Génie Chimique

ENGLISH: GCA / THERMO

Select Thermodynamic Models for Simulation

2,5 DAYS

PURPOSE

To select and validate, through an efficient methodology, the right thermodynamic model for some given processing conditions.

AUDIENCE

Experienced chemical or process engineers involved in process simulation or design of new processes.

LEARNING OBJECTIVES

- To grasp a practical understanding of **fluid behavior**.
- To understand the link between **molecular structures** and fluid behavior.
- To identify and validate the best **thermodynamic model** with its **parameters** for a number of industry-based cases.

PREREQUISITE

Understanding of fluid phases behavior and process simulation.

WAYS AND MEANS

- Pre-requirement based on an e-learning site and a handbook. The different subjects are presented from a practical point of view.
- Specific data file including data, diagrams, charts and correlations used in the different technical areas of chemical engineering.
- Many practical applications based on real data.

OBSERVATION

From October 13th (1:30 pm) till October 15th (5:00 pm)

Instructor is Jean-Charles DE HEMPTINE, world-class expert in Thermodynamics from IFP Energies nouvelles.

COORDINATOR

Mathilde Mercier

AGENDA

PHYSICO-CHEMICAL PROPERTIES AND CHARACTERIZATION OF PURE COMPONENTS — 0.25 d

Ideal gas behavior and equations of states; the corresponding states principle (ex: the Lee&Kesler method).
Useful correlations for vapor pressure (ex: Antoine), liquid molar volume (ex: Rackett), heat capacity (ex: Aly & Lee), enthalpy of vaporization (ex: use of the Clapeyron equation).
Group contribution methods (ex: Joback).
***Application**: compute the normal boiling temperature, heat of vaporization and liquid molar volume of a complex compound.*

VAPOR-LIQUID EQUILIBRIUM OF IDEAL MIXTURES — 0.5 d

Phase diagrams (PT, isobaric, isothermal) and main laws (Raoult, Henry).
Computation principles (ex: Rachford-Rice).
Applications:

- *calculate LPG entrainment using a liquid solvent*
- *calculate the process conditions in a distillation column, using bubble or dew temperatures.*

PHASE EQUILIBRIUM OF NON-IDEAL MIXTURES — 0.5 d

Use of activity coefficient and significance of infinite dilution properties (relationship with Henry's law).
Azeotropy and its molecular significance.
Parameter fitting using a simple model (ex: Margules).
***Application**: hexane + acetone mixture.*
Liquid-liquid phase split with the example of water-hydrocarbon.
***Application**: recognize and read binary phase diagrams.*

CURRENT AND ADVANCED THERMODYNAMIC MODELS — 0.75 d

Definition of fugacity; homogeneous and heterogeneous models.
Main activity coefficient models, their theoretical foundations and their parameters: Margules; Flory; Regular solutions; Flory-Hugins; NRTL; UNIQUAC; UNIFAC.
Cubic equations of state, their parameters and limitations (PengRobinson, SoaveRedlichKwong): alfa functions and mixing rules.
Some advanced models and their molecular significance.

CASE STUDIES FOR MODELS SELECTION — 0.5 d

Case-studies for chemistry and oil refining:

- *C4 distillation: comparison of the efficiency without and with a solvent (extractive distillation, butadiene or acetonitrile)*
- *biofuels: esterification process and separations of alcohol/ester systems.*

LANGUAGE	DATES	LOCATION	FEES	REGISTRATION CONTACT	
EN	13 - 15 Oct	Rueil	1 500 €	RRU	rc.rueil@ifptraining.com