



ESDU-SPD-M6-1

Apr.08: Thermodynamic modelling of asphaltene-oil systems using SAFT

**Unamended
Issued October 2010**

**Imperial College
London**

Copyright Engineering Sciences Data Unit
Provided by IHS Markit under license with ESDU
No reproduction or networking permitted without license from IHS
Full document details: ESDU SPD-M6-1 2010



Documents
Document Sharing Hub

Licensee=/, User=,
Not for Resale.

Sub-Project D: Thermodynamics and
molecular modelling

**Thermodynamic modelling
of asphaltene-oil systems
using SAFT**

Andrew Haslam

Amparo Galindo, George Jackson, Julio Jover, Erich
Müller and Stephen Richardson

Outline

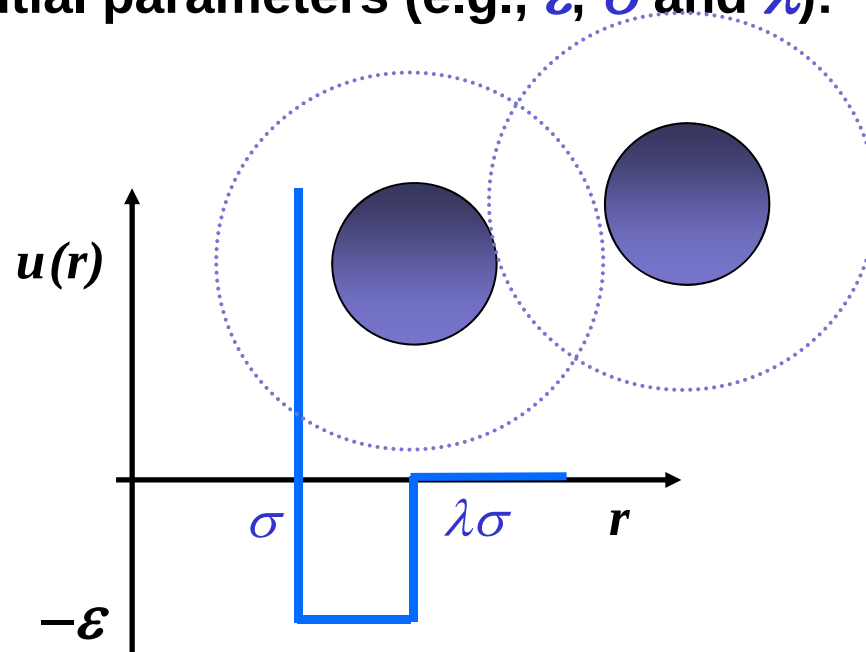
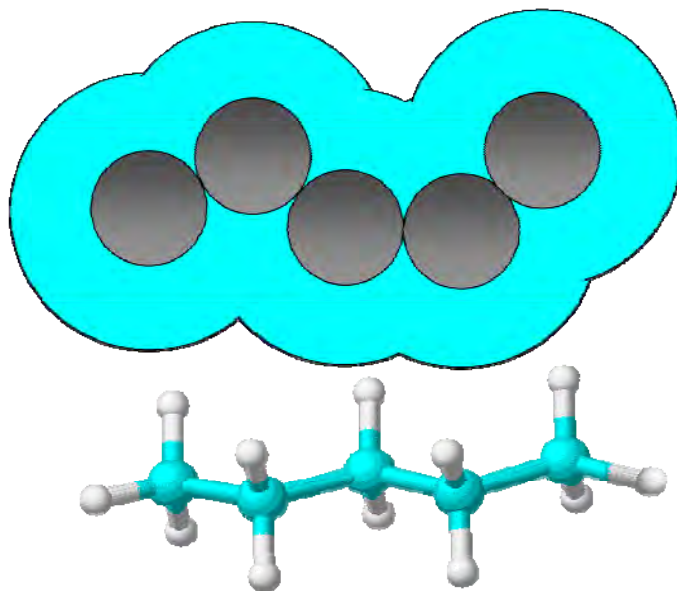
- **SAFT-VR: brief reminder of relevant details**
- **Modelling mixtures**
 - mixture intermolecular potential parameters
 - binary-interaction parameters and combining rules
- **Application to modelling asphaltene-containing systems**
- **Demonstration using experimental crude-oil data**

SAFT-VR equation of state

- Free-energy Equation of State

- from statistical thermodynamics $\Rightarrow$ *molecular based*
- free energy A is a function of m (#(chain segments)) and the intermolecular-potential parameters (e.g., ϵ , σ and λ):

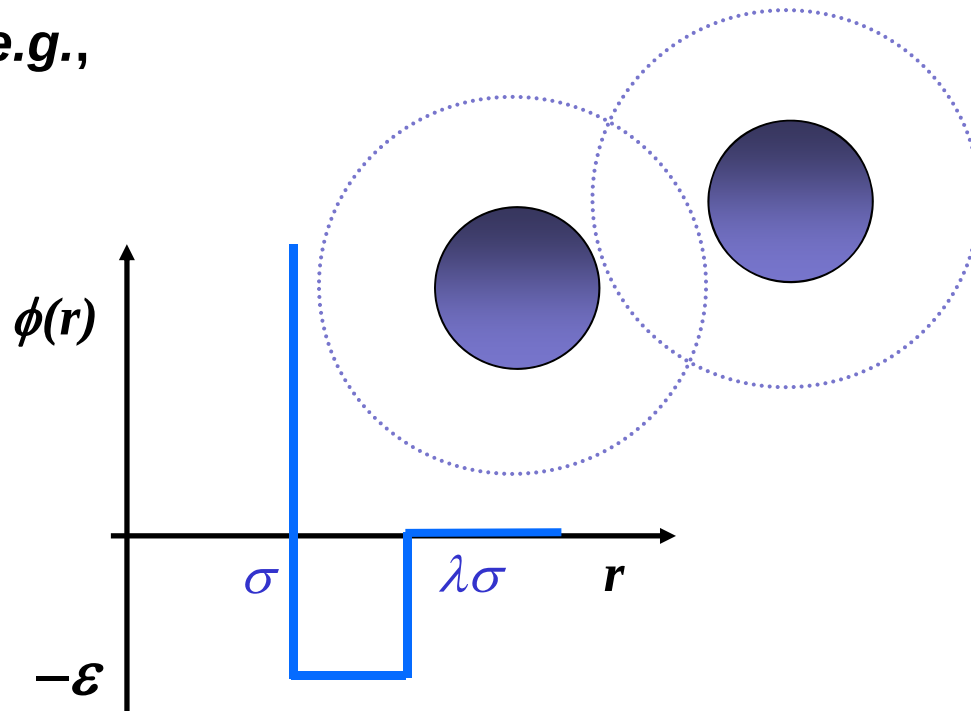
“MW”



- e.g., $p = -\left(\frac{\partial A}{\partial V}\right)_{N,T}$

Modelling real fluids

- Choose an intermolecular potential (the model):
e.g.,



Potential parameters then define the fluid:

$$\epsilon; \lambda; \sigma$$

Modelling real fluids: pures

1. Assign values to potential parameters

Modelling real fluids: pures

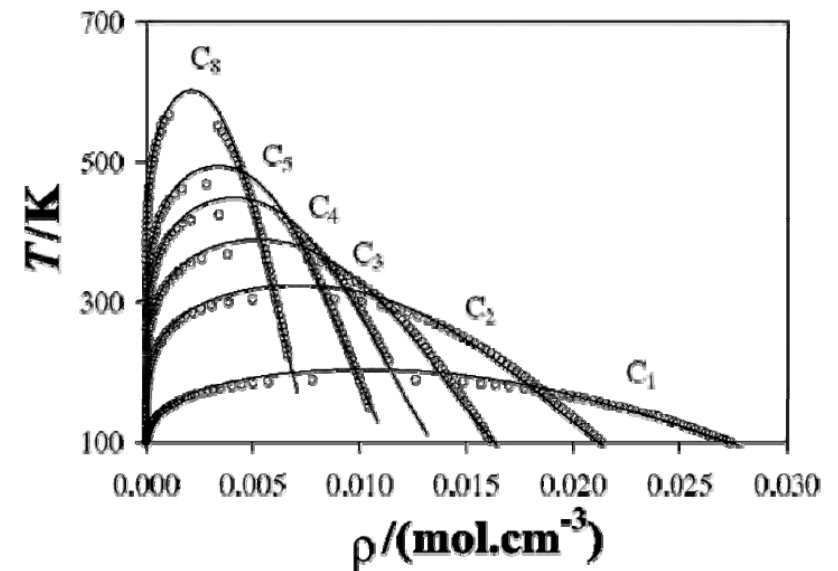
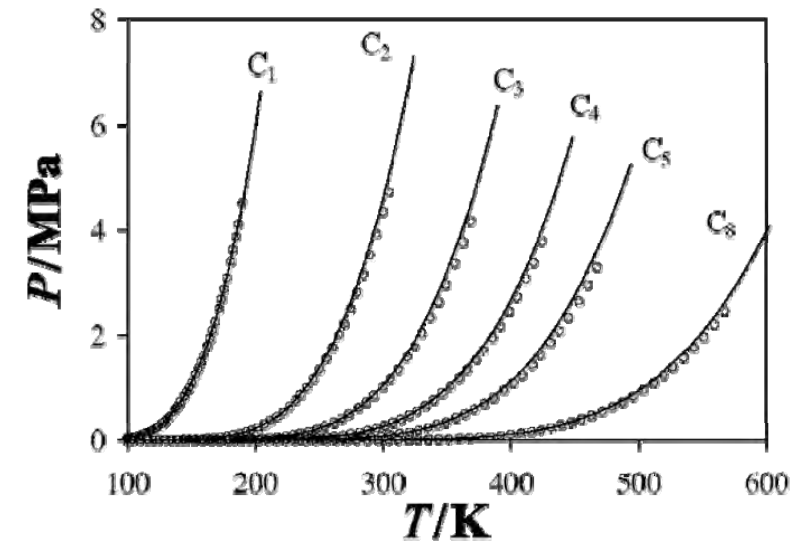
1. Assign values to potential parameters
2. Plug into your theory

Modelling real fluids: pures

1. Assign values to potential parameters
2. Plug into your theory
3. Calculate fluid properties
 - vapour pressure
 - liquid density

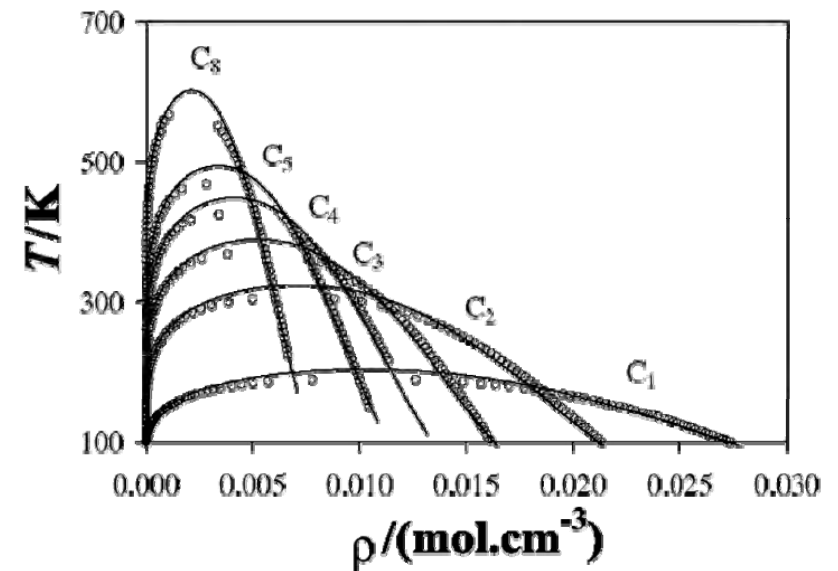
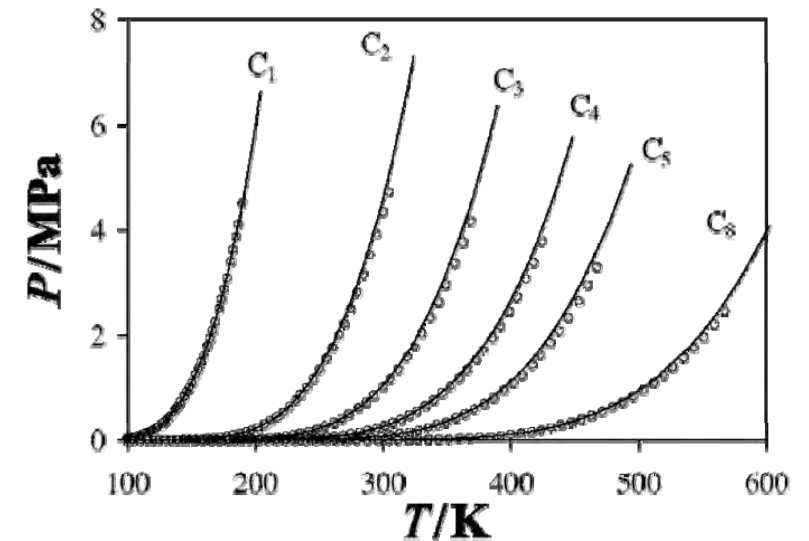
Modelling real fluids: pures

1. Assign values to potential parameters
2. Plug into your theory
3. Calculate fluid properties
 - vapour pressure
 - liquid density
4. Compare with real fluid



Modelling real fluids: pures

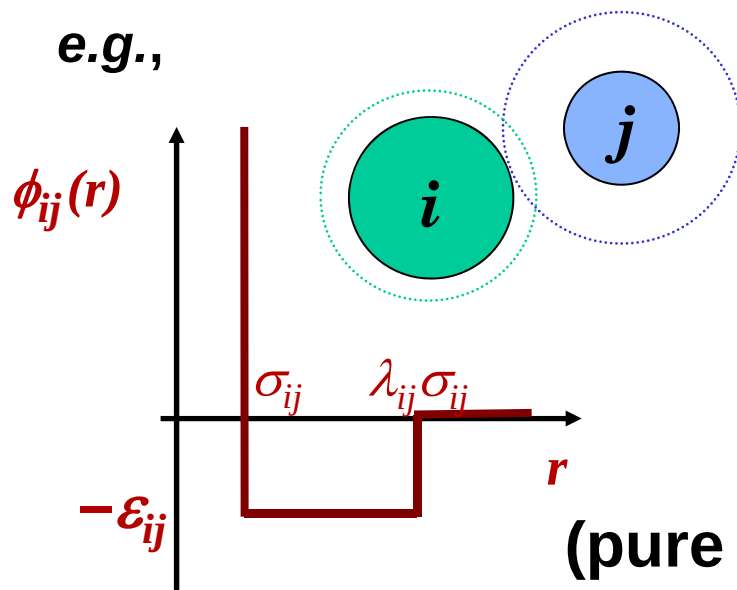
1. Assign values to potential parameters
2. Plug into your theory
3. Calculate fluid properties
 - vapour pressure
 - liquid density
4. Compare with real fluid
5. If necessary, revise parameters; return to (1)



Modelling real fluids: mixtures

- Pure-component model predetermined
- Choose an intermolecular potential (the model):
 - almost invariably of same form as pure-component potential

e.g.,



Potential parameters
(pure and **mixture**) then define the fluid:

$$\sigma_i; \epsilon_i; \lambda_i; \sigma_j; \epsilon_j; \lambda_j; \sigma_{ij}; \epsilon_{ij}; \lambda_{ij}$$

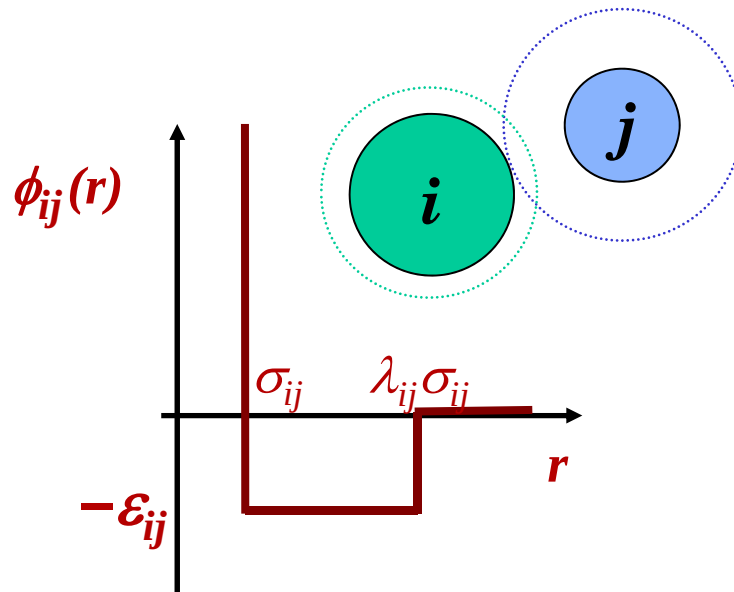
Modelling real fluids: mixtures

- Assume Lorentz rule for σ_{ij} :
$$\sigma_{ij} = \frac{1}{2}(\sigma_i + \sigma_j)$$

- Obtain ϵ_{ij} ; λ_{ij}
 - Expressed as k_{ij} and l_{ij} , where:

$$\epsilon_{ij} = (1 - k_{ij}) \sqrt{\epsilon_i \epsilon_j}$$

$$\lambda_{ij} = (1 - l_{ij}) \frac{(\lambda_i \sigma_i + \lambda_j \sigma_j)}{(\sigma_i + \sigma_j)}$$



Modelling real fluids: mixtures

1. Assign values to potential parameters

Modelling real fluids: mixtures

1. Assign values to potential parameters
2. Plug into your theory

Modelling real fluids: mixtures

1. Assign values to potential parameters
2. Plug into your theory
3. Calculate fluid properties
 - e.g., composition slice from phase diagram