



ESDU-SPD-M6-3

Apr.08: Phase behavior of complex mixtures

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

Phase behaviour of complex mixtures

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Objectives

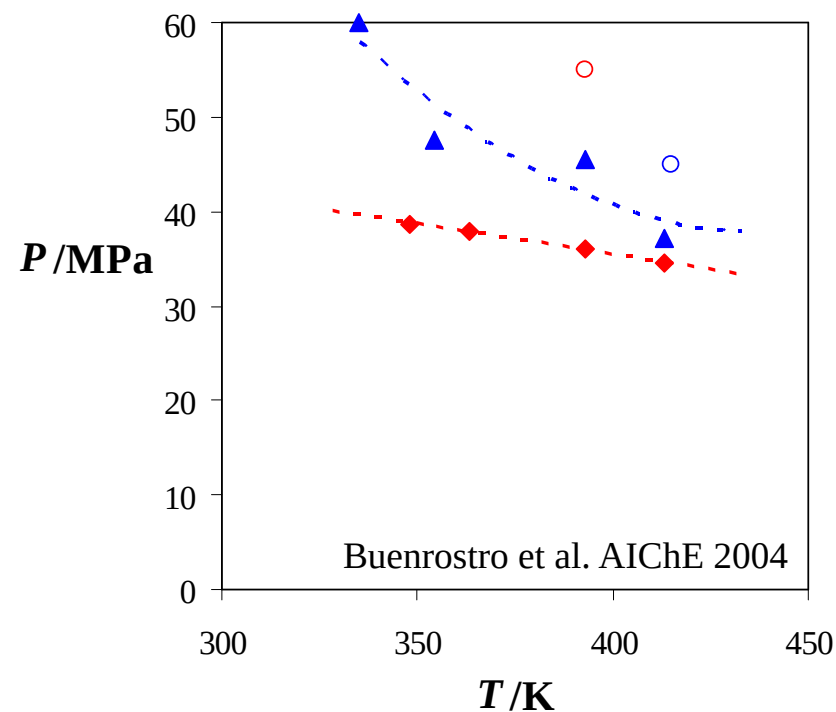
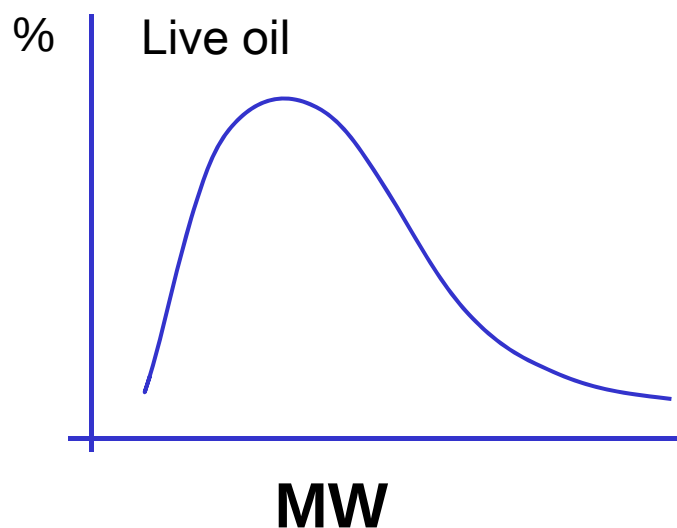
- **Develop an ability to predict the limit of stability of asphaltene-oil mixtures with respect to demixing (precipitation) in exploration and processing**
 - As a function of pressure, temperature and composition
 - And addition of solvents
- **Focus on modelling the crude as a pseudo-fluid whose rough average properties are representative of the collective.**
 - The effect of the polydispersity of the oil (hydrocarbon composition distribution) and the asphaltene (molecular weight distribution) will be examined. (Andrew)
 - There is no unique topology which encompasses what is currently thought to be the “average” asphaltene model. (Julio)

Outline

- **Brief introduction to phase equilibria in complex mixtures (Amparo)**
- **Modelling experimental asphaltene + oil phase equilibria with SAFT (Andrew)**
- **Molecular dynamics simulations of equivalent systems (Julio)**

Asphaltene precipitation envelope

- During natural oil production an asphaltene phase “drops-out” as pressure decreases
 - The onset of precipitation is lower for higher temperature



Dead oil data

- Asphaltene precipitated through the addition of solvents ($n\text{-C}_5, n\text{-C}_6, n\text{-C}_7$) at $P \sim 0.1 \text{ MPa}$, $T \sim 298 \text{ K}$

