

ESDU SPD-M8-3

Predicting adsorption isotherms using a two-dimensional Statistical Associating Fluid Theory

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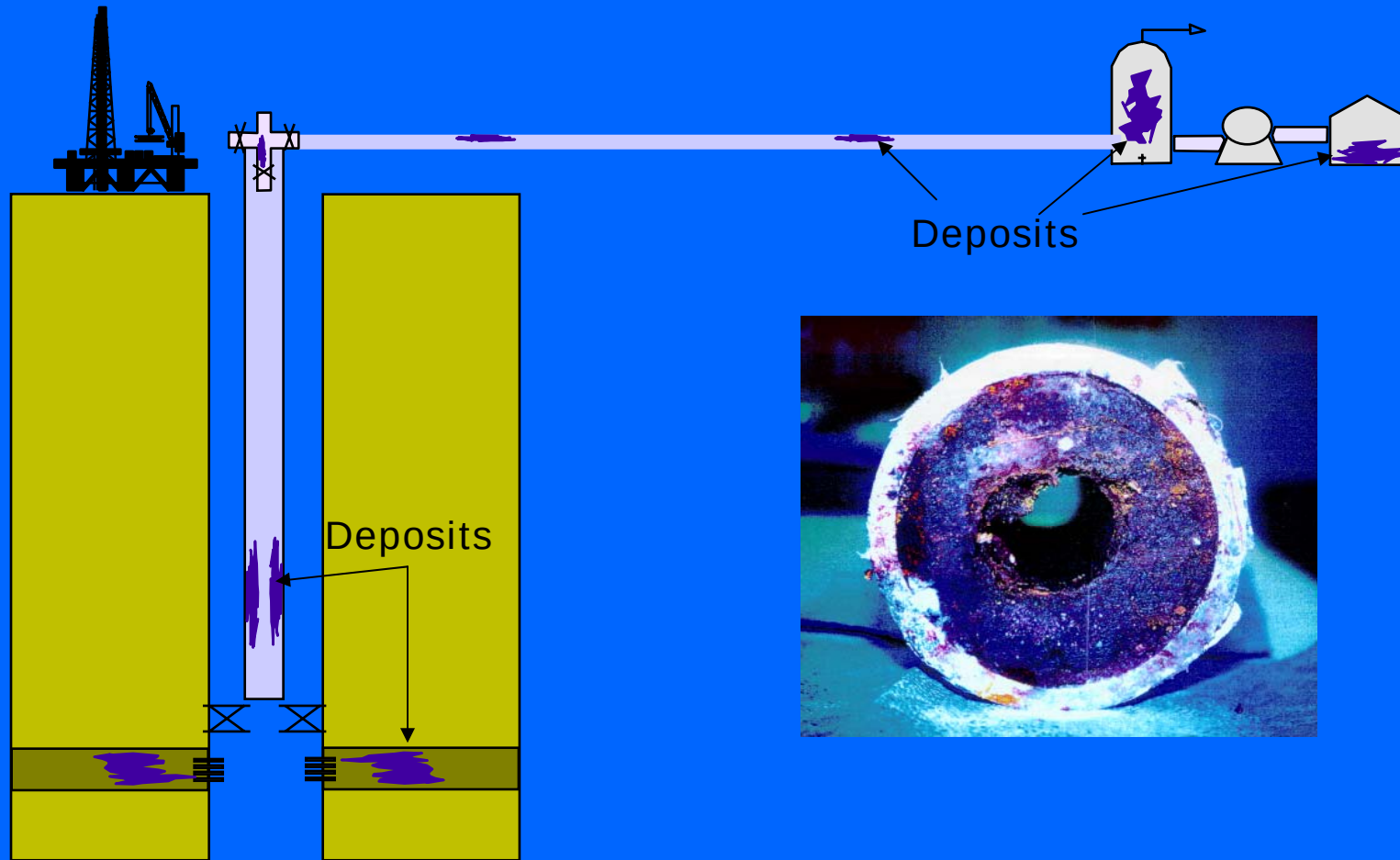
Alejandro Gil-Villegas
Institute of Physics,
University of Guanajuato, México

**Imperial College
September 2008**

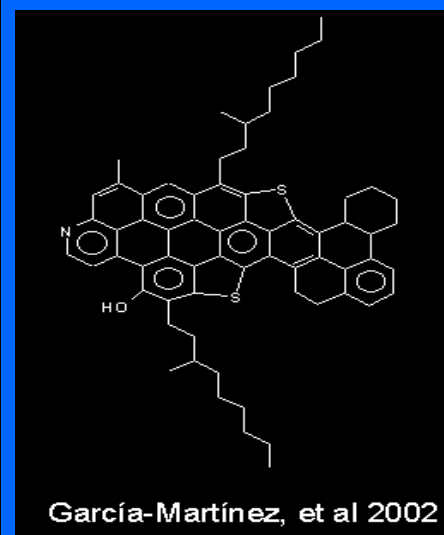
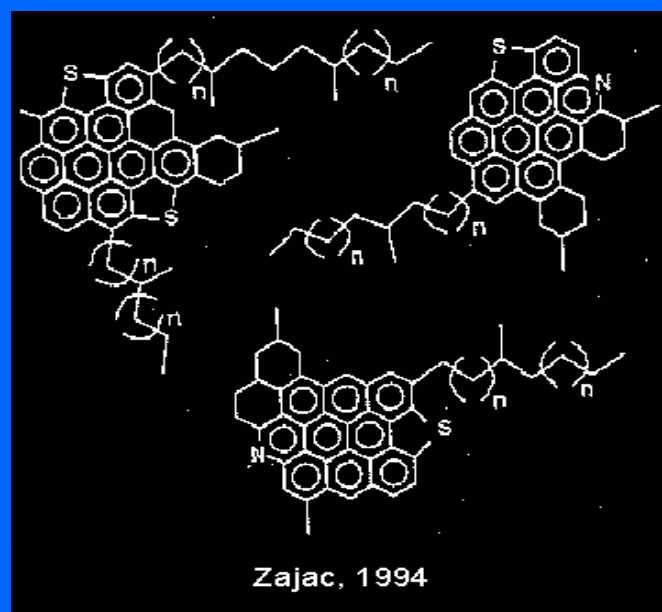
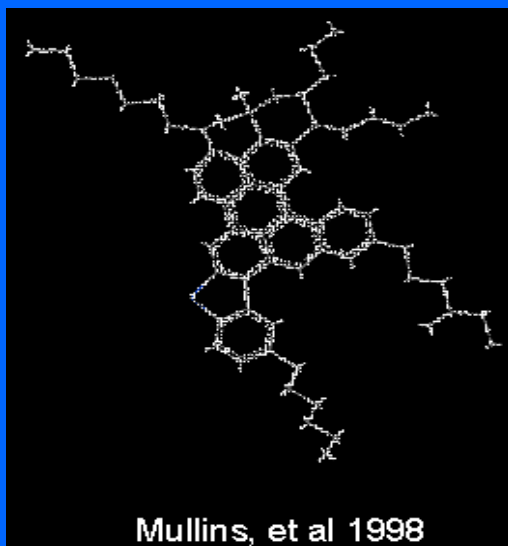
Outline:

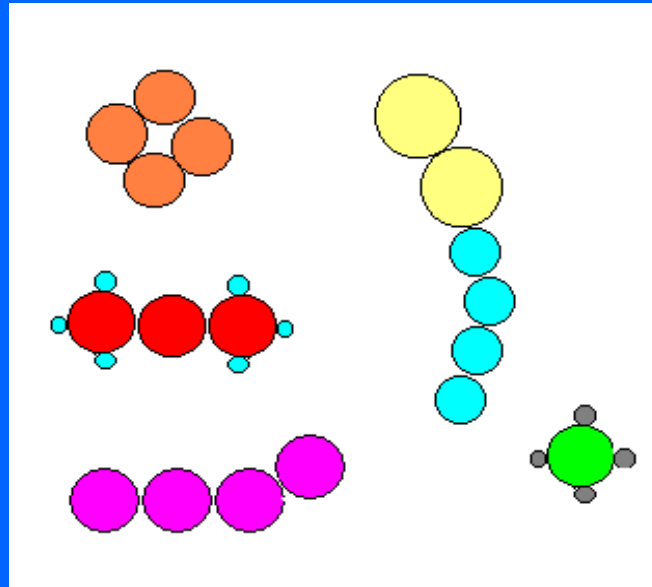
1. Introduction: asphaltenes
2. Two-dimensional SAFT-VR
3. Prediction of adsorption isotherms
4. Conclusions

Asphaltenes



Molecular Models for asphaltenes





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

Michael Wertheim:
Fluids with highly directional attractive forces
J. Stat. Phys. (1984-1986)

Statistical Associating Fluid Theory.
 Chapman, Jackson, Gubbins & Radosz,
Ind. Eng. Chem. Res. (1990).

SAFT- VR
 Gil-Villegas, Galindo, Whitehead, Mills, Jackson & Burgess
J. Chem. Phys. (1997)