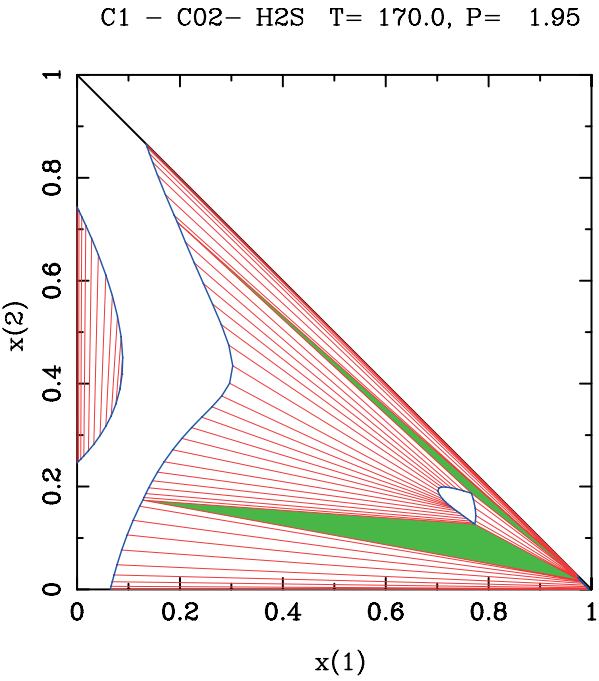
Advanced Course on Thermodynamic Models: Fundamentals & Computational Aspects



August 5 - 16, 2024

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, and 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 calculating of phase equilibrium 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 developing and implementing thermodynamic models for process simulation or for those who 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/GE 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. PT-flash: successive substitution, the Rachford-Rice equation, acceleration, higher order methods and stability analysis.

The Multiphase flash. General state function-based specifications.
Saturation point and phase envelope. Critical point calculation. Chemical equilibrium calculation. Gravitational segregation. Miscible displacement.

Course history

The course is strongly inspired by the book written by Michelsen & Mollerup and the lectures on Computational aspects by prof. Michelsen.

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. One can use other languages like Python or C++ but the support is limited.

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 August 31, 2024.

Further information:
A maximum of 30 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

Textbook:
M.L. Michelsen and J.M. Mollerup, Thermodynamic Models: Fundamentals & Computational Aspects. 2nd Edition December 2007. Tie-Line Publications. Price € 110 (incl VAT) at www.tie-tech.com/shop - Students will receive a discount of 50%.

General course information

Venue:
Department of Chemical & Biochemical Engineering, DTU, Lyngby, Denmark

Information about course site and links will be provided in advance to the course participants.
Registration: www.cere.dtu.dk/education/phd-courses

Further information: Anne Louise Biede (alb@kt.dtu.dk)

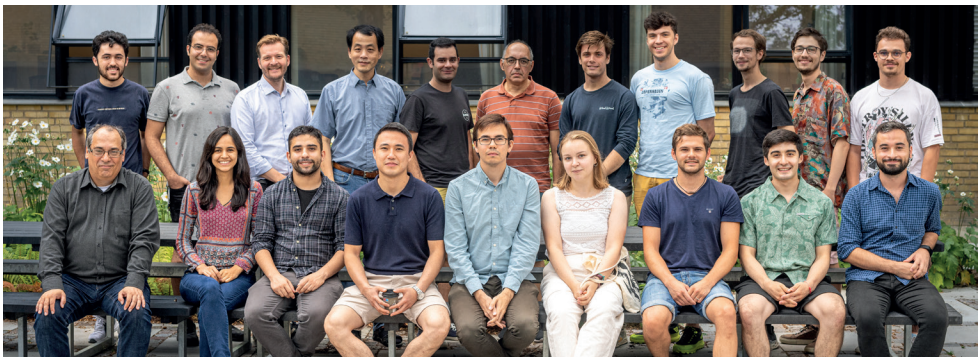


Photo: Christian Ove Carlsson

Registration deadline: June 14 2024
Payment deadline July 1, 2024

Prices:

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

Since there is a maximum of about 30 participants, an early registration is recommended.

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