EPFL

ENG-609 **Numerical Methods for Physical Properties Evaluation**

Heyen Georges

Cursus	Sem.	Type
Energy		Obl.

Language of teaching	English
Credits	1
Session	
Exam	Project report
Workload	30h
Hours	**14**
Courses	14
Number of positions	

Frequency

Every 3 years

Remark

Next time: Winter 2019

Summary

The learning outcome is to learn the numerical methods that are used to evaluate thermophysical properties of pure components and mixtures and there applications for fluid phase changes and separation problems.

Content

Day 1 :
How nanoscale interactions influence the macroscale properties
Concept of equation of state
Ideal behaviour and residual properties
Corresponding state principle
How equations of state are designed
Review of some equations of state (virial, BWR type, cubic equations)

Day 2 :
Mixture properties
Ideal mixture and excess properties
Phase equilibria
Application of equations of state to mixtures

Day 3 :
Excess properties for strongly nonideal mixtures
Excess Gibbs free energy models :
  • Scatchard-Hildebrand
  • Wilson
  • NRTL
  • UNIQUAC
Calculation of phase equilibria for strongly nonideal mixtures at moderate pressure
Parameter estimation in phase equilibrium models
Predictive method (UNIFAC, UNIQUAC)

Day 4 :
Modelling strongly nonideal mixtures at high pressure
Huron-Vidal mixing rules, MHV1, MHV2
Coupling phase equililibria with chemical reaction : electrolyte models

Modelling separation processes
- Flash separation
- Batch distillation
- Continuous distillation

Keywords

Thermodynamic methods, physical properties of fluids and mixtures

Learning Prerequisites

Recommended courses

Thermodynamics