LUNDS UNIVERSITET
Lunds Tekniska Högskola

Course syllabus

Molekylära drivkrafter 1: Termodynamik
Molecular Driving Forces 1: Thermodynamics

KFKA05, 7,5 credits, G1 (First Cycle)

Valid for: 2023/24
Faculty: Faculty of Engineering, LTH
Decided by: PLED B/K
Date of Decision: 2023-04-18

General Information

Main field: Technology.
Compulsory for: B2, K2
Language of instruction: The course will be given in Swedish

Aim

The course aims at providing a solid physical-chemical basis for futher studies in chemical separation and analysis, meterial chemistry, reaktion- and heat engineering and molecular biotechnlology. It

1. introduces both classical and statistical thermodynamics.
2. gives an understanding of the thermodynamic concepts and theories on the basis of molecular properties.
3. has a strong focus on problem-solving using these insights.

Learning outcomes

Knowledge and understanding
For a passing grade the student must

1. be able to describe and explain central thermodynamic concepts and quantities phenomenologically.
2. be able to describe and explain central thermodynamic concepts and quantities from a molecular perspective.
3. be able to make simple qualitative predictions of how the equilibrium properties of a system are affected by changes.

Competences and skills

For a passing grade the student must

1. be able to analyze a problem and be able to perform relevant calculations using the models and equations presented in the course.
2. be able to use a pocket calculator and computer to solve common numerical problems.
3. be able to peform chemical laboration in a safe and accurate manner, including use of laboratory equipment.
4. be able to write simple, but complete, reports of laboratory experiments according to given instructions, including correct presentation of data and error estimates.

Judgement and approach
For a passing grade the student must

1. be able to discuss everyday phenomena on the basis of sound statistical-thermodynamical reasoning.
2. be able to judge the validity of the fundamental thermodynamic models presented.
3. be able to judge the plausibility of the results found in problem solving.

Contents

- Basic concepts of thermodynamics such as work and heat, temperature, entropy, enthalpy, free energy, heat capacity and chemical potential are treated both from a molecular statistical end thermodynamic perspective. Ideal gases are treated exactly with the help of the molecular partition function. The Boltzmann distribution law is derived and applied to a number of different type of problems.
- Reversible and irreversible processes.
- The strategy for thermodynamic calculations: subdivision of a complex process into parts that can be treated as adiabatic, isobaric, isochoric, isentropic or isolated. Thermodynamic cycles.
- Integration of the differential relations to handle changes of state.
- Qualitative and quantitative treatment of phase equilibrium in systems of one component: Clapeyron and Clausius-Clapeyron equations and intepretation of phase diagrams for one component.
- Quantitative calculations of the relations between pressure, temperature and composition in ideal systems of two components with one or more phases. This includes concepts such as partial molar quantities and activity, calculations of colligative properties (boiling point elevation, freezing point depletion and osmosis) as well as vapour pressure above mixtures. Roault's and Henry's laws. The non-ideal cases are treated using the concepts of activity and activity coefficients.
- Thermodynamic treatment of chemical equilibrium.
- Three laboratory exercises treating chemichal equilibrium, vapor pressure and destillation and everyday thermodynamics. At least one laboratory report is written that includes basic statistical analysis and error propagation using the Monte Carlo method.
- One computer excercise treating the Boltzmann distribution law.
- Numerical problems, such as integration, derivation, equation solving and least-squares fitting, are solved using both pocket calculator and desktop computer.
- In the laboratory practicals, the student train spectrophotometric concentration determination, refractomeric determination of concentration, use of evacuated systems, readout of pressure meters, thermometers, hygrometers and more.

Examination details

Grading scale: TH - (U,3,4,5) - (Fail, Three, Four, Five)
Assessment: Written exam and laboratory exercises. Final grade is based on the written examination. The examination is constructed so that good understanding and basic problem solving skills on all parts of the course are required for the passing grade. For higher grades, problem solving skills on a more complex level are required. Bonus points to the written exam may be awarded for performed tasks. The bonus points are then valid only for the ordinary exam and the following two re-exams. Students who are awarded bonus points for performed tasks cannot be awarded bonus points for the same tasks once again when re-registered.

The examiner, in consultation with Disability Support Services, may deviate from the regular form of examination in order to provide a permanently disabled student with a form of examination equivalent to that of a student without a disability.

Parts
Code: 0115. **Name:** Written Examination.
Credits: 6,5. **Grading scale:** TH. **Assessment:** Written examination.
Code: 0215. **Name:** Laboratory Exercises.
Credits: 1. **Grading scale:** UG. **Assessment:** For passing grade, every task is performed and presented according to the instructions, which may mean either as a written report or orally, in Swedish or English. For passing grade, the written reports should be simple but correct and to the point, have a proper structure and contain a relevant discussion of the results. **Contents:** The laboratory part of the course contains three "wet" laboratory experiments and one computer task.

Admission

Assumed prior knowledge: FMAA05 Calculus in One Variable, FMAA20 Linear Algebra with Introduction to Computer Tools, KOOA15 General Chemistry.
The number of participants is limited to: No
The course overlaps following course/s: KFK080, KFK090

Reading list

- Dill, K and Bromberg, S: Molecular Driving Forces, Statistical Thermodynamics in Chemistry, Physics, Biology and Nanoscience. 2nd edition. Garland Publishing Inc, 2010, ISBN: 9780815344308.
- Complementary compendium, produced at Biopphysical Chemistry.

Contact and other information

Course coordinator: Kristofer Modig, kristofer.modig@bpc.lu.se
Course homepage: https://www.cmps.lu.se/education/
Further information: Some teaching might be held in English.