



ESDU-SPD-M6-2

Apr.08: Coarse-Grained simulation of asphaltene-hydrocarbon containing systems

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Documents
Document Sharing Hub

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

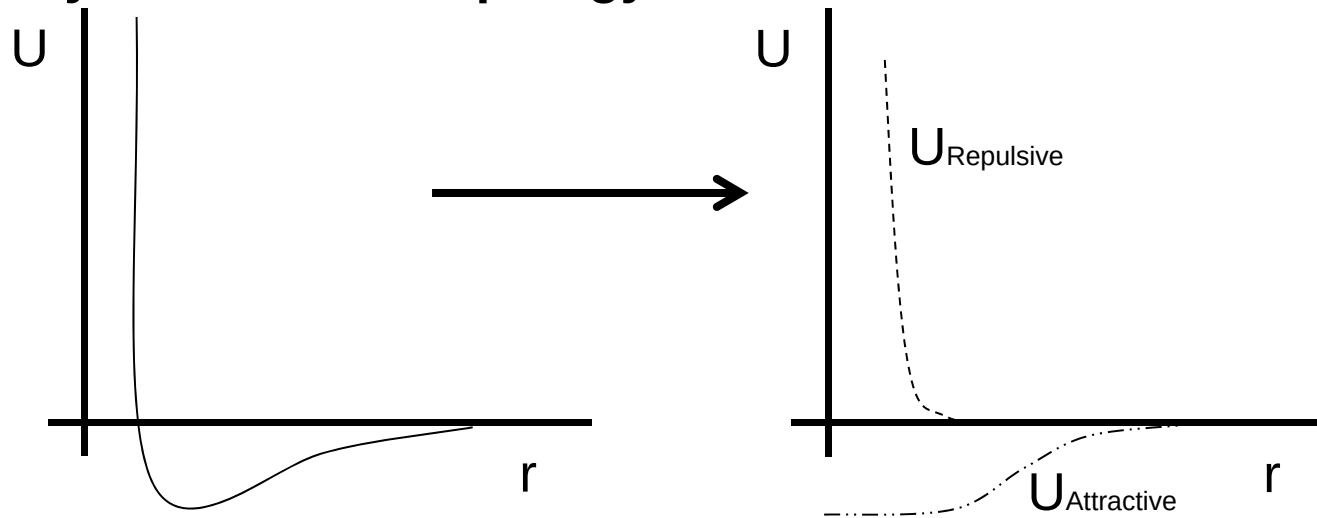
**Coarse-Grained Simulation of
Asphaltene-Hydrocarbon containing
Systems**

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Müller and Stephen Richardson**

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.
 - 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

Progress to Date

- Asphaltene Models

