



ESDU SPD-M2-1

Modelling asphaltenes using soft or related approaches

Unamended
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Sub-Project D: Thermodynamics and molecular modelling

Modelling Asphaltenes using SAFT or related approaches

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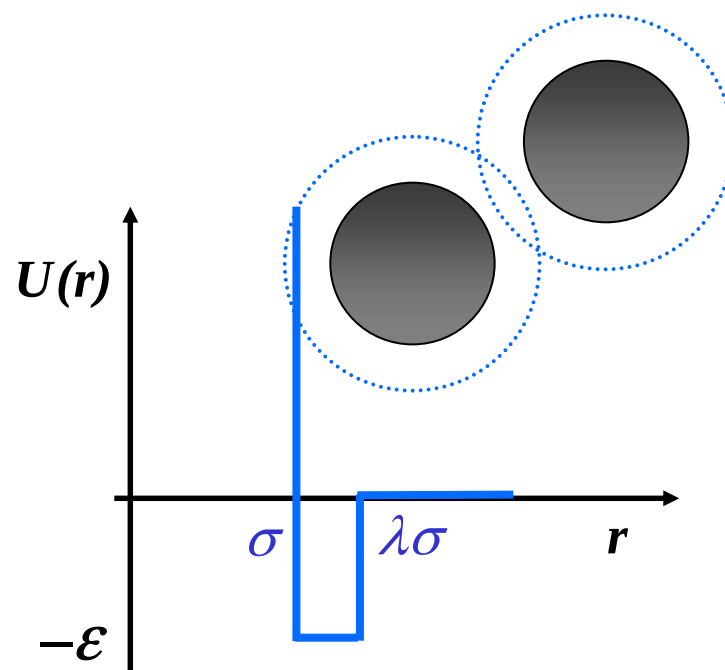
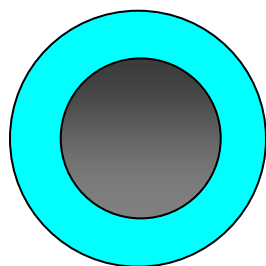
Outline

- **Statistical Associating Fluid Theory (SAFT)**
 - Free-energy equation of state
 - SAFT-VR
- **Previous successful applications of SAFT**
 - complex, multicomponent fluid-phase equilibria
 - strong predictive capabilities
 - linkable to other thermodynamic models
- **Application to asphaltenes**

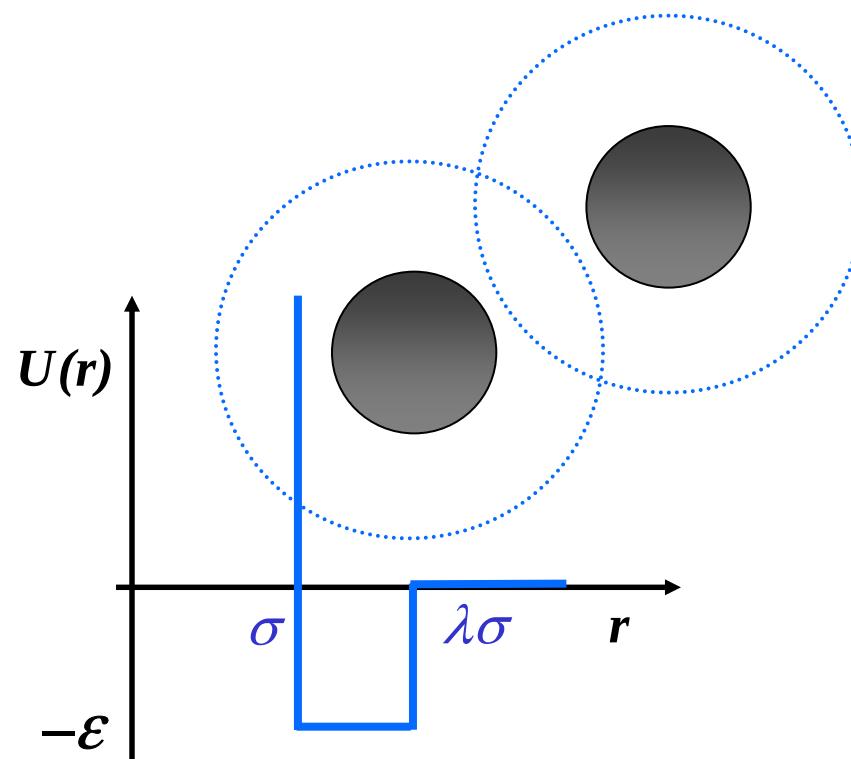
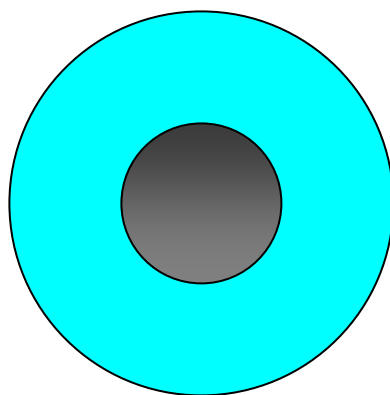
Advanced thermodynamic modelling

- **Statistical Associating Fluid Theory (SAFT)**
 - **Original Theory**
Chapman, Gubbins, Jackson, Radosz,
Ind. Eng. Chem. Res., 29, 1709 (1990)
 - **SAFT-VR (potentials with variable range)**
Gil-Villegas, Galindo, Whitehead, Mills, Jackson, Burgess,
J. Chem. Phys., 106, 4168 (1997)
 - **Numerous other versions (soft-SAFT, PC-SAFT)**
Blas and Vega (1997), Gross and Sadowski (2001)

**Gil-Villegas, Galindo, Whitehead, Mills, Jackson,
Burgess, *J. Chem. Phys.*, 106, 4168 (1997)**



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Burgess, *J. Chem. Phys.*, 106, 4168 (1997)

- Free Energy**

$$\frac{A}{NkT} = \frac{A^{ideal}}{NkT} + \frac{A^{mono.}}{NkT} + \frac{A^{chain}}{NkT} + \frac{A^{assoc.}}{NkT}$$

Gil-Villegas, Galindo, Whitehead, Mills, Jackson,
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- Free Energy**

$$\frac{A}{NkT} = \frac{A^{ideal}}{NkT} + \frac{A^{mono.}}{NkT} + \frac{A^{chain}}{NkT} + \frac{A^{assoc.}}{NkT}$$

$$\frac{A^{ideal}}{NkT} = \ln\left(\frac{\rho\mathcal{V}}{\Omega}\right) - 1 \quad \text{(free Energy of an "ideal" gas)}$$

Gil-Villegas, Galindo, Whitehead, Mills, Jackson,
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- Free Energy

$$\frac{A}{NkT} = \frac{A^{ideal}}{NkT} + \frac{A^{mono.}}{NkT} + \frac{A^{chain}}{NkT} + \frac{A^{assoc.}}{NkT}$$

Perturbation theory

Barker and Henderson (1975)

$$A^{mono.} = A^{hs} + \left(\frac{1}{kT} \right) A_1(u(r), \dots) + \left(\frac{1}{kT} \right)^2 A_2(u(r), \dots)$$

$$\frac{A^{hs}}{N_s kT} = \frac{4\eta - 3\eta^2}{(1 - \eta)^2}$$

Hard sphere

Carnahan and Starling (1969)