

Course title: Phase Equilibria for Process Design – selectable / ~~regular~~ course

Number of contact hours: 60 hours (18h lectures/24 Lab/ 12 CompLab/ 6 Project)

ETCS credits: 6

Course description: The aims of the module are: 1. To enable the student to identify and carry out experimental methods for the measurement of phase equilibria, both from the analytic and practical point of views. 2. To provide students the ability to collect experimental phase equilibria data, and evaluate their quality through the application of coherence and consistency tests. 3. To develop student's skills in the selection of databases and estimation methods, to predict relevant thermodynamic data for the design of chemical processes.

Education effects (P6S_UW, P7S_WG):

At the end of the module, the learner is expected to be able to:

1. Identify, choose, and apply experimental methods for the measurement of phase equilibria.
2. Collect, assess and evaluate experimental phase equilibria data.
3. Know, select and use databases, and estimation methods, to predict thermodynamic data.

Literature:

- 1) R. D. Weir; T. W. de Loos, "Measurement of the Thermodynamic Properties of Multiple Phases", Elsevier, 2005.
- 2) G .T. Hefter; R. P. T. Tomkins, "The Experimental Determination of Solubilities", John Wiley and Sons, 2003.
- 3) R. Dohrn; J. M. S. Fonseca; S. Peper, "Experimental Methods for Phase Equilibria at High Pressures", Annu. Rev. Chem. Biomol. Eng. 2012, 343-367.
- 4) J. W. Kang; V. Diky; R. D. Chirico; J. W. Magee; C. D. Muzny; I. Abdulagatov; A. F. Kazakov; M. Frenkel, "Quality Assessment Algorithm for Vapor-Liquid Equilibrium Data", J. Chem. Eng. Data 2010, 3631–3640.
- 5) J. W. Kang; V. Diky; R. D. Chirico; J. W. Magee; C. D. Muzny; I. Abdulagatov; A. F. Kazakov; M. Frenkel, "Algorithmic Framework for Quality Assessment of Phase Equilibrium Data", J. Chem. Eng. Data 2014, 2283–2293.
- 6) M. Prausnitz; R. N Lichtenthaler, E. G. Azevedo, "Molecular Thermodynamics of Fluid-Phase Equilibria", 3rd edition, Prentice-Hall, 1999.
- 7) S. I. Sandler, Chemical, Biochemical, and Engineering Thermodynamics, 4th edition, John Wiley and Sons, 2006.

Assessment method:

LOs	Assessment methods	Weight
1	Written and practical test	40
2	Project and discussion	20
3	Project work and presentation	40

Prerequisites: Before the course unit the learner is expected to be able to:

1. Recognize and describe the formalism for the thermodynamic description of multicomponent systems.
2. Explain, identify and illustrate the main types of phase diagrams.
3. Develop and interpret phase equilibria calculations: liquid-vapor, liquid-liquid, liquid-liquid-vapor, solid-liquid and solid-vapor.

Primary target group:

Lecturer: Maria Olga de Amorim e Sá Ferreira e Simão Pedro de Almeida Pinho - Polytechnic Institute of Bragança