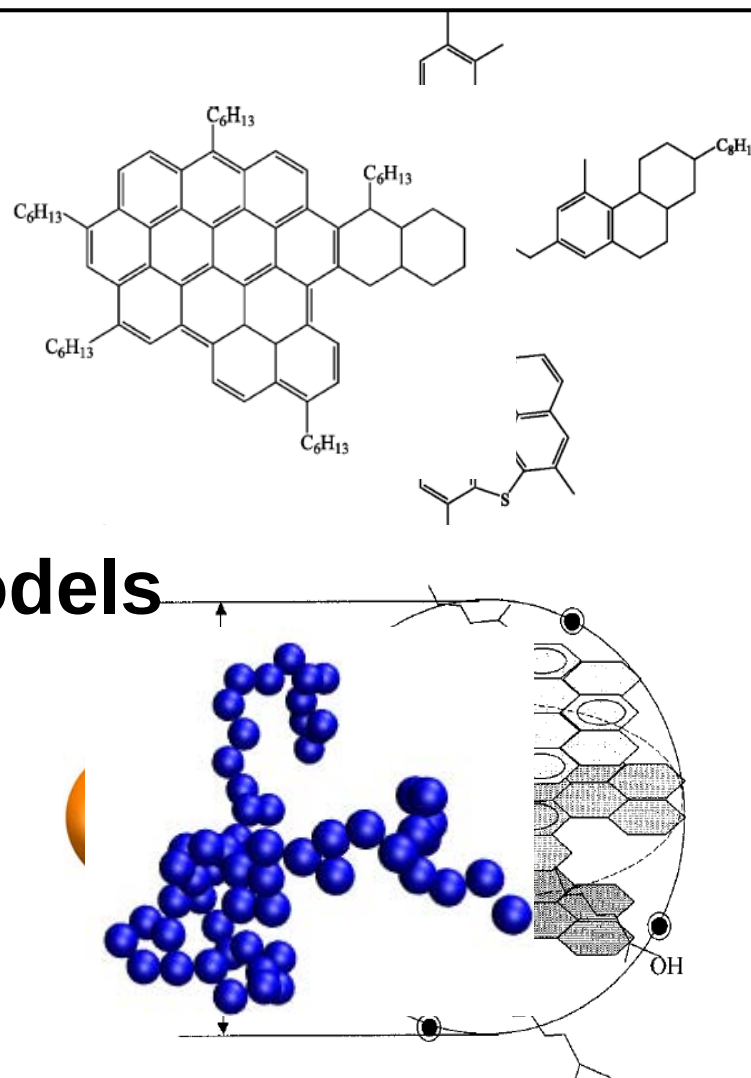
Objective

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



Models of Asphaltenes

- **Molecular Models**
 - Continental
 - Archipelago
- **Coarse grained models**
 - Colloidal
 - Polymer
 - Discotic



Models of Asphaltenes

- **Asphaltene in oil as Colloid-Polymer systems**
 - **Wu, Prausnitz, Firoozabad (1998) AIChE J., 44, 1188 (1998)**
 - Sigma Asphaltene 30 Å
 - Sigma Resin 5 Å
 - Number of Segments in resin 16
 - **Buenrostro-Gonzalez, Lira-Galeana, Gil-Villegas, Wu; AIChE J., 50, 2552 (2004)**
 - Sigma Asphaltene 17 Å
 - Sigma Resin 5 Å
 - Number of Segments in resin 10