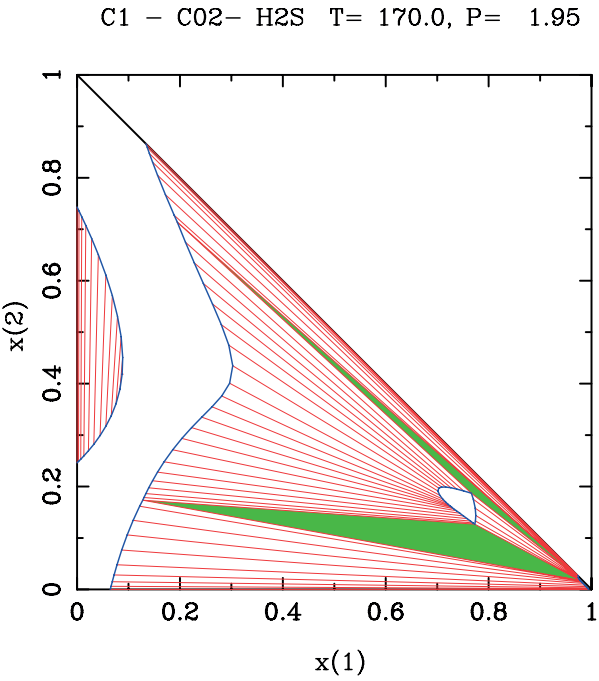
Advanced Course on Thermodynamic Models: Fundamentals & Computational Aspects



August 14 - 25, 2017

CERE
Dept. of Chemical & Biochemical Engineering
Dept. of Chemistry
Technical University of Denmark

Course description

The course will provide the participants with a knowledge of the fundamentals of thermodynamics, an overview of the most important thermodynamic models currently used in industrial practice, including how efficient computer codes for such models are written and checked for errors. In addition the course will emphasize the development of efficient procedures for calculation of phase equilibria under a variety of conditions. The practical part of the course, where the participants have to develop their own codes, emphasizes in particular this aspect. The course is of relevance for researchers engaged in the development and implementation of thermodynamic models for process simulation or for those who just want to learn how to develop and write an efficient and consistent computer code.

Fundamentals:

The state functions, conditions of equilibrium and stability, properties of mixtures, calculation of the derivatives of the thermodynamic functions, checking model expressions and model consistency.

Models:

Equations of state and activity coefficient models, EoS/G^E mixing rules, association models (the CPA and SAFT equations of state), mixtures with electrolytes and polymers, applications including Carbon Capture and Storage as well as flow assurance and trends in thermodynamic models

Computational methods:

General equilibrium relations and material balances. The PT-flash: Successive substitution, the Rachford-Rice equation, acceleration, higher order methods and stability analysis. The multiphase flash. General state function based specifications.

Dew- and bubble points, stability analysis. Chemical equilibrium calculation. Gravitational segregation. Miscible displacement.

Course history & style

The course is strongly inspired by the book written by Michelsen & Mollerup and the lectures on Computational aspects by prof. Michelsen. These lectures will be available in the course website during the course and for a short period after that.

Prerequisites

Basic chemical engineering thermodynamics, including knowledge about Equations of State, the concept of fugacity, and basic chemical equilibrium. For the practical part, a working knowledge of Fortran or Matlab is needed.

Curriculum and exam:

Two weeks of lectures, classroom problems and computer exercises (in teams of two). A third week, which does not require presence at DTU, for completing the exercises. A report is due at latest September 4, 2017.

Further information:

A maximum of 25 participants can be accepted. The course credits are 7.5 ECTS points.

Teachers:

Wei Yan - weya@kemi.dtu.dk
Georgios Kontogeorgis - gk@kt.dtu.dk
Alexander Shapiro ash@kt.dtu.dk
Philip L. Fosbøl - plf@kt.dtu.dk
Consultant: *Michael L. Michelsen - mlm@kt.dtu.dk*

Textbook:

M.L. Michelsen and J.M. Mollerup, Thermodynamic Models: Fundamentals & Computational Aspects. 2nd Edition December 2007. Tie-Line Publications.
Price € 97 (incl VAT) at www.tie-tech.com/shop or by contacting Louise Biede at alb@kt.dtu.dk - Students will receive a discount of 50%.

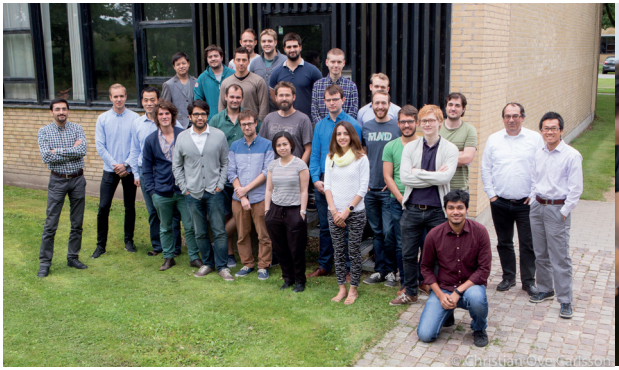
General course information

Venue:

Department of Chemical & Biochemical Engineering, Building 229, DTU, Lyngby, Denmark

Registration and further information:
Please contact Anne Louise Biede

email: alb@kt.dtu.dk



Registration deadline: 1 June 2017

Prices:	Before 1 May	After 1 May
Industrial participant	€ 2,400	€ 2,500
CERE consortium member	€ 1,300	€ 1,400
PhD student	€ 250	€ 300
Academic	€ 1,300	€ 1,400

Since there is a maximum in the number of participants, an early registration is recommended.

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Photo: Christian Ove Carlsson